







May 18–22, 2009 Arlington, Virginia

Hydrogen Program

2009 Annual Merit Review and Peer Evaluation Report

DOE/GO-102009-2920 October 2009

About the Cover

Photo collage (from top to bottom):

Molten carbonate fuel cells installed at Sierra Nevada Brewery, Chico, CA. Photo courtesy of Sierra Nevada Brewery (NREL PIX 16602)

Young interest in fuel cell technology. Photo courtesy of Mr. Antonio Ruiz, U.S. Department of Energy (NREL PIX 16719)

Solar Two power tower in Daggert, CA, depicting potential for renewable hydrogen production. Photo courtesy of Sandia National Laboratories (NREL PIX 02186)

Fuel cell installations for telecommunication back-up power. Photo courtesy of ReliOn (NREL PIX 16642)

Hydrogen adsorption within MOF-74. Image courtesy of the National Institute of Standards and Technology

Hydrogen refueling. Photo courtesy of the California Fuel Cell Partnership (NREL PIX 16640)

Fuel-cell-powered forklift. Photo courtesy of the Defense Logistics Agency (NREL PIX 16601)

Photo on right:

Lincoln Memorial, Washington, DC (iStockphoto)

ERRATA SHEET

NREL REPORT/PROJECT NUMBER: BK-6A1-46600 DOE NUMBER: DOE/GO-102009-2920 TITLE: DOE Hydrogen Program: 2009 Annual Merit Review and Peer Evaluation Report AUTHOR(S): Satyapal, S. ORIGINAL PUBLICATION DATE: October 2009 DATE OF CORRECTIONS: May 2010

The following corrections were made to the Fuel Cells section of this report:

Page 386

The last paragraph was replaced.

Page 448

Christina Johnston was added to the list of authors.

Pages 597-598

Corrections to text in several bullet points were made, starting with Question 1. There were no changes to graph or project scores.

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NOTICE

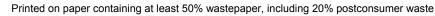
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Dear Colleague:

This document summarizes the comments provided by peer reviewers on hydrogen and fuel cell projects presented at the FY 2009 U.S. Department of Energy (DOE) Hydrogen Program and Vehicle Technologies Program Annual Merit Review and Peer Evaluation Meeting (AMR), held on May 18-22, 2009 in Arlington, Virginia. In response to direction from various stakeholders, including the National Academies, this review process provides evaluations of the Program's projects in applied research, development, demonstration and analysis of hydrogen, fuel cells and infrastructure technologies. The plenary included overview presentations from the Office of Energy Efficiency & Renewable Energy (EERE), Hydrogen Program, Vehicle Technologies Program, and Office of Basic Energy Sciences, as well as international presentations from government organizations in Germany, Japan, and the European Commission.

The recommendations of the reviewers have been taken into consideration by DOE Technology Development Managers in generating future work plans. The table below lists the projects presented at the review, evaluation scores, and the major actions to be taken during the upcoming fiscal year (October 1, 2009 to September 30, 2010). The projects have been grouped according to subprogram (i.e., Production and Delivery, Hydrogen Storage, Fuel Cells, Systems Analysis, Manufacturing) and reviewed according to the five evaluation criteria. The weighted scores are based on a four-point scale. To furnish all principal investigators (PIs) with direct feedback, all evaluations and comments are provided to each presenter; however, the authors of the individual comments remain anonymous. The PI of each project is instructed by DOE to fully consider these summary evaluation comments, as appropriate, in their FY 2010 plans.

I would like to express my sincere appreciation to the reviewers. You make this report possible, and we rely on your comments to help make project decisions for the new fiscal year. We look forward to your participation in the FY 2010 Annual Merit Review, which is presently scheduled for June 7-11, 2010 at the Washington Marriott Wardman Park in Washington, DC. Thank you for participating in the FY 2009 Annual Merit Review and Peer Evaluation Meeting.

Sincerely,

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Sunita Satyapal Acting Program Manager DOE Hydrogen Program Office of Energy Efficiency and Renewable Energy

Hydrogen Production and Delivery

Project Number	Project Title PI Name & Organization	Final Score	Continue	Discontinue	Other	Summary Comment
PD-02	Bio-Derived Liquids Reforming Yong Wang; Pacific Northwest National Laboratory	2.9	х			The researchers understand the role of variables such as space velocity, catalyst, and steam/carbon ratio in reforming and in achieving project goals for sugar and alcohol reforming. The basic catalyst approaches are sound but the catalyst lifetime needs to be included in the economic analysis. The project will continue catalyst modifications and performance characterizations with a focus on the APR systems.
PD-03	Hydrogen Generation from Biomass-Derived Carbohydrates via the Aqueous-Phase Reforming Process <i>Bob Rozmiarek; Virent</i> <i>Energy Systems, Inc.</i>	2.9	X			The project team is heading in the proper direction with a goal of commercializing the aqueous phase reforming process and there is good coordination of catalyst development theory with evaluation. The reviewers noted it was difficult to review this project because of project secrecy. The project is in the final budget period and will continue through the end of the agreement.
PD-04	Investigation of Reaction Networks and Active Sites in Bio-Ethanol Steam Reforming over Co-based Catalysts <i>Umit S. Ozkan; Ohio</i> <i>State University</i>	3.3	x			Non-precious metal catalyst development is necessary to achieve long-term DOE cost targets. The catalyst development activity will provide a sound basis for a decision on the efficiency and effectiveness of the non precious metal catalyst at the end of the project. A concern remains regarding the lifetime of the catalyst. Next steps include long- term (> 100 hrs) time-on-stream experiments and accelerated deactivation and regeneration studies.
PD-05	Distributed Reforming of Renewable Liquids Using Gas Transport Membranes U. (Balu) Balachandran; Argonne National Laboratory	2.3			Х	The project aims to develop an oxygen transport membrane (OTM) for distributed reforming of bio-derived liquids to produce hydrogen. Module-scale modeling will be needed to understand the potential hydrogen pressure that might be achieved. Recommendations include addressing flux and heat management issues and third party analysis of costs. The project will continue to optimize OTM for hydrogen production and chemical stability, and will develop an H2A techno-economic analysis of the process. This work will undergo an interim review in 2010 to determine if the project will continue.
PD-06	Zeolite Membrane Reactor for Water-Gas- Shift Reaction for Hydrogen Production Jerry Y.S. Lin; Arizona State University	3.3	X			Materials development in the photo-electrochemical arena is clearly relevant, especially if such materials show improvements over photovoltaics/electrolyzer systems. The membrane development team has shown good technical success. A cost analysis is needed to validate the potential for significant cost reductions in hydrogen production. Research would benefit from increased focus on the catalytic aspect and from partnering with industry. The project and will continue modifications of membrane materials to improve performance.
PD-07	High-Performance, Durable, Palladium Alloy Membrane for Hydrogen Separation and Purification <i>Jim Acquaviva; Pall</i> <i>Corporation</i>	3.2	х			The team shows strong collaboration and steady progress in the development of a Pd-alloy membrane that enables the production of 99.99% pure hydrogen from reformate, particularly with the flux rate. Next steps include the evaluation of the membrane durability, membrane formation process improvement, and techno-economic analysis.

Project Number	Project Title PI Name & Organization	Final Score	Continue	Discontinue	Other	Summary Comment
PD-08	Solar Cadmium Hydrogen Production Cycle Bunsen Wong; General Atomics	2.7	х			Progress has been made on identifying whether the cadmium quench step of this solar thermochemical process can be accomplished without significant back reaction with oxygen and identified a solar receiver in which the reaction can take place on the ground. The reviewers recommend evaluating alternative approaches to the rotating machinery for the hydrogen production step.
PD-09	Solar High-Temperature Water-Splitting Cycle with Quantum Boost <i>Ali T-Raissi; Florida</i> <i>Solar Energy Center</i>	2.9	X			The sulfur-ammonia thermochemical cycle team has identified the critical path in this technology to be the electrolyzer development and will focus on this barrier as the project continues. The reviewers recommend that the solar field work be delayed until the electrochemical process is finalized.
PD-10	Solar-Thermal Ferrite- Based Water Splitting Cycles Alan W. Weimer; University of Colorado, Boulder	2.8	Х			Significant achievements in the use of ferrites for solar thermochemical water splitting processes include the development and testing of the aerosol reactor and the decrease of 200°C in the ferrite reduction temperature. Next steps in this project will focus on cycling the ferrite materials to define particle degradation.
PD-11	R&D Status for the Cu- Cl Thermochemical Cycle Michele Lewis; Argonne National Laboratory	3.2			x	The reviewers note that the Cu-Cl cycle is one of the most promising thermochemical cycles and that the team has a solid approach to their work. Recommendations include focusing on the elctrolyzer membrane and on materials compatible with a corrosive environment. The Nuclear Hydrogen Initiative is cancelled as of the end of FY 2009. The Fuel Cell program may continue funding this project subject to appropriations.
PD-12	Sulfur-Iodine Thermochemical Cycle Paul Pickard; Sandia National Laboratories	3.3			x	The team has made significant progress in the S-I thermochemical cycle but the reviewers identify the need for improved catalysis, separation of the reaction products, removal of the product gases, and a comprehensive cost analysis. The Nuclear Hydrogen Initiative is cancelled as of the end of FY 2009. Recommend continued R&D if the Fuel Cell program is able to provide funding due to relevance for solar high temperature cycles.
PD-13	Hybrid Sulfur Thermochemical Cycle William A. Summers; Savannah River National Laboratory	3.3			x	Good progress has been made on the hybrid sulfur thermochemical cycle and the team was commended for the clever solution to minimize sulfur crossover. Future work should include long term durability testing. The Nuclear Hydrogen Initiative is cancelled as of the end of FY 2009. Recommend continued R&D if the Fuel Cell program is able to provide funding due to relevance for solar high temperature cycles.
PD-14	High Temperature Electrolysis System Steve Herring; Idaho National Laboratory	3.1			X	The demonstration of the multi kilowatt electrolyzer stacks was noted as a significant achievement by the team. However, the issues of cell performance need to be addressed before proceeding to future large stack demonstrations. The Nuclear Hydrogen Initiative is cancelled as of the end of FY 2009. Recommend continued R&D if Fuel Cell program is able to provide funding due to relevance for solar high temperature cycles.

PROLOGUE Project Title

Project Number	Project Title PI Name & Organization	Final Sco	Continue	Discontin	Other	Summary Comment
PD-15	Technoeconomic Boundary Analysis of Photobiological Hydrogen Producing Systems Brian D. James; Directed Technologies, Inc.	3.4			X	A technoeconomic boundary analysis was completed to evaluate four different hydrogen production option using biological processes: 1) photosynthesis with algae and bacteria; 2) water algae fermentation; 3) lignocellulose fermentation; and 4) microbial electrolysis. These approaches included not only single systems but also multiple system embodiments and system integrations. A final report needs to be completed to close out the project.
PD-16	Maximizing Light Utilization Efficiency and Hydrogen Production in Microalgal Cultures <i>Tasios Melis; University</i> of California, Berkeley	3.5	Х			The project continues to make excellent progress toward the goal to enhance light usage by shortening the light receptor antenna. Cloning of previously identified genes demonstrates the value and validity of the work with efficiency targets achieved ahead of schedule. Work on this project toward cloning newly identified genes to meet long term targets will continue.
PD-17	Biological Systems for Hydrogen Photoproduction Maria L. Ghirardi; National Renewable Energy Laboratory	2.7	х			The project continues to make progress on optimizing photosynthetic water-splitting biological hydrogen production and increasing catalyst stability while improving oxygen tolerance. The partnership between various universities, an international institution, and a national lab is good. However, the reviewers noted that additional progress was expected based upon the funding level.
PD-18	Fermentative and Electrohydrogenic Approaches to Hydrogen Production Pin-Ching Maness; National Renewable Energy Laboratory	3.6	х			This project has a very good combination of novel fermentation with MEC technology, which allows for better feedstock utilization. The systematic inhibitor study was excellent in this project, and the molar yields are quite impressive.
PD-19	Development of Water Splitting Catalysts Using a Novel Molecular Evolution Approach Neal Woodbury; Arizona State University	2.9	Х			Much progress has been made in producing and testing numerous formulations in this project, and automation has enhanced sample throughput. However, the reviewers note that significant progress was not reported since the last review and recommend that a more focused approach should be taken.
PD-20	High-Capacity, High Pressure Electrolysis System with Renewable Power Sources <i>Martin Shimko;</i> <i>Avalence LLC.</i>	2.8	Х			This is a relatively new project with a unique electrolysis system design. The project focuses on high-pressure electrolysis from potentially renewable sources. It was initiated in May 2008 and is currently on track with respect to its planned schedule of accomplishments. Future work continues current activities. The project should develop a detailed cost estimate, assuming success of their design.
PD-21	PEM Electrolyzer Incorporating an Advanced Low Cost Membrane <i>Monjid Hamdan; Giner</i> <i>Electrochemical</i> <i>Systems, LLC</i>	3.7	Х			This new project is targeted at developing a high-efficiency, low-cost membrane, a long life lower cost cell separator, and reducing the cost and improving the efficiency of the BOP. The dimensionally stabilized membrane is one step in this direction. The reviewers recommend that the team focus on larger cell stacks and understand the cause of cell degradation.
PD-22	Photoelectrochemical Hydrogen Production: DOE PEC Working Group Overview Eric L. Miller; Univ. of Hawaii at Manoa	3.3	х			The photoelectrochemical (PEC) working group is an important effort aimed at coordinating research from a dozen institutions. This project shows good integration of theory, synthesis, surface science, and electrochemistry. This project is encouraged to bring industrial partners into the working group.

vi FY 2009 Merit Review and Peer Evaluation Report

Project Number	Project Title PI Name & Organization	Final Score	Continue	Discontinue	Other	Summary Comment
PD-23	Technoeconomic Boundary Analysis of Photoelectrochemical (PEC) Hydrogen Producing Systems Brian James; Directed Technologies Inc.	3.2			х	The team has a strong background in H2A type economic analysis and the technoeconomic model is well designed. The PEC systems are still conceptual and will come into the focus when materials are identified. At that point, industrial partners will need to be integrated into the project. A final report needs to be completed to close out the project.
PD-24	Characterization of Materials for Photoelectrochemical Hydrogen Production (PEC) Clemens Heske; University of Nevada, Las Vegas	3.3	х			The project is important for the development and analysis of PEC materials, and the team is successfully applying and developing state-of-the art measurement techniques and equipment to achieve required experimental results. Project collaboration and information dissemination is very good. Future work will add abilities to further understand surface chemistry of PEC.
PD-25	Nanostructured MoS2 and WS2 for the Solar Production of Hydrogen <i>Thomas F. Jaramillo;</i> <i>Stanford University</i>	3.5	x			The approach of quantum confinement is a novel and unique way to address the search for the optimum PEC material. The project is showing significant progress towards meeting the goal of a 2.0 eV band gap for photo cathodes. Durability needs to be addressed at some point. Future work should include a demonstration of improved photoelectrochemical behavior of the synthesized materials.
PD-26	Development of Hydrogen Selective Membranes/Modules as Reactors/Separators for Distributed Hydrogen Production Paul KT Liu; Media and Process Technology Inc.	3.0	х			Design, fabrication, evaluation and economic analysis of H_2 selective membranes work has progressed through the laboratory stage and the project will move to field testing in July. The reviewers recommend that membrane performance measurements be reported in consistent units and that the investigators review the impact of compression on the cost of the process.
PD-28	A Novel Slurry Based Biomass Reforming Process T.H. Vanderspurt; United Technologies Research Center	2.3			х	Since the last review, the project changed direction from an acid, which was not yielding positive results, to a base hydrolysis reaction with initial results showing >95% conversion of yellow poplar and 74% H ₂ selectivity. The reviews ranged from very positive to disbelief and the final score reflects this difference. The investigators will need to show that the flow through reactor works as well as the batch reactor and a follow up evaluation will determine if progress warrants continuation.
PD-30	Hydrogen Delivery Infrastructure Analysis Marianne Mintz; Argonne National Laboratory	3.5	X			Delivery represents a significant portion of the consumers' cost of hydrogen; it is necessary that we understand the costs associated with the various options. The project showed that significant cost reductions are available through flattening the hydrogen demand profile. A recommendation is to add chemical hydrides as a delivery option.
PD-31	H2A Delivery Components Mode Olga Sozinova; National Renewable Energy Laboratory	3.2	х			The Hydrogen Delivery Components Model is a well-used tool by the hydrogen community and is essential for cost analysis of hydrogen delivery components and systems on the basis of common and transparent assumptions. The project accomplishments have been steady. The reviewers recommend calibrating the model against an actual installation to determine model accuracy.

Project Number	Project Title PI Name & Organization	Final Score	Continue	Discontinue	Other	Summary Comment
PD-32	Hydrogen Energy Station Analysis in Northeastern US and Hydrogen Sensors for Infrastructure <i>Eileen Schmura;</i> <i>Concurrent</i> <i>Technologies</i> <i>Corporation</i>	2.1			Х	This project is nearing completion. The majority of the work focuses on analysis of stationary fuel cell sites powered by biogas (landfill and digester gas) in the northeastern U.S. corridor for combined heat and power (CHP) and combined heat, hydrogen, and power (CHHP). A secondary aspect was the evaluation of hydrogen sensors. The reviewers noted little progress on the hydrogen sensors. (This is a congressionally directed project).
PD-34	Oil-Free Centrifugal Hydrogen Compression Technology Demonstration <i>Hooshang Heshmat,</i> <i>Ph.D.; Mohawk</i> <i>Innovative Technology,</i> <i>Inc.</i>	3.2	х			Industrial compressors are one of the key barriers to cost effective hydrogen supply and distribution. This new project is pursuing an innovative high-speed supercritical design. The project has good technical competency and industrial players. Future work is focused on design, fabrication, and testing, in support of a down-select decision.
PD-35	Development of a Centrifugal Hydrogen Pipeline Gas Compressor <i>Francis A. Di Bella;</i> <i>Concepts NREC</i>	3.3	х			This new project targets the design and demonstration of an advanced centrifugal compressor for high-pressure hydrogen pipeline transport. It is taking a methodical approach to system design and involves industry partners. The design of a system and end rotor seems novel and well thought out. Future work will include materials testing, compressor design, and addressing gearbox issues.
PD-36	Advanced Hydrogen Liquefaction Process Jerry Jankowiak; Praxair	2.6	х			This new project is pursuing a reduced energy process targeted to make liquid hydrogen more economically viable as a transportation fuel. The project has a proprietary approach, the details of which need to be made public at some point. The project is in its early stages. Future plans have not been described in sufficient detail.
PD-37	Active Magnetic Regenerative Liquefier John A. Barclay; Prometheus Energy Company	3.0	Х			This new project is investigating a novel, non-compression technique for hydrogen liquefaction. Good technical results have been achieved. The project team will complete assembly tests by 4th quarter 2009. A detailed system analysis to calculate expected performance and evaluate advantages/disadvantages with respect to conventional liquefaction process will be performed.
PD-38	Reversible Liquid Carriers for an Integrated Production, Storage and Delivery of Hydrogen Bernie Toseland; Air Products and Chemicals, Inc.	2.6	X			This project addresses hydrogen carriers for both onboard and off board hydrogen regeneration, but its potential to meet hydrogen production, delivery, and storage targets is not well defined. Also, the evaluation is being performed using a compound that will not be used commercially. The investigators should identify and test the compound of interest. An evaluation is warranted to determine whether a non toxic carrier exists.
PD-39	Inexpensive Delivery of Cold Hydrogen in High Performance Glass Fiber Composite Pressure Vessels Andrew Weisberg; Lawrence Livermore National Laboratory	3.1	х			The project seeks to demonstrate inexpensive hydrogen delivery through synergy between low-temperature (200 K) hydrogen densification and glass fiber strengthening, to reduce the cost of storage and tube trailer delivery. The team has made good progress. The selection of the operating regime to reduce delivery cost should be reviewed in the context of total cost.

Project Number	Project Title PI Name & Organization	Final Score	Continue	Discontinue	Other	Summary Comment
PD-40	Development of High Pressure Hydrogen Storage Tank for Storage and Gaseous Truck Delivery Don Baldwin; Lincoln Composite Inc.	3.0	х			The project approach begins with the design and qualification of 3600 psi tanks, then will move to 5000 psi tanks. Cost reduction and risk mitigation are the primary objectives. Progress has been made on development and qualification of the 3600 psi tank. Collaboration in the area of testing to ensure the damage tolerance of the design to realistic scenarios should be incorporated.
PD-41	A Combined Materials Science/Mechanics Approach to the Study of Hydrogen Embrittlement of Pipeline Steels <i>P. Sofronis; University</i> of Illinois at Urbana- Champaign	3.4	x			The work has generated considerable insight regarding the mechanism of steel pipeline failures due to hydrogen transport. The researchers used pipeline samples supplied by manufacturers (Air Products, Air Liquide, OSM steels) to provide a basis for further work. The experimental and theoretical methods were noted as being very strong.
PD-42	Fiber Reinforced Composite Pipelines Dr. Thad M. Adams and G. Rawls; Savannah River National Laboratory	2.5	х			The hydrogen permeation and integrity part of this project is complete. Test samples were prepared and tested for hydrogen solubility, diffusivity and permeability. The team should focus on the requirements needed by authorities with jurisdiction for installing FRP for hydrogen service. The investigators should consider partnering with stakeholders and begin field tests.
PD-43	H ₂ Permeability and Integrity of Steel Welds Z. Feng; Oak Ridge National Laboratory	3.6	х			The project aims to analyze the fracture behavior of welds in the presence of hydrogen. The approach of analysis for fracture toughness of welds in the presence of hydrogen may need better definition. Baseline fracture tests with notched cylindrical bars of 4340 steel microstructures have been performed. More emphasis should be put on conventional welding processes, in addition to friction stir welding.
PD-44	Composite Pd and Alloy Porous Stainless Steel Membranes for Hydrogen Production and Process Intensification <i>Yi Hua Ma; Worcester</i> <i>Polytechnic Institute</i>	2.9	Х			The project has shown good progress regarding synthesis, fabrication and testing of Pd and Pd alloy composites membranes for applications in WGS reactors. The experimental testing methods are adequate and carefully performed. The modeling simulations are very useful for predicting the performance of the membrane in a broad range of conditions. Reported test results of the membranes, using simplified gas mixtures, indicate very good long-term H ₂ selectivity and stability. However these tests should be extended to gas mixtures that are more realistic and similar in compositions with syngas.
PD-45	Development of Robust Metal Membranes for Hydrogen Separation Brian D. Morreale; National Energy Technology Laboratory	2.9	х			A test protocol has been developed to standardize membrane testing and to enable comparison in coal conversion processes. Several alloy compositions have been fabricated and screened for performance, and some alloys have shown potential for S-tolerance. Comments suggested the project team should consider developing a list of selection criteria in trying to optimize membrane development, and testing with real syngas from a gasifier.
PD-46	Scale-up of Hydrogen Transport Membranes for IGCC and FutureGen Plants Doug S. Jack; Eltron Research & Development Inc.	2.4			х	The project has shown progress in the development of an H_2/CO_2 separation system for coal gasifier systems. Comments suggested that the project has high potential if successful, but reviewers thought more information and data to support the highlighted results was required to more accurately review this project. Most reviewers believed that additional testing of the membranes is needed before scaling up.

Project Number	Project Title PI Name & Organization	Final Score	Continue	Discontinue	Other	Summary Comment
PD-47	High Permeability Ternary Palladium Alloy Membranes with Improved Sulfur and Halide Tolerance <i>Kent Coulter, Ph.D.;</i> <i>Southwest Research</i> <i>Institute</i> [®]	3.2	х			The experimental and computational modeling approaches employed in this project are generally well planned and effective and the project team is working with a number of very capable groups, with complementary expertise. It was recommended that the computational modeling efforts become more coordinated with laboratory studies. Additionally, more emphasis should be given to improving and validating the modeling procedures for predicting hydrogen permeability of various alloys under different temperature and pressure conditions, and to investigating methods that improve membrane durability. Overall, the project was considered to have significant value to industry by providing a powerful tool to make alloy compositions with high precision.
PD-48	Experimental Demonstration of Advanced Palladium Membrane Separators for Central High-Purity Hydrogen Production S.C. Emerson; United Technologies Research Center	2.9			X	The objective of this project is to develop, construct and experimentally validate the performance of 0.1 kg H_2 /day PdCu trimetallic alloy membrane separators at feed pressures of 2 MPa (290 psia) in the presence of H ₂ S, NH ₃ , and HCl. In this study, The project team has a good approach to develop a sulfur, halide, and ammonia resistant alloy membrane for hydrogen separation. A large number of contaminants in the test gases have been used, making the test results more realistic. Project completion occurs in FY2009.
PD-49	Integration of a Structural Water Gas Shift Catalyst with a Vanadium Alloy Hydrogen Transport Device <i>Tom Barton; Western</i> <i>Research Institute</i>	3.0			х	Objectives of this project include development and testing of WGS catalysts capable of operating at high pressures and manufacturing an integrated WGS membrane system to produce 10,000 liters/day of hydrogen from coal-derived syngas. Overall, the technical accomplishments of the project have been good and the team had good collaboration among universities, national laboratories, and industry. It was recommended that the performance tests for the WGS catalysts and membranes should be extended to conditions that better mimic more realistic syngas compositions. Project completion occurs in FY2009.
PD-50	Hydrogen Delivery in Steel Pipelines Doug Stalheim; Secat, Inc.	2.8		Х		The identification, development and analysis of promising modern low-carbon steel microstructures were identified by the reviewers as a strength of this project. Recommendations are to focus on fracture toughness assessments and the effect of impurities on metal integrity. The project ends in FY2009.
PDP-01	Development and Optimization of Cost Effective Material Systems for Photoelectrochemical Hydrogen Production <i>Eric McFarland;</i> <i>University of California,</i> <i>Santa Barbara</i>	3.2	X			This project is advancing many areas of understanding and technology in photoelectrochemical hydrogen production and has made progress in understanding Fe_2O_3 that may also be useful when developing other low gap oxide materials or for using Fe_2O_3 in a tandem system. The team is working toward finding an adequate photoelectrochemical material prior to engineering a complete system.

Project Number	Project Title PI Name & Organization	Final Score	Continue	Discontinue	Other	Summary Comment
PDP-02	Semiconductor Materials for Photoelectrolysis John A. Turner; National Renewable Energy Laboratory	3.0	х			This project targets cheap, durable and efficient materials for PEC. Stabilization of the III-V materials class is the central focus, but other important classes are also under investigation. There was progress in the synthesis and characterization of InGaN-based materials. Future work needs to focus strongly both on improving the stability and reducing the cost of the III-V materials.
PDP-03	PEC Materials: Theory and Modeling Yanfa Yan; National Renewable Energy Laboratory	3.1	X			The focus of the project is to understand the performance of PEC materials and provide guidance and solutions for performance improvement, design and new materials discovery. Density functional theory (DFT) is the right approach to perform material discovery. The project has good coordination between theory and experiments.
PDP-04	Progress in the Study of Amorphous Silicon Carbide (a-SiC) as a Photoelectrode in Photoelectrochemical (PEC) Cells Arun Madan; MVSystems, Inc.	3.0	X			The objective of the project is to fabricate a hybrid a-Si tandem solar cell/a-SiC photoelectrode (PV/a-SiC) device. The approach of tailoring the bandgap with deposition control and multilayer films is a good strategy for capturing the solar spectrum. The project has made good progress in materials development and testing. The project would benefit from a cost assessment to ensure the technology is on the path to achieving overall hydrogen production cost targets.
PDP-05	Progress in the Study of Tungsten Oxide Compounds as Photoelectrodes in Photoelectrochemical Cells Nicolas Gaillard; University of Hawaii	3.3	х			The project is relevant to establishing the next steps for photoelectrochemical hydrogen production (PEC) electrode structures. There is a methodical approach that evaluates the individual layers of the PEC electrode. An improvement in WO ₃ -based PEC electrode performance has been demonstrated via new materials/fabrication techniques, and this will be pursued to further improve PEC performance.
PDP-06	Photoelectremical Hydrogen Production Jess Kaneshiro; University of Hawaii at Manoa	3.1	х			The investigation of copper chalcopyrite is good since these materials are inexpensive and durable. High currents have been achieved, but stability needs to be addressed. Voltage bias has been reduced by sulfur incorporation in the materials. The project will continue to focus on the reduction of voltage bias by investigating new and/or different materials.
PDP-07	Critical Research for Cost-Effective Photoelectrochemical Production of Hydrogen William B. Ingler, Jr.; University of Toledo	2.5	х			The project seeks to develop critical technologies required for cost-effective production of hydrogen from sunlight and water using thin film (tf)-Si-based photoelectrodes. Only some of the project tasks are directly relevant to the goals of PEC hydrogen production. The project shows some good potential and results, but significant technical barriers still exist. With regard to future activities, there may not be enough time and funding to achieve the project goals.
PDP-10	Composite Bulk Amorphous Hydrogen Purification Membranes T. Adams; Savannah River National Laboratory	2.8	Х			The project focus on using low-cost metallic glass membranes instead of high-cost palladium is in line with DOE programmatic goals. The currently measured hydrogen flux rates are generally an order of magnitude below those of palladium. Work is in progress to generate thin films of the metallic glass to improve hydrogen flux rates. Future plans include work to generate and measure flux rates in thin films, additional modeling work, and testing of alloys suggested by the modeling work.

Project Number	Project Title PI Name & Organization	Final Score	Continue	Discontinue	Other	Summary Comment
PDP-12	Catalytic Solubilization and Conversion of Lignocellulosic Feedstocks <i>T.A. Semelsberger; Los</i> <i>Alamos National</i> <i>Laboratory</i>	3.0	X			The project focus on biomass from non-food/feed crops is an excellent approach for feedstocks for the production of hydrogen. The screening experiments with an array of potential catalysts using solid biomass and potential biomass digestion products to look for evidence of biomass breakdown have resulted in some encouraging results. The future plan includes both additional screening experiments and some focused work on lignin, which has proven to be the most difficult part of the biomass to digest.
PDP-13	Novel Low-Temperature Proton Transport Membranes Andrew Payzant; Oak Ridge National Laboratory	2.5		Х		The project has successfully synthesized 10 micron films on Y-stabilized zirconia. The reviewers indicated that the results were modest with very low hydrogen fluxes to-date, and that targets, milestones and performance metrics for the project were lacking. This project will be discontinued.
PDP-14	Ultra-thin Proton Conduction Membranes for H ₂ Stream Purification with Protective Getter Coatings Dr. Margaret E. Welk; Sandia National Laboratories	2.6			X	The reviewers commented that the project team's integrated/monolithic approach to S gettering/H ₂ purification should provide a simplified system design and good robustness. Reviewers recommended that the membranes be tested under real in-service operating conditions and that performance and cost comparisons be made with alternative technologies. An interim review will be conducted in FY 2010 to determine if this project will continue.
PDP-15	Distributed Bio-Oil Reforming S. Czernik; National Renewable Energy Laboratory	3.2	Х			The project was found to be very well thought out and has shown progress in producing hydrogen from pyrolysis oil. The catalyst development work and reducing the methanol concentration were particularly noteworthy. Recommendations for future work include evaluating lower cost catalysts and the life cycle cost of the process.
PDP-16	Pressurized Steam Reforming of Bio- Derived Liquids for Distributed Hydrogen Production Shabbir Ahmed; Argonne National Laboratory	2.4			х	The modeling effort over the past year has provided insight into options for pressurized steam reforming of ethanol. However, the reviewers note that the minimal funding that was available in FY 2009 was not sufficient to experimentally verify the model. This work will be evaluated further to determine whether to continue the funding in FY 2010.
PDP-17	Renewable Electrolysis Integrated System Development and Testing <i>Kevin W. Harrison;</i> <i>National Renewable</i> <i>Energy Laboratory</i>	3.3	х			The team addresses a key area of hydrogen use with renewable energy sources and provides a good combination of analysis and experimental results. The reviewers feel that long term data generation is critical to the success of this project and that the compressor and fueling station work are diluting the focus.
PDP-18	Hydrogen from Water in a Novel Recombinant Oxygen-Tolerant Cyanobacterial System <i>Qing Xu; J. Craig</i> <i>Venter Institute</i>	3.2	Х			The team has a well developed plan to identify, isolate, and express oxygen tolerant hydrogenase genes and a vast library and tools for their use. A better explanation should be provided to understand how the results from this project will apply to commercial hydrogen production systems.

Project Number	Project Title PI Name & Organization	Final Score	Continue	Discontinue	Other	Summary Comment
PDP-19	Use of Biological Materials and Biologically Inspired Materials for H ₂ Catalysis John W. Peters; Montana State University	3.1	х			The focus on improving hydrogenase stability and on enzymes and catalyst supports is good and the investigators have made progress on well defined goals. However, the coordination and even the relationship between the different parts of this project are not clear. The project team should focus more on down selecting different configurations for the biomimetic device.
PDP-20	Hydrogen Embrittlement of Structural Steels Brian Somerday; Sandia National Laboratories	2.7	х			The project has shown the dependence of the degree of hydrogen embrittlement on the type of steel. However, questions arise on the variation in the round robin testing and whether all participating labs were calibrating in the same manner. Additional planning and coordination are recommended before proceeding much further.
PDP-21	Oil-Free Rotor-Bearings for Hydrogen Transportation & Delivery <i>Hooshang Heshmat,</i> <i>Ph.D.; Mohawk</i> <i>Innovative Technology,</i> <i>Inc.</i>	3.1			х	The project is a Phase II SBIR project aimed at the development of foil bearings (journal and thrust) for hydrogen pipeline compressors. The project has made steady progress and is on its way to the next prototype setup and testing phase. Future activities will focus on a final report of the overall project and dynamic seal tests at high pressures, speeds, and temperature.
PDP-22	Development of Highly Efficient Solid State Electrochemical Hydrogen Compressor (EHC) Ludwig Lipp; FuelCell Energy, Inc.	3.5	х			The project will continue as a Phase II SBIR. The project supports a critical delivery objective within the Hydrogen Program. Good progress is being made. The ability to provide a 300:1 compression ratio is impressive. Durability studies (1000 cycles to 3000 psi) demonstrate good durability. The project should establish cost goals in addition to performance in order to focus future work.
PDP-24	Composite Technology for Hydrogen Pipelines Barton Smith; Oak Ridge National Laboratory	3.3	Х			This project appears to have significant potential to reduce the cost of hydrogen pipelines to meet the DOE targets. Composites experience in the natural gas industry provides a good basis for this work. Surface treatments and associated testing will yield valuable data on the ability to improve the permeability of polymer pipelines. A strong collaboration with pipe, liner, and coupling manufacturers will be pursued moving forward into next year.
PDP-25	Coatings for Centrifugal Compression George Fenske; Argonne National Laboratory	3.0	Х			The team has used a very practical approach to material failure in a reducing environment and several promising coatings have been tested side-by-side to provide comparisons. The reviewers recommend that the project should focus on understanding the mechanisms by which hydrogen affects the tribological features of interfaces.
PDP-26	Purdue Hydrogen Systems Laboratory J. Gore; Purdue University	2.5			X	The project objectives are very broad and wide-ranging. There has been progress towards the objective of identifying ideal process parameters. The bio approach generally suffers from low hydrogen yields, low kinetics, and scale-up issues. There is no clearly described path for taking this technology forward into a commercially viable, scalable process. Future work is a continuation of the current efforts. (This is a congressionally directed project).

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PDP-27	Developing Improved Materials to Support the Hydrogen Economy Michael Martin; Edison Materials Technology Center	2.2			Х	The objectives of this project are to demonstrate feasibility with job creation potential, identify cross-cutting breakthrough materials technologies, and stimulate near- term manufacturing-based commercialization. A small number of the projects appear to be generating revenue, which may be a sign of some technical success. The project is essentially complete. (This is a congressionally directed project).
PDP-28	Hydrogen Production and Fuel Cell Research D. Yogi Goswami; University of South Florida	1.9			х	The project objectives are to investigate the feasibility of the UT-3 thermochemical cycle theoretically and experimentally, develop calcium oxide reactants with favorable characteristics and better performance, conduct kinetic studies of gas-solid reactions to examine and improve cyclic stability and performance of solid reactants, and lower hydrogen production cost by increasing hydrogen yield with an improved solid reactant. These objectives are too broad and diverse. There is no clear project management organization. Most of the hydrogen production schemes attempted have already been thoroughly studied. Future work needs more focus on overcoming DOE barriers. (This is a congressionally directed project).
PDP-29	Integrated Hydrogen Production, Purification and Compression System Satish Tamhankar; Linde North America Inc.	2.8	х			The project approach combines good engineering and pilot scale testing with the complex integration of the membrane reactor and metal hydride compressor (MHC) systems. Needs for additional performance data, particularly with the MHC, and more detailed cost estimates were identified. Suggestions include testing a Pall membrane.

Hydrogen Storage

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ST-01	Metal Hydride Center of Excellence Lennie Klebanoff; Sandia National Laboratories	3.2			X	The Metal Hydride Center of Excellence (MHCoE) is scheduled to be completed in FY2010. The reviewers found the MHCoE to be well coordinated and managed and to have shown flexibility in performing down-selection of materials and refocusing efforts. Efforts going forward will be focused on completing the highest priority activities and documenting all MHCoE work for use by the Program in the future.

Project Number	Project Title PI Name & Organization	Final Score	Continue	Discontinue	Other	Summary Comment
ST-02	Thermodynamically Tuned Nanophase Materials for Reversible Hydrogen Storage: Structure and Kinetics of Nanoparticle and Model System Materials Bruce Clemens; Stanford University	2.4			х	This project will conclude in FY2010 and is a partner in the MHCoE focused on using model systems to investigate sorption kinetics, thermodynamics and sorption induced phase changes. The reviewers found that the experimental and analytical work has been very well carried out. However there are questions as to the applicability of the materials and model systems to the materials being investigated within the MHCoE, and progress has been slow. The remaining work should focus on material systems that will be most relevant to the MHCoE and demonstrate the applicability of the results to bulk materials.
ST-03	Discovery and Development of Metal Hydrides for Reversible On-board Hydrogen Storage Mark Allendorf; Sandia National Laboratories	3.0			x	This project will conclude in FY2010 and is a partner in the MHCoE directed at discovery of new hydrogen storage materials and improving the kinetics, thermodynamics and sorption properties of storage materials. The project was found to have good coordination between theory and experimental work. Going forward in the limited time remaining, the project should focus on completing tasks associated with the materials with greatest promise.
ST-04	Chemical Vapor Synthesis and Discovery of H ₂ Storage Materials: Li-Mg-N-H System Z. Zak Fang; University of Utah	3.2			X	This project will conclude in FY2010 and is a partner in the MHCoE focused on investigating new hydride materials with an emphasis on LiMgN. The project was found to be well carried out. With the remaining time, the project should focus on completing the current investigations, including carrying out cycling studies of the material systems.
ST-05	Aluminum Hydride Regeneration Jason Graetz; Brookhaven National Laboratory	3.3			х	This project will conclude in FY2010 and is a partner in the MHCoE focused on investigating the desorption and regeneration processes for alane (AlH ₃). The project is considered to be well managed, organized and executed. The project should continue as planned. However, closer work with the Hydrogen Storage Engineering Center of Excellence and System Analysis Working Group is encouraged to assess energy balances and feasibility of the regeneration schemes, and the use of slurries.
ST-06	Electrochemical Reversible Formation of Alane Ragaiy Zidan, Savannah River National Laboratory	3.1			X	This project will conclude in FY2010 and is a partner in the MHCoE focused on developing electrochemical routes for the regeneration of alane. The project was found to have made tremendous progress over the past year, being able to produce gram quantities of pure α -alane. With the remaining time in the project, it should focus on assessing and improving the well-to-tank energy efficiency of the process, including consideration of improved electrochemical cell design.
ST-07	Fundamental Studies of Advanced, High- Capacity Reversible Metal Hydrides <i>Craig M. Jensen;</i> <i>University of Hawaii</i>	3.0			Х	This project will conclude in FY2010 and is a partner in the MHCoE focused on developing new reversible hydride materials. The project team is highly respected and has many collaborations around the world. The team has made significant progress. However, due to the breadth of materials it works on, it would benefit by narrowing the scope of materials for future efforts.

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ST-08	First-Principles Modeling of Hydrogen Storage in Metal Hydride Systems J. Karl Johnson; University of Pittsburgh/Georgia Institute of Technology	3.4			Х	This project will conclude in FY2010 and is a partner in the MHCoE focused on computational modeling to identify promising material systems for focus by MHCoE experimentalists. The coordination between the project and the MHCoE is considered excellent. The team was commended for incorporating gas phase species in their models. It is recommended that the team consider incorporation of entropy in their models and validate their modeling of amorphous materials.
ST-09	Thermodynamically Tuned Nanophase Materials for Reversible Hydrogen Storage <i>Ping Liu; HRL</i> <i>Laboratories, LLC</i>	3.0			х	This project will conclude in FY2010 and is a partner in the MHCoE focused on development of reversible hydrides materials through destabilization and nanoconfinement approaches. The work is considered novel and well conducted. With the time remaining, it is recommended that the project focus on fully characterizing the current systems and developing a more complete understanding of the role of the scaffolds.
ST-10	Catalyzed Nano- Framework Stabilized High Density Reversible Hydrogen Storage Systems X. Tang; United Technologies Research Center	2.9			х	This project will conclude in FY2010 and is a partner in the MHCoE focused on the development of metal hydride/catalyzed nanoframework combinations that result in reversible hydrogen storage with targeted properties. The project incorporated computational modeling with experimental validation. In the remaining time, this project should focus on completing the incorporation of the hydride into the zirconia frameworks and characterizing the properties of these materials to validate their modeled predictions.
ST-11	Neutron Characterization and Calphad in Support of the Metal Hydride Center of Excellence <i>Terrence J. Udovic;</i> <i>National Institute of</i> <i>Standards and</i> <i>Technology</i>	3.4			X	This project will conclude in FY2010. NIST provides characterization resources for both the Metal Hydride Center of Excellence (P.I. Terrence Udovic) and the Hydrogen Sorption Center of Excellence (P.I.s D. Neumann and C. Brown) as well as independent projects within the EERE applied hydrogen storage program as part of an Interagency Agreement. This project provides unique capabilities that employ neutron-based measurement methods for hydrogen storage materials R&D.
ST-12	Analyses of Hydrogen Storage Materials and On-Board Systems Stephen Lasher; TIAX LLC	3.2			Х	This project is fully funded in 2009, and will complete work in FY2010. Their assessments of storage systems have consistently received high reviews. They are finalizing summary reports with ANL: Compressed Storage (350, 700 bar), Cryocompressed, AX-21, MOF 177, Liquid, N- ethylcarbazole, and an Alane Slurry based system.
ST-13	System Level Analysis of Hydrogen Storage Options <i>R.K. Ahluwalia;</i> <i>Argonne National</i> <i>Laboratory</i>	3.6	X			ANL will complete several summary reports with TIAX in FY2010. Analyses will be performed on the most promising materials developed in the Material Centers. Coordination with the Engineering Center will continue.

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ST-15	2009 Overview - DOE Chemical Hydrogen Storage Center of Excellence Kevin Ott; Los Alamos National Laboratory	3.8			х	The Chemical Hydrogen Storage Center of Excellence (CoE) will conclude at the end of FY2010. This is a very productive CoE, with excellent interaction and coordination among partners. It is well focused on virtually all DOE targets and technical barriers. The CoE should continue to improve release kinetics, thermochemistry, liquid fuel and efficient AB regeneration, and continue to down-select and focus resources on winning strategies.
ST-16	Amineborane-Based Chemical Hydrogen Storage Larry Sneddon; University of Pennsylvania	3.6			х	This project will conclude in FY2010. The project should down-select and converge storage systems as appropriate, and focus AB release R&D in the most promising system. Emphasis should be to investigate effects of additives on AB regeneration, continue to address hydrogen purity, and continue efforts to retain spent fuel in the liquid phase.
ST-17	Chemical Hydrogen Storage R&D at Los Alamos National Laboratory Anthony Burrell; Los Alamos National Laboratory	3.8			х	This project will conclude in FY2010. The project should continue to further advance the new AB regeneration system towards DOE targets and update the cost analysis; and continue to improve hydrogen release parameters, liquid fuel and address impurity release from AB. Coordinate with the Engineering CoE to address the on-board system requirements for the AB system.
ST-18	PNNL Progress as Part of the Chemical Hydrogen Storage Center of Excellence <i>Tom Autrey; Pacific</i> <i>Northwest National</i> <i>Laboratory</i>	3.6			х	This project will conclude in FY2010. The project should complete the investigation of the AB regeneration scheme and document its efficiency; conduct a cost analysis for AB regeneration scheme; continue to improve hydrogen release parameters, focusing on promising materials, and address impurity release from AB; and document more detailed results/benefits from the IPHE collaboration.
ST-19	Main Group Element and Organic Chemistry for Hydrogen Storage and Activation David A. Dixon; University of Alabama	2.7			х	This project will conclude in FY2010. The computational approaches are yielding important results on thermodynamic properties, hydrogen release, and spent fuel regeneration pathways which are vital to the overall success of the CHSCoE. The project should prioritize future work for better focus and use of remaining resources.
ST-20	Low-Cost Precursors to Novel Hydrogen Storage Materials <i>S. Linehan; Rohm and</i> <i>Haas Company</i>	3.4			х	This project will conclude in FY2010. The project should down-select between the metal reduction and the carbothermal process; conduct a cost analysis of NaBH ₄ as the AB first fill raw material, for the selected process; and conduct a cost analysis for the most promising AB regeneration scheme.
ST-21	Ammonia Borane Regeneration and Market Analysis of Hydrogen Storage Materials David Schubert; U.S. Borax	3.1			Х	This project will conclude in FY2010. The project should update the projection for worldwide boron market demand, assuming fuel cell vehicles are widely adopted throughout the rest of the world and not only in the United States.

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ST-22	Overview of the DOE Hydrogen Sorption Center of Excellence Anne C. Dillon and Lin Simpson; National Renewable Energy Laboratory	2.5			х	The Hydrogen Sorption Center of Excellence will conclude at the end of FY2010. In the remaining time, the CoE should focus on go/no-go recommendations of materials of interest to the Hydrogen Storage Engineering CoE based upon experimental data. Gaps should be closed for spillover materials addressing the lack of reproducibility of synthesis (and performance) across laboratories. Go/no-go recommendations should be made to DOE. Theory efforts should continue to incorporate experimental synthesis experience and experimental measurements to validate and update the models. CoE should close gaps such as, "what is the ideal-predicted %B content" and "ideal specific surface area" and "how do these predictions compare with current experimental values."
ST-23	A Biomimetic Approach to Metal-Organic Frameworks with High H ₂ Uptake <i>Hong-Cai (Joe) Zhou;</i> <i>Texas A&M University</i>	3.1	x			This project was selected after the initiation of the Sorption CoE; it will continue in FY2010. Good progress has been made. Progress should be accelerated by reducing the empiricism of the approach through collaboration with theory and detailed characterization. Establish trends on the polarizability of dihydrogen to entatic metal centers versus metal type to streamline synthesis options. Have promising results reproduced externally as soon as possible.
ST-24	Hydrogen Storage by Spillover Ralph T. Yang; University of Michigan	2.0			X	This project will conclude in FY2010. In the remaining period, the team should focus on reproducibility of synthesis and performance measurements by collaborating with external groups (e.g. round-robin activities). Increased characterization work should be used to understand barriers to increasing kinetics of hydrogen uptake.
ST-25	Optimization of Nano- Carbon Materials for Hydrogen Sorption Boris I. Yakobson, R. Hauge; Rice University	2.6			X	This project will conclude in FY2010. Spillover simulations are the key piece of this project. In the remaining period, theory efforts should continue to incorporate experimental synthesis experience and measurement of performance from partners and collaborators to validate and update the theoretical models.
ST-26	NREL Research as Part of the Hydrogen Sorption Center of Excellence L.J. Simpson; National Renewable Energy Laboratory	2.9			x	This project will conclude in FY2010. In the remaining period, NREL should put forward a sharply focused effort on improving synthesis and performance measurement reproducibility of spillover materials, including external parties (e.g. round robin efforts). Experimental verification efforts should be prioritized such as the Ca-COFs. Theory efforts should continue to stress verification using experimental data.
ST-27	Hydrogen Storage through Nanostructured Polymeric Materials <i>Di-Jia Liu; Argonne</i> <i>National Laboratory</i>	3.4	х			This project was selected after the initiation of the Sorption CoE; it will continue in FY2010. Good progress has been made. The team should increase collaborations with theory and external testing of materials for reproducibility. Efforts should also stress understanding trends such as limits of specific surface area and potential for higher temperature operation (e.g. >77K).
ST-28	Discovery of Materials with a Practical Heat of H ₂ Adsorption <i>Alan Cooper. H. Cheng</i> <i>et al.; Air Products and</i> <i>Chemicals, Inc. (APCI)</i>	2.4			х	This project will conclude in FY2010. In the remaining period, APCI should focus its efforts on the most promising areas and in summarizing trends identified to date. Effort on finishing the study of the promising aspect of BC ₃ spillover is recommended but further work on exploration of higher surface area BCx materials, that have not been successful to date, should be deemphasized.

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ST-29	Optimizing the Binding Energy of Hydrogen on Nanostructured Carbon Materials through Structure Control and Chemical Doping <i>Jie Liu; Duke University</i>	2.7			х	This project will conclude in FY2010. In the remaining period, the team should focus on doped carbon materials rather than on spillover catalysts. Emphasize sufficient characterization work in addition to performance measurements.
ST-30	Nanoengineered Graphene Scaffolds with Alternating Metal- Carbon Layers for H ₂ Uptake at Ambient Temperatures James Tour and Carter Kittrell; Rice University	2.6			х	This project will conclude in FY2010. In the remaining period, the team should focus on graphene dynamic multilayer work. The team should work within and outside the CoE, as appropriate, to obtain a broader range of measurements for pressure-concentration-temperature characterization of the most promising materials.
ST-32	A Synergistic Approach to the Development of New Hydrogen Storage Materials, Part I Jeffrey R. Long; University of California, Berkeley	2.7			х	This project will conclude in FY2009. The project team should establish priorities for the remainder of the project based on the most critical technical barriers and the materials most capable of meeting those challenges. Work on destabilization of metal hydrides has been adequately addressed. Results of R&D should be summarized, and physical property data shared with the Engineering Center.
ST-33	Hydrogen Storage in Metal-Organic Frameworks O. Yaghi (Pl), Chris Doonan; University of California, Los Angeles	2.7	X			This project started in FY2009 and the focus to-date has been on the most significant challenge, i.e., increasing binding energy. The project team should focus on refining theory based on experimental results and on collaboration and leveraging of work with other R&D groups for optimum results.
ST-34	Compact (L)H ₂ Storage with Extended Dormancy in Cryogenic Pressure Vessels <i>Gene Berry; Lawrence</i> <i>Livermore National</i> <i>Laboratory</i>	2.7	х			LLNL will continue to work with industry on tank cycling tests and investigations of ortho-para hydrogen states as a function of temperature and time. Work will continue to achieve further improvements beyond the 30% lower cost and more than double system capacity over 350 bar tanks currently projected by TIAX and ANL.
STP-01	Lifecycle Verification of Polymeric Storage Liners Barton Smith; Oak Ridge National Laboratory	2.9	х			ORNL will continue to make use of their automated test bed and explore a wide range of temperatures and pressures to assess polymer liners. Permeability data and projecting durability of the materials are the highest priorities for the coming year.
STP-02	Electron-Charged Hydrogen Storage Materials Chinbay Q. Fan; Gas Technology Institute	2.5			Х	This project will continue to develop materials pending the results of an upcoming go/no-go decision milestone to demonstrate 6wt% storage. Next steps include obtaining a better theoretical understanding of the mechanisms behind this storage process.
STP-03	Polymer-Based Activated Carbon Nanostructures for H ₂ Storage Dr. Israel Cabasso; State University of New York	2.6	х			This project will continue to explore avenues to increase binding energies. They will also need to show more data on uptake near room temperature (-25C) and improve the accuracy of these measurements. Their material may be tested at SWRI for independent verification. A 2010 go/ no- go decision point will be identified.

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STP-04	Low-Cost High- Efficiency High- Pressure H ₂ Storage Carter Liu; Quantum Fuel Systems Technologies Worldwide Inc.	2.7			х	This project is ending in FY2009. Remaining work in 2009 will focus on reducing component weight, volume and cost, and communicating results in a final report.
STP-17	Solutions for Chemical Hydrogen Storage: Hydrogenation/Dehydro genation of B-N Bonds Karen Goldberg; University of Washington	3.4			х	This project will conclude in FY2010. The team should use rationale design to provide more focus on how and on what basis ligand and metal selections for future catalysts will be made; and develop performance targets and assess catalyst performance to guide more efficient catalyst development.
STP-18	Chemical Hydrogen Storage Using Ultra- High Surface Area Main Group Materials & The Development of Efficient Amine-Borane Regeneration Cycles <i>Philip P. Power;</i> <i>University of California,</i> <i>Davis</i>	2.8			X	This project will conclude in FY2010. The team should investigate the optimum amount of nano-BN additions to AB to maximize storage capacity and quantify release of impurities; and redirect the effort for AB regeneration to address and reflect that of the current Center AB regeneration scheme.
STP-19	Electrochemical Hydrogen Storage Systems Dr. Digby Macdonald,; Pennsylvania State University	2.2			Х	This project will conclude in FY2010. The team should validate the EIS model for complex reaction systems; and increase focus on AB regeneration efforts where it is most relevant.
STP-20	Chemical Hydrogen Storage Using Aluminum Ammonia- Borane Complexes <i>M. Frederick</i> Hawthorne; University of Missouri - Columbia	3.0			Х	This project will conclude in FY2010. The team should determine the long-term stability, release kinetics, and solid state structure of new materials; and investigate impurity effects in hydrogen release.
STP-21	Novel Metal Perhydrides for Hydrogen Storage Jiann-Yang Hwang; Michigan Technological University	2.7			Х	This project has a go/no-go decision point at the end of FY2009. The project focus should be to check the reversibility of H_2 adsorption, and determine that the gas desorbed is 100% H_2 . The team should collaborate with others for validation of adsorption/desorption measurements on these materials.
STP-22	Purdue Hydrogen Systems Laboratory J. Gore; Purdue University	2.4			X	This is a Congressionally-directed project. Investigate and account for Me ₃ SiOTf in the AB regeneration scheme. Account for potential inefficiency resulting from the formation of a Si-O bond during AB regeneration. Because the slurry reactor product is likely to be solid, investigate removal of solid products from reactor.
STP-23	Hydrogen Storage Research Lee Stefanakos; University of South Florida	2.6			Х	This is a Congressionally-directed project. Investigate and eliminate experimental artifacts to obtain accurate and reliable PCT measurements for the LiBH ₄ /LiNH ₂ /MgH ₂ complex hydride and nanoporous PANI systems. Validate ab initio calculations. Focus future tasks on the most noteworthy remaining barriers.

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STP-25	Carbon Aerogels for Hydrogen Storage T.F. Baumann; Lawrence Livermore National Laboratory	2.9			X	This project will conclude in FY2010. The project has contributed to both the Metal Hydride and Sorption Centers of Excellence. In the remaining period. LLNL should continue to focus on strategies to improve heat conductivity and H_2 transport, and work on aerogels as nanoscale hosts for complex hydrides.
STP-26	Single-Walled Carbon Nanohorns for Hydrogen Storage and Catalyst Supports David B. Geohegan; Oak Ridge National Laboratory	3.4			Х	This project will conclude in FY2010. In the remaining period, ORNL should continue to stress reproducibility of synthesis and performance by participating with other CoE partners and independent organizations to perform independent measurement on its most promising materials. Theory work should continue to stress incorporation of experimental data to validate predictions.
STP-27	Enhanced Hydrogen Dipole Physisorption: Constant Isosteric Heats and Hydrogen Diffusion in Physisorbents <i>Channing Ahn;</i> <i>California Institute of</i> <i>Technology</i>	3.2			Х	This project will conclude in FY2010. In the remaining period, CalTech should focus on obtaining a better understanding of the thermodynamic properties of these materials and shedding light on the interrelations of pore size/distribution, enthalpies, temperature and pressure effects, and their influence on hydrogen uptake and release. Emphasis should be placed on the pore-slit/graphitic structures in collaboration with Rice University.
STP-28	Characterization of Hydrogen Adsorption by NMR Yue Wu; University of North Carolina	3.2			X	This project will conclude in FY2010. The NMR tool developed in this project is a unique approach to understanding fundamental material properties and their relationship to H_2 uptake. In the remaining period, the PI should work with NREL to prioritize the most important samples for study.
STP-29	Advanced Boron and Metal Loaded High Porosity Carbons <i>T. C. Mike Chung;</i> <i>Pennsylvania State</i> <i>University</i>	2.9			Х	This project will conclude in FY2010. In the remaining period, Penn State should emphasize obtaining validation of their most promising samples, with increased participation with CoE partners. The project team has demonstrated increased hydrogen capacity in B-doped materials over pure carbon for equivalent surface area. Penn State should make recommendations for a go/go-no decision on further research into these B-containing carbons based upon the limited surface area achieved and other factors.
STP-30	Best Practices for Characterizing Hydrogen Storage Properties of Materials <i>Karl Gross; H</i> ₂ <i>Technology Consulting</i> <i>LLC</i>	3.6	х			This project has developed a long-needed general guide on hydrogen storage measurements for broad distribution. Contributors to this effort are known experts in the field. Remaining planned chapters address cycling measurements and thermodynamics.
STP-36	Reversible Hydrogen Storage Materials: Structure, Chemistry, and Electronic Structure Ian Robertson; University of Illinois, Urbana-Champaign	3.4			Х	This project will conclude in FY2010 and is a partner in the MHCoE focused on providing microstructural characterizations and understanding of complex hydride materials to MHCoE partners, and on providing computational modeling of systems. The work is considered of very high quality and a valuable resource to the MHCoE. With the approaching end of the MHCoE, priorities should be placed on materials of greatest import to the MHCoE and efforts should be made to complete characterizations of systems and dissemination of results.

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STP-37	Metal Borohydrides, Ammines, and Aluminum Hydrides as Hydrogen Storage Materials <i>Gilbert M. Brown; Oak</i> <i>Ridge National</i> <i>Laboratory</i>	3.1			Х	This project will conclude in FY2010 and is a partner in the MHCoE focused on developing reversible hydrogen storage materials, specifically borohydrides, amides/imides, alane and light alanates. While the research team is highly competent with reactive materials and produces high quality work, the work plan was thought to be insufficiently focused and too broad in scope. Future work should focus on materials and approaches that have the highest probability of producing materials of interest.
STP-38	Development and Evaluation of Advanced Hydride Systems for Reversible Hydrogen Storage Joseph W. Reiter; Jet Propulsion Laboratory	3.2			Х	This project will conclude in FY2010 and is a partner in the MHCoE providing NMR analysis to MHCoE partners. The project validates material sorption properties and projects storage system characteristics. The NMR characterization is considered to be of very high value to the MHCoE, with some of the best hydride characterization capabilities anywhere in the world. The project is very well coordinated and collaborates effectively with the MHCoE. The team should focus on completing the characterization, documentation and dissemination of results to date and be prepared to quickly perform characterizations on MHCoE systems identified as partners complete their efforts.
STP-39	Effect of Trace Elements on Long-Term Cycling/Aging Properties and Thermodynamic Studies of Complex Hydrides for Hydrogen Storage Dhanesh Chandra; University of Nevada, Reno	3.6			X	This project will conclude in FY2010 and is a partner in the MHCoE focused on characterizing the effects of impurities and long-term cycling on reversible metal hydride materials, and on determining phase diagrams and vapor behavior in these systems. The high quality and volume of results for the past year and the quality and extent of collaborations, including international, were highly commended. Going forward it was recommended that the project try to extend their cycling analysis to new materials of high interest to the MHCoE.
STP-40	Amide and Combined Amide/Borohydride Investigations Don Anton, Savannah River National Laboratory	2.0			X	This project will conclude in FY2010 and is a partner in the MHCoE focused on the characterization of LiMgN and identification of dopants/additives to catalyze its sorption reactions. With the time remaining, the project should complete the characterization work and focus on aiding the MHCoE coordinate with the Hydrogen Storage Engineering Center of Excellence. A go/no-go decision on this material will be made by the end of Q2 FY2010.
STP-41	Synthesis of Nanophase Materials for Thermodynamically Tuned Reversible Hydrogen Storage <i>Channing Ahn;</i> <i>California Institute of</i> <i>Technology</i>	3.2			х	This project will conclude in FY2010 and is a partner in the MHCoE focused on understanding why material systems theoretically predicted to be reversible are not. The project team is considered highly talented and performs a useful service to the MHCoE. With the remaining time, it is recommended that the team focus on scaffolding effects and understanding the role they play in aiding and/or modifying sorption properties.
STP-42	Lightweight Borohydrides for Hydrogen Storage JC. Zhao; Ohio State University	3.1	Х			This project is a partner in the MHCoE and is focused on developing borohydride materials. In 2008 the project was expanded to include aluminoborane compounds. The project team should complete their original scope of work for the MHCoE, wrap up their Mg(BH ₄) ₂ work, and then focus on the aluminoborane efforts.

Project Number	Project Title PI Name & Organization	Final Score	Continue	Discontinue	Other	Summary Comment
STP-43	Center for Hydrogen Storage Research at Delaware State University Andrew Goudy; Delaware State University	2.6			Х	This is a Congressionally-directed project that involves the preparation and characterization of complex hydride materials for hydrogen storage. Many of the systems being investigated are similar to materials under investigation within the MHCoE and therefore the PI would benefit from stronger collaboration with MHCoE partners. The project team should focus on the most promising material systems and try to complement and avoid duplication of other efforts being carried out within the program.
STP-44	Solid-State Hydriding and Dehydriding of LiBH ₄ + MgH ₂ Enabled via Mechanical Activation and Nano- Engineering Leon Shaw; University of Connecticut	2.9		х		This is an independent project that involves the mechanical activation and nano-engineering of complex hydride materials for improved hydrogen storage properties. The project has reached an end of a phase and is being completed in December 2009. The systems being investigated are similar to materials under investigation within the MHCoE and the PI has been encouraged to and has collaborated more strongly with MHCoE partners. The project team should wrap up their current efforts and prepare their results for dissemination to the hydrogen storage community.
STP-45	Standardized Testing Program for Solid-State Hydrogen Storage Technologies <i>Michael Miller;</i> <i>Southwest Research</i> <i>Institute</i> [®]	3.2	х			This is an independent project that supports the Hydrogen Program through the operation of a national-level testing facility for the assessing and validating hydrogen storage properties of materials. This facility is a valuable resource to the program. The project team needs to develop additional characterization methods to validate results on samples that have proven difficult to reproduce, such as spillover materials, and help develop an understanding of the reason for the spurious results. With many of the Program's projects coming to completion, SwRI needs to be prepared to process samples more quickly as a higher volume of samples analyzed may be required.
STP-46	An Integrated Approach of Hydrogen Storage in Complex Hydrides of Transitional Elements <i>Tansel Karabacak;</i> University of Arkansas at Little Rock	2.6			х	This is a Congressionally-directed project focused on developing novel complex hydrides for hydrogen storage. The project has investigated a wide-range of materials using some interesting preparation techniques. Going forward, it is recommended that the project perform a down-selection and discontinue efforts on less promising materials, such as the metal-decorated and Mg-nanoblades.

Fuel Cells

Project Number	Project Title PI Name & Organization	Final Score	Continue	Discontinue	Other	Summary Comment
FC-01	Lead Research and Development Activity for DOE's High Temperature, Low Relative Humidity Membrane Program James Fenton; University of Central Florida	2.9	х			Not all reviewers feel the HTMWG coordination has been as successful as needed. Reviewers were divided on the future plans for centralized fuel cell testing of HTMWG materials, but generally support an expansion of the lead group's standardized characterization methodologies to include membrane durability and stability testing. The project has also worked to develop new membranes, and reviewers note that questions remain on acid leaching and the development path to low relative humidity performance. The membrane portion of the project will not be continued in FY2010 due to programmatic priorities.
FC-02	Dimensionally Stable Membranes Cortney K. Mittelsteadt; Giner Electochemical, LLC	3.4	X			This highly rated project's milestones for the year were achieved and interim conductivity targets have been met. Improvements in fuel cell performance have been shown, including electrodes. Reviewers believe future plans, including focus on cost of manufacturing, cycling durability and improved performance, are appropriate.
FC-03	New Polymer/Inorganic Proton Conductive Composite Membranes for PEMFC Serguei Lvov; Pennsylvania State University	2.1		x		The project was unable to meet conductivity targets or significantly improve upon Nafion®, and the membranes developed have poor chemical stability. The project will not be continued.
FC-04	Poly(cyclohexadiene)- Based Polymer Electrolyte Membranes for Fuel Cell Applications Jimmy Mays; University of Tennessee Mohammad Hassan and Kenneth Mauritz; University of Southern Mississippi	2.2		x		The project was unable to meet conductivity targets or significantly improve upon Nafion® and the materials developed have poor chemical stability. The project will not be continued.
FC-05	Advanced Materials for Proton Exchange Membranes James E. McGrath; Virginia Polytechnic Institute and State University	2.8		х		VPI has systematically developed copolymer membranes that have good mechanical properties and durability, but less than necessary conductivity. The project will not be continued.
FC-06	Protic Salt Polymer Membranes: High- Temperature Water-Free Proton-Conducting Membranes D. Gervasio; Arizona State University	2.2	х			Effort was placed on fuel cell fabrication and testing too early, and the basic materials were unable to meet conductivity targets or significantly improve upon Nafion®. ASU has added a new approach to anhydrous operation based on indium tin phosphate (ITP) that shows higher conductivity, but reviewers believe issues will be crossover, mechanical stability of the pure ITP, and low-temperature performance.

Project Number	Project Title PI Name & Organization	Final Score	Continue	Discontinue	Other	Summary Comment
FC-07	Fluoroalkyl-Phosphonic- Acid-Based Proton Conductors Stephen Creager; Clemson University	2.7		X		Progress was made in molecular dynamics modeling of model compounds, but the membranes synthesized failed in testing and did not meet the conductivity targets. The project will not be continued.
FC-08	Rigid Rod Polyelectrolytes: Effect on Physical Properties Frozen-in Free Volume: High Conductivity at Low RH Morton Litt; Case Western Reserve University	2.9	X			CWRU demonstrated membranes with high in-plane conductivity, but through-plane conductivity has not been experimentally demonstrated for these anisotropic materials. Mechanical stability remains an issue and chemical stability has not been demonstrated. Reviewers recommend increased collaboration.
FC-09	NanoCapillary Network Proton Conducting Membranes for High Temperature Hydrogen/Air Fuel Cells Peter Pintauro; Vanderbilt University	3.4	Х			This highly rated project has met its interim milestones and is on track. Reviewers rate the approach and future plans favorably, and consider electrospinning of conducting polymers to be a notable advance.
FC-10	High Temperature Membrane with Humidification- Independent Cluster Structure Ludwig Lipp; FuelCell Energy, Inc.	3.3	х			FCE's proprietary materials meet or exceed the interim DOE targets. Durability and fuel cell performance data and cost projections have not yet been presented.
FC-11	Novel Approaches to Immobilized Heteropoly Acid (HPA) Systems for High Temperature, Low Relative Humidity Polymer-Type Membranes Andrew M. Herring; Colorado School of Mines	2.9	X			The project is meeting conductivity milestones but needs to address mechanical and chemical stability. Reviewers found future work plans lacking in specifics.
FC-12	Improved, Low-Cost, Durable Fuel Cell Membranes James Goldbach; Arkema	2.4	Х			Membrane conductivity has been significantly below target. Reviewers question the ability to improve conductivity sufficiently with these materials.
FC-13	Membranes and MEAs for Dry, Hot Operating Conditions Steven Hamrock; Fuel Cell Components	3.3	X			Membranes have been fabricated with promising conductivity at 50% RH and 80°C, and several approaches are underway to improve mechanical durability and water solubility. Reviewers believe the project will need to narrow its focus in future work.
FC-14	New Polyelectrolyte Materials for High Temperature Fuel Cells John B. Kerr; Lawrence Berkeley National Laboratory	2.9	Х			Membrane conductivities with anhydrous proton conductors are below target and some reviewers question whether the approach can lead to materials that are stable.

Project Number	Project Title PI Name & Organization	Final Score	Continue	Discontinue	Other	Summary Comment
FC-15	Development of Novel PEM Membrane and Multiphase CFD Modeling of PEM Fuel Cell Susanta K. Das; Kettering University	1.8			х	This project received the second lowest overall ranking of fuel cell projects at this year's review. Reviewers questioned the characterization methods used and noted the independently measured membrane conductivity was far below target (project is not aligned with DOE goals). Reviewers felt the CFD modeling added nothing new and would require collaboration with a stack developer for relevance and validation. (Congressionally directed project)
FC-16	Applied Science for Electrode Cost, Performance, and Durability Christina Johnston; Los Alamos National Laboratory	3.0			х	Reviewers generally commend the sophistication of the experimental techniques and the quality of the science, and note that insights obtained can be used to improve both mass transport and kinetic performance. However, reviewers would like to see collaboration with industrial MEA manufacturers to address high-volume processing. This project will be combined with other similar activities at LANL.
FC-17	Advanced Cathode Catalysts and Supports for PEM Fuel Cells <i>Mark K. Debe; 3M</i> <i>Company</i>	3.6	X			This project tied with two others for the highest ranking amongst fuel cell projects in this year's review. This year, single-cell test results show that a 3M membrane electrode assembly has <u>exceeded</u> several key 2015 targets for cost, performance, and durability, hence showing promise for automotive-scale fuel cell stacks. Reviewers generally consider water management to be the toughest remaining challenge.
FC-18	Highly Dispersed Alloy Catalyst for Durability Vivek S. Murthi; UTC Power	3.0	Х			Alloys under study include iridium, and reviewers continue to question the value of replacing Pt with even less abundant metals, though researchers are working to replace a portion of the Ir with less expensive metals such as Co or Cr. Reviewers believe the approach including fundamental studies/modeling, catalyst synthesis, and cell testing will lead to improved understanding of ORR, but felt plans for future work are weak. In particular, durability of core-shell structures needs further attention.
FC-19	Development of Alternative and Durable High Performance Cathode Supports for PEM Fuel Cells Yong Wang; Pacific Northwest National Laboratory	2.7	X			While progress on support stability has been made, some reviewers are concerned that the focus on stability may overlook the effect of the support on necessary catalyst activity and electrode performance. Reviewers also recommend that cost be more explicitly addressed in support screening.
FC-20	Non-Platinum Bimetallic Cathode Electrocatalysts D. Myers; Argonne National Laboratory	3.1	Х			While reviewers commend the quality of the science, the best performing catalyst is still below the state-of-the-art and comparable performance on a platinum group metal mass activity basis may not be achieved. Reviewers would like to see more focus on durability and more fuel cell testing.
FC-21	Advanced Cathode Catalysts Piotr Zelenay; Los Alamos National Laboratory	3.5	X			This project tied with three others for the second highest ranking amongst fuel cell projects in this year's review. Several reviewers deemed the progress "impressive." Reviewers note the complexity of the project and some believe a narrowing of scope would be beneficial, while other reviewers comment on the strength and value in the individual team member contributions. Reviewer recommendations reflect this diversity of opinion.

Project Number	Project Title PI Name & Organization	Final Score	Continue	Discontinue	Other	Summary Comment
FC-22	Effects of Fuel and Air Impurities on PEM Fuel Cell Performance Fernando Garzon; Los Alamos National Laboratory	3.5	х			This project tied with three others for the second highest ranking in this year's review. Reviewers generally commended the approach, progress, and plans. Recommendations included incorporation of gas mixtures in the test program and reviewers encourage publication of data and models as soon as possible to aid developers.
FC-23	Effects of Impurities on Fuel Cell Performance and Durability J.G. Goodwin, Jr.; Clemson University	3.2	X			Reviewers recommended changes in testing approach and urged lower impurity concentrations to be more relevant to the hydrogen quality effort. Reviewers note lack of completed or planned work on mitigation strategies, and recommended closer collaboration with other institutions working on impurity effects.
FC-24	The Effects of Impurities on Fuel Cell Performance and Durability <i>Trent M. Molter, Ph.D.;</i> <i>University of</i> <i>Connecticut</i>	3.2	х			The project had difficulty with its commercially supplied membrane electrode assemblies, which hindered progress this year. Reviewers urged lower catalyst loadings and lower impurity concentrations to make the project more relevant to the transportation application. Reviewers recommended closer collaboration with other institutions working on impurity effects.
FC-25	Development and Demonstration of a New-Generation High Efficiency 1-10 kW Stationary PEM Fuel Cell System Durai Swamy, Ph.D.; Intelligent Energy	2.7	х			Reviewers note the team continues to work on absorption enhanced reforming, but have shifted the project baseline to steam methane reforming with pressure swing adsorption for gas clean-up. Use of a low-temperature PEMFC for a heat recovery application was questioned. As with many industrial product development projects, technical detail and data shared are limited and progress is hard to assess.
FC-26	Stationary PEM Fuel Cell Power Plant Verification <i>Eric Strayer; UTC</i> <i>Power</i>	3.3	х			The advanced system undergoing field testing has reduced parts count, higher efficiency power conditioning, improved air, thermal and water management, a cost reduction of more than 30%, and a power density more than 2.5 times greater than other commercially available systems in the 1 to 5 kW range. Reviewers generally were complimentary of the project and its progress.
FC-27	Intergovernmental Stationary Fuel Cell System Demonstration <i>Richard Chartrand;</i> <i>Plug Power</i>	2.9			x	Reviewers note this project is primarily specifying, procuring and assembling existing components (including a Ballard stack). The project uses a definition of "appropriate performance" as being components that demonstrate their "specified performance." This is a straight-forward demonstration project, but will fall well short of DOE targets.
FC-28	Development of a Low Cost 3-10 kW Tubular SOFC Power System Norman Bessette; Acumentrics Corporation	3.0	Х			Reviewers felt the approach was sound, but had difficulty determining what progress had been achieved under this program as opposed to the preceding project funded by DOE Fossil Energy. As with many industrial product development projects, technical detail and data shared are limited. The micro combined heat and power (mCHP) home appliance demonstrations starting in Europe are certainly of interest.

Project Number	Project Title PI Name & Organization	Final Score	Continue	Discontinue	Other	Summary Comment
FC-29	Fuel Cell Systems Analysis R.K. Ahluwalia; Argonne National Laboratory	3.2	х			Reviewers note that necessarily generic fuel cell stack models may make the model less useful for design-specific issues such as cold start and freeze, though data being developed in the Department's water transport projects may help in making models more widely applicable. Reviewers would like to see the hard problems attacked, such as impurity effects and aging, and recommend validation against DOE-funded system-level projects.
FC-30	Mass-Production Cost Estimation of Automotive Fuel Cell Systems Brian D. James; Directed Technologies, Inc.	3.4	х			This highly rated project is one of two independent system cost estimation efforts funded by the Program. Reviewers note the difficulty in projecting future commodity (for example platinum) cost/pricing, and the difficulty in projecting changing system and component costs without automobile manufacturers and their suppliers being involved. However, reviewers generally commend the effort and approach.
FC-31	Direct Hydrogen PEMFC Manufacturing Cost Estimation for Automotive Applications Jayanti Sinha; TIAX LLC	3.1	X			This project is one of two independent system cost estimation efforts funded by the Program, and differs in component detail and approach from the complementary project, providing the Department with diverse assessments. Reviewers generally had more comments on details of this project compared to FC-30, and noted the changes in the "ANL 2009" system description might significantly affect cost results. However, reviewers generally support the effort and approach.
FC-32	Microstructural Characterization of PEM Fuel Cell Materials <i>Karren L. More; Oak</i> <i>Ridge National</i> <i>Laboratory</i>	3.6	Х			This project tied with two others for the highest ranking of the fuel cell projects in this year's review. Reviewers appreciate the significant increase in capability of and broad access to these state-of-the-art facilities, and note the on- going potential to provide valuable insights into both beginning materials structure and degradation. Reviewers commend the positive feedback from two-way collaboration with users. About the only reviewer concern was whether the open access might crowd out higher priority analyses as the project becomes oversubscribed.
FC-33	Platinum Group Metal Recycling Technology Development <i>Lawrence Shore; BASF</i> <i>Catalysts LLC</i>	3.5		х		This project tied with three others for the second highest ranking of fuel cell projects in this year's review. BASF has achieved the platinum recovery objective, identified room- temperature processing alternatives, and reduced reagent usage for platinum leaching. Reviewers generally consider the project a success, and concerns are limited to questions of whether on-going developments, such as nanostructured thin film catalyst-coated membranes or core-shell structures, will require significant process modifications.
FC-34	Neutron Imaging Study of the Water Transport in Operating Fuel Cells David Jacobson; National Institute of Standards and Technology	3.5	Х			This project tied with three others for the second highest ranking in this year's review. Reviewers commend the high-resolution images shown at this year's review, but note that as membranes continue to get thinner, spatial resolution will need to improve further to provide additional insights. Reviewers also applaud the low-temperature capability demonstrated this year.
FC-35	Water Transport Exploratory Studies Rod Borup; Los Alamos National Laboratory	3.3	Х			Reviewers generally value the imaging, characterization, and modeling efforts. Some reviewers believe the project could benefit from a reduction in scope and sharper focus on a few tasks in more depth.

Project Number	Project Title PI Name & Organization	Final Score	Continue	Discontinue	Other	Summary Comment
FC-36	Water Transport in PEM Fuel Cells: Advanced Modeling, Material Selection, Testing, and Design Optimization J. Vernon Cole; CFD Research Corporation	2.9	х			The project is still in the mode of collecting data and building models. Reviewers are concerned that temperature effects may not be adequately treated, and note analyses at constant low-temperature operation provide little useful information. Reviewers did not find plans for future work to address perceived shortcomings.
FC-37	Visualization of Fuel Cell Water Transport and Performance Characterization Under Freezing Conditions Satish Kandlikar; Rochester Institute of Technology	3.0	х			Reviewers noted significant technical content arising from the studies, but felt insights described to date were lacking. Plans for future work were rated lower than was approach, accomplishments and collaboration.
FC-38	Subfreezing Start/Stop Protocol for an Advanced Metallic Open-Flowfield Fuel Cell Stack Amedeo Conti; Nuvera Fuel Cells, Inc.	3.2	x			Reviewers believe the approach has resulted in data- supported designs that meet DOE targets, but note it is not clear whether or not the design/materials used and the lessons learned from this project are broadly applicable due to the lack of dissemination of details considered proprietary. Fundamental understanding, if it has been obtained, has not been shared. Reviewers do, however, generally consider the project successful.
FC-39	Development of Thermal and Water Management System for PEM Fuel Cells Zia Mirza; Honeywell	2.0		Х		For this low-rated project, reviewers saw little progress and noted that even if successful, testing of available, well- known components will not improve the technical readiness of fuel cell power systems. This project will be discontinued.
FC-40	Nitrided Metallic Bipolar Plates P.F. Tortorelli; Oak Ridge National Laboratory	3.1	X			Reviewers rated the approach high, but rated technical progress and plans below average. There is a concern that the project has not demonstrated that stamped foils can achieve the necessary precise geometry and tolerances. Reviewers recommend characterization of near-surface compositions following stamping for comparison with before-stamped materials to ensure no processing issues interfere with the efficacy of the oxidation and nitridation treatments. Reviewers recommend collaboration with a stack or automotive manufacturer.
FC-41	Next Generation Bipolar Plates for Automotive PEM Fuel Cells Orest Adrianowycz; GrafTech International Ltd.	2.8		X		This project is ending this fiscal year. Reviewers generally feel that the materials developed have not been adequately characterized or tested in conditions relevant to the objective.
FC-42	Low Cost, Durable Seals for PEM Fuel Cells Jason Parsons; UTC Power	2.7		Х		This project is ending this fiscal year. Reviewers note that compositions of seal materials developed have not been disclosed, fuel cell cyclic testing has not been done, and the seals developed for the company's specific material set may not be generically applicable to other stack designs and materials sets.

Project Number	Project Title PI Name & Organization	Final Score	Continue	Discontinue	Other	Summary Comment
FC-43	Diesel Fueled SOFC System for Class 7/Class 8 On-Highway Truck Auxiliary Power Dan Norrick; Cummins Power Generation	3.1		х		The project is making progress and has largely completed design and subsystem testing, including demonstration of dry catalytic partial oxidation reforming of ultra-low sulfur diesel. Projected system characteristics are below DOE targets. As with many industrial product development projects, technical detail and data shared are limited.
FC-44	Solid Oxide Fuel Cell Development for Auxiliary Power in Heavy Duty Vehicle Applications <i>Gary D. Blake; Delphi</i>	3.6	х			This project tied with two others for the highest ranking of the fuel cell projects in this year's review. As with many industrial product development projects, technical detail and data shared are limited, but reviewers commend the two successful on-truck demonstrations, the very good power density, and the complete system packaging. The project is meeting key milestones.
FC-45	Solid Acid Fuel Cell Stack for APU Applications <i>Hau H. Duong;</i> <i>Superprotonic, Inc.</i>	2.4			х	For this project, reviewers note progress in cell/stack development and power density, but have concerns with the high platinum catalyst loading and durability. The project is behind on milestones and costs have not been addressed. Reviewers consider the technology immature. (Congressionally directed project)
FC-46	Low-Cost Co- Production of Hydrogen and Electricity Fred Mitlitsky; Bloom Energy	2.8			х	The focus of this project is on the stationary power demonstration system built in Alaska, and as with many industrial product development projects, technical details and data shared are limited. Integration of a hydrogen pump with a solid oxide fuel cell stack has not been completed. (Congressionally directed project)
FC-47	Development of a Novel Efficient Solid-Oxide Hybrid for Co- Generation of Hydrogen and Electricity Using Nearby Resources for Local Application <i>Greg Tao; Materials and</i> <i>Systems Research, Inc.</i>	3.3			х	Reviewers of this project rated the relevance, approach, progress, collaboration and plans all well above average, and consider the project generally on-track. (Congressionally directed project)
FC-48	Silicon Based Solid Oxide Fuel Cell for Portable Consumer Electronics Alan Ludwiszewski; Lilliputian Systems, Inc.	2.6			х	For this project, reviewers note progress in increasing cell power and improvement in sealing, but note numerous difficult challenges that remain. Reviewers consider the technology immature. (Congressionally directed project)
FC-49	Biogas Fueled Solid Oxide Fuel Cell Stack Praveen Cheekatamarla; NanoDynamics Energy, Inc.	2.6			X	Reviewers note progress in designing, fabricating and testing single cells in hydrogen and simulated biogas, but note the information presented was very generalized. Approach and collaboration were both rated quite low. (Congressionally directed project)
FCP-02	Component Benchmarking Subtask Reported: USFCC Durability Protocols and Technically-Assisted Industrial and University Partners <i>Tommy Rockward; Los</i> <i>Alamos National</i> <i>Laboratory</i>	3.4	Х			Reviewers rated the project very high on relevance and collaboration, and high on all other categories. Reviewers generally consider this an important mechanism for the DOE to support researchers and developers.

xxx FY 2009 Merit Review and Peer Evaluation Report

Project Number	Project Title PI Name & Organization	Final Score	Continue	Discontinue	Other	Summary Comment
FCP-03	Research & Development for Off Road Fuel Cell Applications <i>Richard J. Lawrence;</i> <i>IdaTech</i>	2.7	X			The fuel cell was developed with Department of Defense funding, so this project is focused on the demonstration. The project contains relatively little research but is generally on track. Reviewers would like to see a commercialization plan developed.
FCP-04	Renewable and Logistics Fuels for Fuel Cells at the Colorado School of Mines Neal P. Sullivan; Colorado School of Mines	2.6			х	Reviewers made a number of comments that the multiple tasks do not seem integrated and the project lacks focus, making it unlikely that the state-of-the-art will be significantly advanced. (Congressionally directed project)
FCP-06	Fuel Cell Research at the University of South Carolina John W. Van Zee; University of South Carolina	2.9			X	This project funds a diverse and unrelated set of tasks under a single university project. Approach, progress, and collaboration received average scores based on the individual tasks. The project is scheduled to end this fiscal year. (Congressionally directed project)
FCP-07	Development of Kilowatt-Scale Fuel Cell Technology Steven S.C. Chuang; The University of Akron	2.1			х	The focus of this project is on direct conversion of coal resulted in a very low score for relevance to the DOE Hydrogen Program. The university has built a high- temperature cell and operated it on hydrogen, but the concept of coal conversion has not been demonstrated. Reviewers note the lack of collaborators with solid oxide fuel cell experience and consider the plans optimistic for the funding available. (Congressionally directed project)
FCP-08	Center for Fundamental and Applied Research in Nanostructured and Lightweight Materials Drs. Mullins, et al.; Michigan Technological University	2.0			х	This is a project funding a diverse and unrelated set of tasks developing materials to be used in fuel cell applications and energy storage. The project rated very low on approach due to lack of coordination between tasks, very low on accomplishments for the lack of progress toward relevant DOE targets, and received only slightly better scores for collaboration and plans. (Congressionally directed project)
FCP-09	Engineered Nanostructured MEA Technology for Low Temperature Fuel Cells <i>Yimin Zhu; Nanosys,</i> <i>Inc.</i>	2.4			Х	The project rated very low on approach and collaboration. It rated below average on progress. Although some milestones were met, progress toward DOE targets was not evident. This project has ended. (Congressionally directed project)
FCP-10	Alternative Fuel Cell Membranes for Energy Independence <i>K.A. Mauritz; University</i> of Southern Mississippi	2.6			х	Reviewers rated the relevance high, but the approach and accomplishments below average, and collaborations very low, while plans scored above average. Polymers have been synthesized, but no membranes have been made. (Congressionally directed project)
FCP-11	Extended Durability Testing of an External Fuel Processor for SOFC Mark A. Perna; Rolls Royce Fuel Systems (US) Inc.	2.3			х	Reviewers rated the relevance below average, largely because of the system scale, rated the approach and accomplishments well below average, and rated collaboration very low. There was concern that the tests seem to lack diagnostic instrumentation, metrics, and post- test characterization plans. (Congressionally directed project)

Project Number	Project Title PI Name & Organization	Final Score	Continue	Discontinue	Other	Summary Comment
FCP-12	Hydrogen Fuel Cell Development in Columbia (SC) Kenneth Reifsnider; University of South Carolina	2.5			X	This is a project that funds a diverse and unrelated set of tasks under a single university project, similar to FCP-06. Reviewers scored the project below average in all areas, and had difficultly assessing progress as the poster referenced a number of earlier projects. (Congressionally directed project)
FCP-13	Martin County Hydrogen Fuel Cell Development Jeffrey Bonner-Stewart; Microcell Corporation	1.6			X	This project received the lowest score of the fuel cell projects in this year's review. Essentially no technical data was provided. The project lacks metrics and partners, and reviewers judge the technology not ready for scale-up and manufacturing. The project is complete. (Congressionally directed project)
FCP-14	Fuel Cell Balance of Plant Reliability Testbed Vern Sproat; Stark State College of Technology	2.0			х	Reviewers consider the need for such test beds, the barriers addressed, and the approach to be unclear. Reviewers scored the project low on relevance and very low in all other categories. (Congressionally directed project)

Systems Analysis

Project Number	Project Title PI Name & Organization	Final Score	Continue	Discontinue	Other	Summary Comment
AN-01	HyDRA: Hydrogen Demand and Resource Analysis Tool Johanna Levene; National Renewable Energy Laboratory	3.0	х			Future work will address reviewers' suggestions: (a) develop means to incorporate future resource cost changes in the determination of the future hydrogen cost; and (b) add biogas and renewable fuel resources to the model.
AN-02	Water's Impacts on Hydrogen A.J. Simon; Lawrence Livermore National Laboratory	2.9			X	The project will be completed in FY 2009. The project quantifies the impact of water demand for hydrogen production on hydrogen cost and regional resource impacts.
AN-03	Cost Implications of Hydrogen Quality Requirements S. Ahmed; Argonne National Laboratory	3.2	X			Argonne National Laboratory's future work will focus on analyzing the impact of fuel quality on stationary fuel cell operation from feedstocks such as biogas and renewable fuels; determining optimum levels for impurity species; and evaluating costs requirements.
AN-04	Macro-System Model Victor Diakov; National Renewable Energy Laboratory	3.2	х			Additional work will address reviewers' suggestions of verifying the model outputs and performing validation with industry.

Project Number	Project Title PI Name & Organization	Final Score	Continue	Discontinue	Other	Summary Comment
AN-05	Discrete Choice Analysis of Consumer Preferences for Refueling Availability Marc W. Melaina; National Renewable Energy Laboratory	2.6			х	The project will be completed in FY 2009. The project provides a quantitative representation of the cost penalty for limited refueling availability using discrete choice survey and modeling methodology.
AN-06	Analysis of Energy Infrastructures and Potential Impacts from an Emergent Hydrogen Fueling Infrastructure Andy Lutz; Sandia National Laboratories	2.9	х			Sandia National Laboratory will address the reviewers' suggestions to consider all-electric vehicles; use an iterative approach for supply and demand; and incorporate biofuels as another competitive choice.
AN-07	Hydrogen Deployment System Modeling Environment (HyDS- ME) Brian W. Bush; National Renewable Energy Laboratory	3.2	х			National Renewable Energy Laboratory will incorporate reviewers' suggestions to include a model validation step, biogas feedstock options and stationary fuel cells as an option for combined heat, power and fuel generation.
AN-08	Analysis of Hydrogen Production and Delivery Infrastructure as a Complex Adaptive System George S. Tolley; RCF Economic and Financial Consulting, Inc.	3.0			х	The project will be completed in FY 2009. The project enables agent based modeling to assess supply of hydrogen fuel and purchase of hydrogen fuel cell vehicles. The purpose is to provide insight regarding the private sector's willingness to invest in hydrogen infrastructure and the policies needed to enable infrastructure construction.
AN-09	Adapting the H2A Hydrogen Production Cost Analysis Model to Stationary Applications <i>Michael Penev; National</i> <i>Renewable Energy</i> <i>Laboratory</i>	3.2	x			National Renewable Energy Laboratory will incorporate reviewers' suggestions to include the impact of potential fuel economy and emission standard legislation of gasoline powered vehicles, and an impact assessment and evaluation of criteria pollutants.
AN-10	Hydrogen and Fuel Cell Analysis: Lessons Learned from Stationary Power Generation S.E. Grasman; Missouri University of Science and Technology	1.8		х		The project considered opportunities for hydrogen in stationary and portable applications, and analyzed different national and international strategies and will be completed in FY 2009. However, the project was not rated favorably. The project received poor reviewer ratings for relevance to the overall DOE objectives and technical accomplishments. The project was determined to be too general and the data analysis was inadequate.
AN-11	Modeling the Transition to Hydrogen Paul N. Leiby; Oak Ridge National Laboratory	3.2	Х			Future work will address reviewers' suggestions: (a) evaluate supply and demand impacts on feedstock cost; and (b) consider the influence of market, technology and regulation drivers.
AN-12	Fuel-Cycle Analysis of Fuel-Cell Vehicles and Fuel-Cell Systems with the GREET Model <i>Michael Wang; Argonne</i> <i>National Laboratory</i>	3.3	Х			Argonne National Laboratory's future work will address reviewers' suggestions: new fuel economy and emission standard regulations will be included; and all the hydrogen production pathways in the GREET model will be included.

PROLOGUE

Project Number	Project Title PI Name & Organization	Final Score	Continue	Discontinue	Other	Summary Comment
AN-13	Evaluation of the Potential Environmental Impacts from Large- Scale Use and Production of Hydrogen in Energy and Transportation Applications Don Wuebbles; University of Illinois at Urbana-Champaign	3.0			х	The project will be completed in FY 2009. The project identified and examined possible ecological and environmental effects from the production and use of hydrogen from various energy sources.
AN-14	Potential Environmental Impacts of Hydrogen- Based Transportation & Power Systems Mark Z. Jacobson; Stanford University	3.0			Х	The project will be completed in FY 2009. The project compared the emissions of hydrogen to six criteria pollutants (CO, SOx, NOx, particulate material (PM), ozone and lead) for near-term and long-term hydrogen production technologies and evaluated the effects of emissions on climate, human health, and the ecosystem.
ANP-01	Pathways to Commercial Success: Technologies and Products Supported by the HFCIT Program Steve Weakley; Pacific Northwest National Laboratory	2.9			X	This project has evaluated the commercial benefits of the Program through 2008. The project has found that 144 patents, over 20 commercial products and over 50 emerging products are attributed to DOE R&D. As fuel cell R&D continues, this project will update annually the commercial benefits due to DOE R&D. The project will be revised to match the future direction of the Fuel Cell Technologies Program.
ANP-03	Thermodynamic, Economic, and Environmental Modeling of Hydrogen (H ₂) Co- Production Integrated with Stationary Fuel Cell Systems (FCS) <i>Whitney Colella; Sandia</i> <i>National Laboratories</i>	3.2	Х			Sandia National Laboratory's future work will address reviewers' suggestions: (a) include the effect of financial incentives related to criteria pollutant emission trading; and (b) consider how to transition from the present situation (conventional stand-alone systems for electricity, heat and hydrogen) to the intermediate scenario of combined heat and power without stranding earlier investments.

Manufacturing R&D

Project Number	Project Title PI Name & Organization	Final Score	Continue	Discontinue	Other	Summary Comment
MF-01	Fuel Cell MEA Manufacturing R&D Michael Ulsh; National Renewable Energy Laboratory	3.2	х			This project is relevant and has a good team with strong collaborations; however additional industrial partners would strengthen the validation of future work. Identification of non-random defect sources in a realistic manufacturing environment using 2-D autocorrelation would benefit the project. The potential impact of in-line MEA defect identification on manufacturing cost should be assessed.

PROLOGUE

Project Number	Project Title PI Name & Organization	Final Score	Continue	Discontinue	Other	Summary Comment
MF-02	Reduction in Fabrication Costs of Gas Diffusion Layers Colleen Legzdins; Ballard Material Products	3.6	X			Reduction of manufacturing costs of the Gas Diffusion Layer is highly relevant and this project has demonstrated reasonable progress during the past year. Plans for future activities such as commissioning of process technology and on-line measurement tools are aggressive and challenging. The cost reductions associated with the developed process should be clearly assessed. The ultimate benefits of the project will be dependent on the effective transfer of the manufacturing processes and on-line measurement techniques to the fuel cell manufacturing community.
MF-03	Modular, High-Volume Fuel Cell Leak-Test Suite and Process <i>Ian Kaye; UltraCell</i> <i>Corporation</i>	3.4	х			Rapid in-line leak testing during fuel cell stack manufacture is very relevant and this project has made reasonable progress in the past six months. Integration of the prototype testing hardware in a realistic assembly process will enable a meaningful go/no-go decision for the project in the future. Emphasis on how this process will improve manufacturing yield should be included in the project.
MF-04	Manufacturing of Low- Cost, Durable Membrane Electrode Assemblies Engineered for Rapid Conditioning <i>F. Colin Busby; W.L</i> <i>Gore and Associates,</i> <i>Inc.</i>	3.3	х			High-volume manufacturing of fuel cell MEAs at low-cost is a relevant goal of this project. Improved integration of the efforts of the individual members of this strong team would enhance the potential benefits of the project. Close coordination between the modeling and experimental efforts will be required to achieve the projected manufacturing cost reductions. Future plans are quite aggressive and project scope and schedule may need to be adjusted.
MF-05	Adaptive Process Controls and Ultrasonics for High Temperature PEM MEA Manufacture Raymond Puffer; Rensselaer Polytechnic Institute	3.3	X			The application of adaptive process control to the manufacture of high temperature MEAs is relevant and the potential of ultrasonic welding to support high-volume production appears promising. In the early stages of this project progress is adequate, however future effort needs to be better defined and meaningful go/no-go decision points included in the project schedule. The potential for manufacturing cost reductions needs to be fully quantified for this project as early as possible.
MF-06	Development of Advanced Manufacturing Technologies for Low Cost Hydrogen Storage Vessels <i>Carter Liu; Quantum</i> <i>Fuel Systems</i> <i>Technologies Worldwide</i> <i>Inc.</i>	2.8	x			This project was considered relevant in terms of it potential to lower the cost of high-pressure hydrogen containment vessels; however it was noted that the focus of the project was "product improvement" and, thus, the relevancy to manufacturing was questionable. A good team with composites expertise was noted. The project suffers from inadequate stress and safety analysis and lack of a credible cost projection and potential manufacturing cost reduction estimate. Testing protocols should have been discussed in greater detail. If continued, the go/no-go decision point should be moved earlier in the schedule.
MF-07	Digital Fabrication of Catalyst Coated Membranes Peter C. Rieke; Pacific Northwest National Laboratory	3.5		х		This project is completed. It is very relevant based on its potential for significant process improvement and cost reduction, however an initial economic assessment would have strengthened the progress to date. A strong team and integrated future plans indicate the potential for significant improvements in the manufacture of catalyst-coated membranes.

Project Number	Project Title PI Name & Organization	Final Score	Continue	Discontinue	Other	Summary Comment
MFP-01	Inexpensive Pressure Vessel Production through Fast Dry Winding Manufacture Andrew Weisberg; Lawrence Livermore National Laboratory	2.4	х			This project was considered to be relevant based on the potential of the "dry-wind" manufacturing process, but supporting evidence of the proposed process and cost benefits would have strengthened validation of the approach and progress to date. More detail regarding process parameters, without disclosing propriety information, was needed to accurately evaluate accomplishments and progress. Additional confirmation of the integration of team effort and specific roles of the project partners was needed. A comprehensive comparison of this process with conventional manufacturing techniques is needed to adequately validate the advantages of this process.

TABLE OF CONTENTS

INTROD	UCTION	-1
HYDROG	GEN PRODUCTION AND DELIVERY	-9
PD-02	Bio-Derived Liquids Reforming	12
PD-03	Hydrogen Generation from Biomass-Derived Carbohydrates via the Aqueous-Phase Reforming Process	
PD-04	Investigation of Reaction Networks and Active Sites in Bio-Ethanol Steam Reforming over Co-based Catalysts	
PD-05	Distributed Reforming of Renewable Liquids Using Gas Transport Membranes	
PD-06	Zeolite Membrane Reactor for Water-Gas-Shift Reaction for Hydrogen Production	
PD-07	High-Performance, Durable, Palladium Alloy Membrane for Hydrogen Separation and Purification	
PD-08	Solar Cadmium Hydrogen Production Cycle	
PD-09	Solar High-Temperature Water-Splitting Cycle with Quantum Boost	34
PD-10	Solar-Thermal Ferrite-Based Water Splitting Cycles	37
PD-11	R&D Status for the Cu-Cl Thermochemical Cycle	
PD-12	Sulfur-Iodine Thermochemical Cycle	
PD-13	Hybrid Sulfur Thermochemical Cycle	46
PD-14	High Temperature Electrolysis System	49
PD-15	Technoeconomic Boundary Analysis of Photobiological Hydrogen Producing Systems	53
PD-16	Maximizing Light Utilization Efficiency and Hydrogen Production in Microalgal Cultures	
PD-17	Biological Systems for Hydrogen Photoproduction	58
PD-18	Fermentative and Electrohydrogenic Approaches to Hydrogen Production	
PD-19	Development of Water Splitting Catalysts Using a Novel Molecular Evolution Approach	
PD-20	High-Capacity, High Pressure Electrolysis System with Renewable Power Sources	65
PD-21	PEM Electrolyzer Incorporating an Advanced Low Cost Membrane	69
PD-22	Photoelectrochemical Hydrogen Production: DOE PEC Working Group Overview	
PD-23	Technoeconomic Boundary Analysis of Photoelectrochemical (PEC) Hydrogen Producing Systems	75
PD-24	Characterization of Materials for Photoelectrochemical Hydrogen Production (PEC)	
PD-25	Nanostructured MoS ₂ and WS ₂ for the Solar Production of Hydrogen	81
PD-26	Development of Hydrogen Selective Membranes/Modules as Reactors/Separators for Distributed Hydrogen Production	81
PD-28	A Novel Slurry Based Biomass Reforming Process	
PD-30	Hydrogen Delivery Infrastructure Analysis	90
PD-31	H2A Delivery Components Mode	02
PD-32	Hydrogen Energy Station Analysis in Northeastern US and Hydrogen Sensors for Infrastructure	
PD-34	Oil-Free Centrifugal Hydrogen Compression Technology Demonstration	
PD-35	Development of a Centrifugal Hydrogen Pipeline Gas Compressor	98
PD-36	Advanced Hydrogen Liquefaction Process1	00
PD-37	Active Magnetic Regenerative Liquefier1	02
PD-38	Reversible Liquid Carriers for an Integrated Production, Storage and Delivery of Hydrogen	
PD-39	Inexpensive Delivery of Cold Hydrogen in High Performance Glass Fiber Composite Pressure Vessels1	
PD-40	Development of High Pressure Hydrogen Storage Tank for Storage and Gaseous Truck Delivery10	
PD-41	A Combined Materials Science/Mechanics Approach to the Study of Hydrogen Embrittlement of	-
	Pipeline Steels1	10
PD-42	Fiber Reinforced Composite Pipelines1	
PD-43	H ₂ Permeability and Integrity of Steel Welds1	
PD-44	Composite Pd and Alloy Porous Stainless Steel Membranes for Hydrogen Production and Process	
	Intensification1	16
PD-45	Development of Robust Metal Membranes for Hydrogen Separation1	
PD-46	Scale-up of Hydrogen Transport Membranes for IGCC and FutureGen Plants12	21
PD-47	High Permeability Ternary Palladium Alloy Membranes with Improved Sulfur and Halide Tolerance 12	

TABLE OF CONTENTS

PD-48	Experimental Demonstration of Advanced Palladium Membrane Separators for Central High-Purity	
	Hydrogen Production	126
PD-49	Integration of a Structural Water Gas Shift Catalyst with a Vanadium Alloy Hydrogen Transport	
	Device	
PD-50	Hydrogen Delivery in Steel Pipelines	
PDP-01	Development and Optimization of Cost Effective Material Systems for Photoelectrochemical Hydro	
	Production	
PDP-02	Semiconductor Materials for Photoelectrolysis	
PDP-03	PEC Materials: Theory and Modeling	139
PDP-04	Progress in the Study of Amorphous Silicon Carbide (a-SiC) as a Photoelectrode in Photoelectroche	mical
	(PEC) Cells	141
PDP-05	Progress in the Study of Tungsten Oxide Compounds as Photoelectrodes in Photoelectrochemical	1 4 2
PDP-06	Cells Photoelectremical Hydrogen Production	145
PDP-06 PDP-07	Critical Research for Cost-Effective Photoelectrochemical Production of Hydrogen	143
PDP-07 PDP-10	Composite Bulk Amorphous Hydrogen Purification Membranes	14/
PDP-10 PDP-12	Catalytic Solubilization and Conversion of Lignocellulosic Feedstocks	
PDP-13	Novel Low-Temperature Proton Transport Membranes	
PDP-13 PDP-14	Ultra-thin Proton Conduction Membranes for H ₂ Stream Purification with Protective Getter	130
PDP-14	Coatings	150
PDP-15	Distributed Bio-Oil Reforming	161
PDP-16	Pressurized Steam Reforming of Bio-Derived Liquids for Distributed Hydrogen Production	
PDP-10 PDP-17	Renewable Electrolysis Integrated System Development and Testing	169
PDP-17	Hydrogen from Water in a Novel Recombinant Oxygen-Tolerant Cyanobacterial System	
PDP-18	Use of Biological Materials and Biologically Inspired Materials for H ₂ Catalysis	
PDP-19 PDP-20	Hydrogen Embrittlement of Structural Steels	177
PDP-21	Oil-Free Rotor-Bearings for Hydrogen Transportation & Delivery	
PDP-21 PDP-22	Development of Highly Efficient Solid State Electrochemical Hydrogen Compressor (EHC)	
PDP-22 PDP-24	Composite Technology for Hydrogen Pipelines	102 194
PDP-25	Control for Centrifugal Compression	
PDP-26	Purdue Hydrogen Systems Laboratory	
PDP-27	Developing Improved Materials to Support the Hydrogen Economy	
PDP-28	Hydrogen Production and Fuel Cell Research	107
PDP-29	Integrated Hydrogen Production, Purification and Compression System	201
1 D1 -27	integrated Hydrogen Hoddetton, Furneation and Compression System	201
HYDRO	GEN STORAGE	205
ST-01	Metal Hydride Center of Excellence	209
ST-02	Thermodynamically Tuned Nanophase Materials for Reversible Hydrogen Storage: Structure and	207
51 02	Kinetics of Nanoparticle and Model System Materials	212
ST-03	Discovery and Development of Metal Hydrides for Reversible On-board Hydrogen Storage	
ST-04	Chemical Vapor Synthesis and Discovery of H_2 Storage Materials: Li-Mg-N-H System	
ST-05	Aluminum Hydride Regeneration	
ST-06	Electrochemical Reversible Formation of Alane	225
ST-07	Fundamental Studies of Advanced, High-Capacity Reversible Metal Hydrides	
ST-08	First-Principles Modeling of Hydrogen Storage in Metal Hydride Systems	232
ST-09	Thermodynamically Tuned Nanophase Materials for Reversible Hydrogen Storage	235
ST-10	Catalyzed Nano-Framework Stabilized High Density Reversible Hydrogen Storage Systems	
ST-11	Neutron Characterization and Calphad in Support of the Metal Hydride Center of Excellence	
ST-12	Analyses of Hydrogen Storage Materials and On-Board Systems	
ST-12	System Level Analysis of Hydrogen Storage Options	
ST-15	2009 Overview - DOE Chemical Hydrogen Storage Center of Excellence	251
ST-16	Amineborane-Based Chemical Hydrogen Storage	
ST-17	Chemical Hydrogen Storage R&D at Los Alamos National Laboratory	
ST-18	PNNL Progress as Part of the Chemical Hydrogen Storage Center of Excellence	261
ST-19	Main Group Element and Organic Chemistry for Hydrogen Storage and Activation	264

ST-20	Low-Cost Precursors to Novel Hydrogen Storage Materials	267
ST-21	Ammonia Borane Regeneration and Market Analysis of Hydrogen Storage Materials	269
ST-22	Overview of the DOE Hydrogen Sorption Center of Excellence	272
ST-23	A Biomimetic Approach to Metal-Organic Frameworks with High H ₂ Uptake	276
ST-24	Hydrogen Storage by Spillover	278
ST-25	Optimization of Nano-Carbon Materials for Hydrogen Sorption	281
ST-26	NREL Research as Part of the Hydrogen Sorption Center of Excellence	284
ST-27	Hydrogen Storage through Nanostructured Polymeric Materials	288
ST-28	Discovery of Materials with a Practical Heat of H_2 Adsorption	
ST-29	Optimizing the Binding Energy of Hydrogen on Nanostructured Carbon Materials through Structu	
51 =>	Control and Chemical Doping	294
ST-30	Nanoengineered Graphene Scaffolds with Alternating Metal-Carbon Layers for H ₂ Uptake at Amb	ient .
51 50	Temperatures	297
ST-32	A Synergistic Approach to the Development of New Hydrogen Storage Materials, Part I	
ST-32	Hydrogen Storage in Metal-Organic Frameworks	
ST-34	Compact (L)H ₂ Storage with Extended Dormancy in Cryogenic Pressure Vessels	302
STP-01	Lifecycle Verification of Polymeric Storage Liners	307
STP-02	Electron-Charged Hydrogen Storage Materials	200
STP-02 STP-03	Polymer-Based Activated Carbon Nanostructures for H ₂ Storage	207
STP-04	Low-Cost High-Efficiency High-Pressure H ₂ Storage	315
STP-17	Solutions for Chemical Hydrogen Storage: Hydrogenation/Dehydrogenation of B-N Bonds	
STP-18	Chemical Hydrogen Storage Using Ultra-High Surface Area Main Group Materials & The Develo	
511-10	of Efficient Amine-Borane Regeneration Cycles	320
STP-19	Electrochemical Hydrogen Storage Systems	272
STP-20	Chemical Hydrogen Storage Using Aluminum Ammonia-Borane Complexes	
STP-20 STP-21	Novel Metal Perhydrides for Hydrogen Storage	220
STP-22	Purdue Hydrogen Systems Laboratory	222
STP-22 STP-23	Hydrogen Storage Research	
STP-25	Carbon Aerogels for Hydrogen Storage	
STP-23 STP-26	Single-Walled Carbon Nanohorns for Hydrogen Storage and Catalyst Supports	
STP-20 STP-27	Enhanced Hydrogen Dipole Physisorption: Constant Isosteric Heats and Hydrogen Diffusion in	343
511-27	Physisorbents	345
STP-28	Characterization of Hydrogen Adsorption by NMR	
STP-28	Advanced Boron and Metal Loaded High Porosity Carbons	250
STP-30	Best Practices for Characterizing Hydrogen Storage Properties of Materials	252
STP-30 STP-36	Dest Flactices for Characterizing Hydrogen Storage Flopenties of Materials	254
	Reversible Hydrogen Storage Materials: Structure, Chemistry, and Electronic Structure Metal Borohydrides, Ammines, and Aluminum Hydrides as Hydrogen Storage Materials	
STP-37		
STP-38 STP-39	Development and Evaluation of Advanced Hydride Systems for Reversible Hydrogen Storage Effect of Trace Elements on Long-Term Cycling/Aging Properties and Thermodynamic Studies of	
518-39		
STP-40	Complex Hydrides for Hydrogen Storage Amide and Combined Amide/Borohydride Investigations	264
STP-41	Synthesis of Nanophase Materials for Thermodynamically Tuned Reversible Hydrogen Storage	
STP-42	Lightweight Borohydrides for Hydrogen Storage Center for Hydrogen Storage Research at Delaware State University	271
STP-43		
STP-44	Solid-State Hydriding and Dehydriding of LiBH ₄ + MgH ₂ Enabled via Mechanical Activation and	
OTD 45	Engineering Standardized Testing Program for Solid-State Hydrogen Storage Technologies	3/4
STP-45		
STP-46	An Integrated Approach of Hydrogen Storage in Complex Hydrides of Transitional Elements	3/9
FUEL C	ELLS	383
FC-01	Lead Research and Development Activity for DOE's High Temperature, Low Relative Humidity	
	Membrane Program	387
FC-02	Dimensionally Stable Membranes	
FC-03	New Polymer/Inorganic Proton Conductive Composite Membranes for PEMFC	
FC-04	Poly(cyclohexadiene)-Based Polymer Electrolyte Membranes for Fuel Cell Applications	400

FC-05	Advanced Materials for Proton Exchange Membranes	404
FC-06	Protic Salt Polymer Membranes: High-Temperature Water-Free Proton-Conducting Membranes	
FC-07	Fluoroalkyl-Phosphonic-Acid-Based Proton Conductors	413
FC-08	Rigid Rod Polyelectrolytes: Effect on Physical Properties Frozen-in Free Volume: High Conductiv	ity at
FC-09	NanoCapillary Network Proton Conducting Membranes for High Temperature Hydrogen/Air Fuel Cells	
FC-10	High Temperature Membrane with Humidification-Independent Cluster Structure	
FC-11	Novel Approaches to Immobilized Heteropoly Acid (HPA) Systems for High Temperature, Low R	
	Humidity Polymer-Type Membranes	
FC-12	Improved, Low-Cost, Durable Fuel Cell Membranes	433
FC-13	Membranes and MEAs for Dry, Hot Operating Conditions	437
FC-14	New Polyelectrolyte Materials for High Temperature Fuel Cells	
FC-15	Development of Novel PEM Membrane and Multiphase CFD Modeling of PEM Fuel Cell	
FC-16	Applied Science for Electrode Cost, Performance, and Durability	
FC-17	Advanced Cathode Catalysts and Supports for PEM Fuel Cells	
FC-18	Highly Dispersed Alloy Catalyst for Durability	435
FC-19	Development of Alternative and Durable High Performance Cathode Supports for PEM Fuel Cells	
FC-20	Non-Platinum Bimetallic Cathode Electrocatalysts	
FC-21	Advanced Cathode Catalysts	405
FC-22	Effects of Fuel and Air Impurities on PEM Fuel Cell Performance	
FC-23	Effects of Impurities on Fuel Cell Performance and Durability	
FC-23 FC-24	The Effects of Impurities on Fuel Cell Performance and Durability	480
FC-24 FC-25	Development and Demonstration of a New-Generation High Efficiency 1-10 kW Stationary PEM I	400 Supl
гС-23	Cell System	102
FC-26	Stationary PEM Fuel Cell Power Plant Verification	
	Stationary PEM Fuel Cell Powel Flant Vernication	480
FC-27	Intergovernmental Stationary Fuel Cell System Demonstration	489
FC-28	Development of a Low Cost 3-10 kW Tubular SOFC Power System	492
FC-29	Fuel Cell Systems Analysis	
FC-30	Mass-Production Cost Estimation of Automotive Fuel Cell Systems	
FC-31	Direct Hydrogen PEMFC Manufacturing Cost Estimation for Automotive Applications	502
FC-32	Microstructural Characterization of PEM Fuel Cell Materials	
FC-33	Platinum Group Metal Recycling Technology Development	508
FC-34	Neutron Imaging Study of the Water Transport in Operating Fuel Cells	511
FC-35	Water Transport Exploratory Studies	513
FC-36	Water Transport in PEM Fuel Cells: Advanced Modeling, Material Selection, Testing, and Design Optimization	517
FC-37	Visualization of Fuel Cell Water Transport and Performance Characterization Under Freezing	
	Conditions	
FC-38	Subfreezing Start/Stop Protocol for an Advanced Metallic Open-Flowfield Fuel Cell Stack	
FC-39	Development of Thermal and Water Management System for PEM Fuel Cells	
FC-40	Nitrided Metallic Bipolar Plates	529
FC-41	Next Generation Bipolar Plates for Automotive PEM Fuel Cells	
FC-42	Low Cost, Durable Seals for PEM Fuel Cells	537
FC-43	Diesel Fueled SOFC System for Class 7/Class 8 On-Highway Truck Auxiliary Power	
FC-44	Solid Oxide Fuel Cell Development for Auxiliary Power in Heavy Duty Vehicle Applications	545
FC-45	Solid Acid Fuel Cell Stack for APU Applications	548
FC-46	Low-Cost Co-Production of Hydrogen and Electricity	552
FC-47	Development of a Novel Efficient Solid-Oxide Hybrid for Co-Generation of Hydrogen and Electric Using Nearby Resources for Local Application	city
FC-48	Silicon Based Solid Oxide Fuel Cell for Portable Consumer Electronics	559
FC-49	Biogas Fueled Solid Oxide Fuel Cell Stack	563
FCP-02	Component Benchmarking Subtask Reported: USFCC Durability Protocols and Technically-Assist	ted
ECD 02	Industrial and University Partners	
FCP-03	Research & Development for Off Road Fuel Cell Applications	
FCP-04	Renewable and Logistics Fuels for Fuel Cells at the Colorado School of Mines	372

FCP-06	Fuel Cell Research at the University of South Carolina	576
FCP-07	Development of Kilowatt-Scale Fuel Cell Technology	579
FCP-08	Center for Fundamental and Applied Research in Nanostructured and Lightweight Materials	
FCP-09	Engineered Nanostructured MEA Technology for Low Temperature Fuel Cells	
FCP-10	Alternative Fuel Cell Membranes for Energy Independence	
FCP-11	Extended Durability Testing of an External Fuel Processor for SOFC	591
FCP-12	Hydrogen Fuel Cell Development in Columbia (SC)	594
FCP-13	Martin County Hydrogen Fuel Cell Development	597
FCP-14	Fuel Cell Balance of Plant Reliability Testbed	599
EDUCAT	ION; SAFETY, CODES AND STANDARDS; AND TECHNOLOGY VALIDATION	601
SYSTEM	S ANALYSIS	611
AN-01	HyDRA: Hydrogen Demand and Resource Analysis Tool	614
AN-02	Water's Impacts on Hydrogen	617
AN-03	Cost Implications of Hydrogen Quality Requirements	620
AN-04	Macro-System Model	622
AN-05	Discrete Choice Analysis of Consumer Preferences for Refueling Availability	
AN-06	Analysis of Energy Infrastructures and Potential Impacts from an Emergent Hydrogen Fueling	025
111,00	Infrastructure	628
AN-07	Hydrogen Deployment System Modeling Environment (HyDS-ME)	631
AN-08	Analysis of Hydrogen Production and Delivery Infrastructure as a Complex Adaptive System	634
AN-09	Adapting the H2A Hydrogen Production Cost Analysis Model to Stationary Applications	637
AN-10	Hydrogen and Fuel Cell Analysis: Lessons Learned from Stationary Power Generation	640
AN-11	Modeling the Transition to Hydrogen	643
AN-12	Fuel-Cycle Analysis of Fuel-Cell Vehicles and Fuel-Cell Systems with the GREET Model	646
AN-13	Evaluation of the Potential Environmental Impacts from Large-Scale Use and Production of	
A NT 14	Hydrogen in Energy and Transportation Applications	
AN-14	Potential Environmental Impacts of Hydrogen-Based Transportation & Power Systems	
ANP-01	Pathways to Commercial Success: Technologies and Products Supported by the HFCIT Program	
ANP-03	Thermodynamic, Economic, and Environmental Modeling of Hydrogen (H ₂) Co-Production Integration (FGS)	ated
	with Stationary Fuel Cell Systems (FCS)	659
MANUFA	ACTURING R&D	663
MF-01	Fuel Cell MEA Manufacturing R&D	665
MF-02	Reduction in Fabrication Costs of Gas Diffusion Layers	668
MF-03	Modular, High-Volume Fuel Cell Leak-Test Suite and Process	671
MF-04	Manufacturing of Low-Cost, Durable Membrane Electrode Assemblies Engineered for Rapid Conditioning	
ME 05		
MF-05	Adaptive Process Controls and Ultrasonics for High Temperature PEM MEA Manufacture	
MF-06	Development of Advanced Manufacturing Technologies for Low Cost Hydrogen Storage Vessels -	0/9
MF-07	Digital Fabrication of Catalyst Coated Membranes	082
MFP-01	Inexpensive Pressure Vessel Production through Fast Dry Winding Manufacture	684
	X A: ATTENDEE LIST	
APPEND	X B: SUBPROGRAM COMMENTS PROVIDED BY REVIEWERS	711
APPEND	X C: GENERAL PROJECT EVALUATION FORM	743
APPEND	X D: LIST OF PROJECTS NOT REVIEWED	749
APPEND	X E: SURVEY QUESTIONNAIRE RESULTS	753

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INTRODUCTION

The FY 2009 U.S. Department of Energy (DOE) Hydrogen Program and Vehicle Technologies Program Annual Merit Review and Peer Evaluation Meeting (AMR) was held on May 18-22, 2009 at the Crystal Gateway Marriott and Crystal City Marriott in Arlington, Virginia. This report is a summary of comments from AMR peer reviewers regarding the hydrogen and fuel cell projects funded by DOE's Office of Energy Efficiency and Renewable Energy (EERE). Hydrogen production projects funded by the Offices of Fossil Energy and Nuclear Energy were also reviewed and included in the report. The work evaluated in this document supports DOE, and the results of this merit review and peer evaluation are major inputs utilized by the DOE in making funding decisions for following fiscal years.

The objectives of this meeting were as follows:

- Review and evaluate FY 2009 accomplishments and FY 2010 plans for DOE laboratory programs, industry/university cooperative agreements, and related research and development (R&D) efforts.
- Provide an opportunity for program stakeholders/participants (e.g., fuel cell manufacturers, component developers, etc.) to shape the DOE-sponsored R&D program in such a way that the highest priority technical barriers are addressed and technology transfer is facilitated.
- Foster interactions among the national laboratories, industry, and universities conducting R&D.

The peer review process followed the guidelines of the Peer Review Guide developed by the Office of Energy Efficiency and Renewable Energy (EERE). The peer review panel members, listed in Table 1, provided comments on the projects presented. These panel members are experts from a variety of related backgrounds related to hydrogen and fuel cells R&D, and they represent national laboratories, universities, various U.S. Government agencies, and manufacturers of hydrogen production, storage, delivery, and fuel cell technologies. Each reviewer was screened for conflicts of interest (COI) as prescribed by the Peer Review Guide. A complete list of the meeting participants is presented as Appendix A.

No.	Last Name, First Name	Organization
1	Aardahl, Christopher	Pacific Northwest National Laboratory
2	Abdel-Baset, Tarek	Chrysler, LLC
3	Aceves, Salvador	Lawrence Livermore National Laboratory
4	Adjemian, Kev	Nissan Technical Center North America, Inc.
5	Adzic, Radoslav	Brookhaven National Laboratory
6	Ahluwalia, Rajesh	Argonne National Laboratory
7	Ahmed, Shabbir	Argonne National Laboratory
8	Ahn, Channing	California Institute of Technology
9	Akiba, Etsuo	Energy Technology Research Institute
10	Anderson, Arlene	U.S. Department of Energy, EERE
11	Anderson, Michele	ONR Naval Materials Division
12	Anderson, Robert	U.S. Environmental Protection Agency
13	Anton, Donald	Savannah River National Laboratory
14	Atanasoski, Radoslav	3M Center

Table 1: Peer Review Panel Members

15	Bailey, Carol	RDS, LLC
16		
	Balachandran, U. (Balu)	Argonne National Laboratory
17	Balema, Viktor	Sigma-Aldrich
18	Bardasz, Ewa	Lubrizol
19	Baturina, Olga	Naval Research Laboratory
20	Bavarian, Farshad	Chevron
21	Benard, Pierre	Institut de recherche sur l'hydrogène
22	Bender, Guido	Hawaii Natural Energy Institute/ University of Hawaii
23	Bendersky, Leonid	National Institute of Standards and Technology
24	Benjamin, Thomas	Argonne National Laboratory
25	Blair, Larry	U.S. Department of Energy
26	Borup, Rod	Los Alamos National Laboratory
27	Bose, Arun	U.S. Department of Energy
28	Bourgeois, Richard	General Electric Global Research Center
29	Bowman, Robert	Oak Ridge National Laboratory
30	Buxbaum, Robert	REB Research & Consulting
31	Cai, Mei	GM Research & Development Center
32	Cairns, Julie	CSA America
33	Carter, J.	Argonne National Laboratory
34	Carter, Robert	GM Fuel Cell Activities
35	Casey, Dan	Chevron
36	Choudhury, Biswajit	DuPont Fuel Cells
37	Cooper, Alan	Air Products and Chemicals, Inc.
38	Cox, Philip	PolyFuel Inc.
39	Cross III, James	Nuvera Fuel Cells, Inc.
40	De Jonghe, Lutgard	Lawrence Berkeley National Laboratory
41	Debe, Mark	3M Company
42		BASF Fuel Cell, Inc.
42	DeCastro, Emory Deutsch, Todd	National Renewable Energy Laboratory
43		** *
-	Dobbins, Tabbetha	Louisiana Tech University
45	Driscoll, Daniel	U.S. Department of Energy
46	Eddaoudi, Mohamed	University of South Florida
47	Eisman, Glenn	Rensselaer Polytechnic Institute
48	Erdle, Erich	EFCECO
49	Ernst, William	Retired, Plug Power
50	Fahr, Askar	National Institute of Standards and Technology
51	Farese, David	Air Products
52	Fenske, George	Argonne National Laboratory
53	Filiou, Constantina	European Commission
54	Fort, William	Shell Global Solutions (U.S.), Inc.
55	Gabrielov, Alexei	Shell Technology Center Houston
56	Ge, Qingfeng	Southern Illinois University
57	Ghirardi, Maria	National Renewable Energy Laboratory
58	Gittleman, Craig	Fuel Cell Research Labs
59	Glass, Robert	Lawrence Livermore National Laboratory
60	Goldbach, James	Arkema, Inc.
61	Goudy, Andrew	Delaware State University
62	Graber, Joe	U.S. Department of Energy
63	Grassilli, Leo	D&L Energy
64	Gross, Karl	Hydrogen Technology Associates
65	Gupta, Nikunj	Shell Hydrogen, LLC
66	Haberman, David	National Energy Technology Laboratory
67	Hamdan Giner, Monjid	Giner, Inc.
		,

68	Hamrock, Steven	3M Fuel Cell Components Program
68 69	Harriock, Steven Hardis, Jonathan	National Institute of Standards and Technology
70	Harrison, Kevin	National Renewable Energy Laboratory
70	Hebling, Christopher	Fraunhofer Institute for Solar Energy Systems
72	Herbert, Thorsten	NOW GmbH
73	Herring, Andy	Colorado School of Mines
74	Hershkowitz, Frank	ExxonMobil Research & Engineering Co.
74		
76	Hesterberg, Tom Hirano, Shinichi	Navistar, Inc. Ford Motor Company
70	Holladay, Jamie	
78	Hua, Thanh	U.S. Department of Energy
78	Imam, M.	Argonne National Laboratory
80	Jacobson, David	Naval Research Laboratory
81		National Institute of Standards and Technology
	James, Brian	Directed Technologies, Inc.
82	Jensen, Craig	University of Hawaii
83	Johnston, Christina	Los Alamos National Laboratory
84	Jorgensen, Scott	GM R&D
85	Kabir, Zakiul	ClearEdge Power
86	Kabza, Alexander	Zentrum für Sonnenenergie- und Wasserstoff-
07	Kananaja lina	Forschung (ZSW) Baden-Württembergix
87	Kegerreis, Jim	Exxon Mobil
88	Kerr, John	Lawrence Berkeley National Laboratory
89	King, Dave	PNNL Annual National Laboration
90	Kopasz, John	Argonne National Laboratory
91	Kumar, Romesh	Argonne National Laboratory
92	Kuriyama, Nobuhiro	National Institute of Advanced Industrial Science and
02	Loobor Stophon	Technology Research
93 94	Lasher, Stephen	TIAX, LLC
	Lewis, Michele	Argonne National Laboratory
95	Lipp, Ludwig	FuelCell Energy, Inc.
96 97	Maness, Pin-Ching	National Renewable Energy Laboratory
97 98	Mann, Margaret	National Renewable Energy Laboratory
	Markovic, Nenad	Argonne National Laboratory
99	Maroni, Victor	Argonne National Laboratory
100	Masten, David	General Motors, Fuel Cell Activities
101	Mazumder, Malay	University of Arkansas
102	McFarland, Eric	University of California, Santa Barbara
103	McQueen, Shawna	Energetics Incorporated
104	Mehall, Mark	Ford Motor Company
105	Meisner, Gregory	GM Research & Development Center
106	Melis, Tasios	University of California, Berkeley
107	Merritt, James	Department of Transportation
108	Mettes, Jacques	Power and Energy
109	Meyers, Jeremy	University of Texas, Austin
110	Miller, Eric	University of Hawaii at Manoa, HNEI
111	Miller, James	Argonne National Laboratory
112	Miller, Michael	Southwest Research Institute
113	Minh, Nguyen	Consultant
114	Mitchell, George	GM Solutions, LLC
115	Mohtadi, Rana	Toyota Motor Engineering and Manufacturing of
140		North America
116	More, Karren	Oak Ridge National Laboratory
117	Moreland, Greg	Retired, Consultant (Sentech)
118	Myers, Deborah	Argonne National Laboratory

119	Nguyen, Kevin	Chevron Energy Technology Company		
120	Nkansah, Asare			
120		Chicago State University		
121	Olson, Greg	Retired, HRL		
	Ozkan, Umit	Ohio State University		
123	Ozolins, Vidvuds	University of California, Los Angeles		
124	Padro, Catherine	Los Alamos National Laboratory		
125	Parks, George	FuelScience, LLC		
126	Paster, Mark	Consultant, Retired DOE		
127	Patel, Pinakin	Fuel Cell Energy		
128	Pecharsky, Vitalij	Iowa State University		
130	Penev, Michael	National Renewable Energy Laboratory		
131	Perret, Robert	Nevada Technical Services, LLC		
132	Peters, John	Montana State University		
133	Petrovic, John	Petrovic and Associates		
134	Pinkerton, Frederick	General Motors Research and Development Center		
135	Pintauro, Peter	Vanderbilt University		
136	Pivovar, Bryan	National Renewable Energy Laboratory		
137	Podolski, Walt	Argonne National Laboratory		
138	Quah, Cheng-Guan Michael	Concurrent Technologies		
139	Ronnebro, Ewa	Pacific Northwest National Laboratory		
140	Ramani, Vijay K.	Illinois Institute of Technology		
141	Rambach, Glenn	Third Orbite Power Systems, Inc.		
142	Remick, Robert	National Renewable Energy Lab		
143	Richards, Mark	Versa Power Systems		
144	Roan, Vernon	Retired, National Academies Member		
145	Rocheleau, Richard	University of Hawaii at Manoa		
146	Rossmeissl, Neil	U.S. Department of Energy		
147	Saber, Jim	NextEnergy		
148	Sandrock, Gary	Oak Ridge National Laboratory		
149	Shultz, Travis	U.S. Department of Energy		
150	Siegel, Don	University of Michigan		
151	Simnick, James	BP Global Fuels Technology		
152	Sink, Carl	U.S. Department of Energy		
153	Sofronis, Petros	University of Illinois, Urbana-Champaign		
154	Spendelow, Jacob	Los Alamos National Laboratory		
155	Stanfield, Eric	National Institute of Standards and Technology		
156	Stevenson, Jeff	Pacific Northwest National Laboratory		
157	Steward, Darlene	Hydrogen Technologies & Systems Center		
158	Stolten, Detlef	Forschungszentrum Jülich, GmbH		
159	Stroh, Ken	Sentech, Inc.		
160	Stubos, Thanos	NCSR Demokritos		
161	Sudik, Andrea	Ford Motor Company		
162	Summers, William	Savannah River National Laboratory		
163	Surdoval, Wayne	U. S. Department of Energy		
164	Swider Lyons, Karen	Naval Research Laboratory		
165	Tao, Greg	Materials and Systems Research, Inc.		
166	T-Raissi, Ali	University of Central Florida		
167	Tran, Thanh	NSWC Carderock		
168	Tumas, William	Los Alamos National Laboratory		
169	Turner, John	National Renewable Energy Laboratory		
170	Uddin, Nasim	Global Automotive Management Council, Inc.		
170	Vanderborgh, Nicholas	Los Alamos National Laboratory, retired		
172	Veenstra, Mike	Ford Motor Company		
112				

173	Voecks, Gerald	Retired, GM		
174	Wainright, Jesse	Dept of Chemical Engineering, Case Western		
		Reserve University		
175	Waldecker, James	Ford Motor Company		
176	Walker, Gavin	University of Nottingham		
177	Wang, Yong	Pacific Northwest National Laboratory		
178	Weeks, Brian	Advanced Energy Systems		
179	Weidner, John	University of South Carolina		
180	Wheeler, Douglas	DJW Technology, LLC		
181	Williams, Mark	Retired, National Energy Technology Laboratory		
182	Wipke, Keith	National Renewable Energy Laboratory		
183	Wolverton, Christopher	Northwestern University		
184	Woodbury, Neal	Arizona State University		
185	Xu, Qing	J. Craig Venter Institute		
186	Yvon, Klaus	Université de Genève		
187	Zawodzinski, Thomas	Case Western Reserve University		
188	Zelenay, Piotr	Los Alamos National Laboratory		
189	Zhao, Yiping	University of Georgia		

SUMMARY OF PEER REVIEW PANEL'S CROSS-CUTTING COMMENTS AND RECOMMENDATIONS

AMR panel members provided comments and recommendations regarding selected DOE hydrogen and fuel cell projects, overall management of the Program, and the AMR peer evaluation process. Project comments and scores are provided in the following sections of the report. Comments on subprogram management are provided in Appendix B.

ANALYSIS METHODOLOGY

A total of **216** projects were reviewed at the meeting. As shown above, **189** panel members participated in the AMR process providing a total of **1,066** project evaluations (not every panel member reviewed every project). These reviewers were asked to provide numeric scores (on a scale of 1 to 4, with 4 being the highest) for five aspects of the research presented. Sample evaluation forms are provided in Appendix C. Scores and comments were submitted on a provided laptop to an online, private database allowing for real time tracking of the review process. A list of projects that were presented at the AMR but were not reviewed is provided in Appendix D.

Project scores were based on the following five criteria and weights:

Score 1: Relevance to overall DOE objectives (20%)

Score 2: Approach to performing the R&D (20%)

Score 3: Technical accomplishments and progress toward achieving the project and DOE goals (40%)

Score 4: Technology transfer and collaborations with industry, universities, and other laboratories (10%)

Score 5: Approach to and relevance of proposed future research (10%)

INTRODUCTION

For each project, an average score was calculated (from the scores of individual reviewers) for each of the five aforementioned criteria. These average scores were then weighted and combined to produce a final overall score for each project. In this manner, a project's final overall score can be meaningfully compared to that of another project. The following formula was used to calculate the weighted, overall score:

```
Final Score = [Score 1 x 0.20] + [Score 2 x 0.20] + [Score 3 x 0.40] + [Score 4 x 0.10] + [Score 5 x 0.10]
```

Some new projects were reviewed, for which the third criterion (Technical Accomplishments) did not apply because of the projects' recent startup. In this case, the other four criteria were scaled proportionately in the weighting calculation. The weighting value for the remaining scores [weight + (40/60 * weight)] was used to establish a final score formula for these projects. The result was the following:

```
Final Score = Score 1 \times \{0.20 + [(40/60) \times 0.20]\} + Score 2 \times \{0.20 + [(40/60) \times 0.20]\} + Score 4 \times \{0.10 + [(40/60) \times 0.10]\} + Score 5 \times \{0.10 + [(40/60) \times 0.10]\}
```

A perfect, overall score of "4" would indicate that a project satisfied the five criteria to the fullest possible extent; the lowest possible, overall score of "1" would indicate that a project did not satisfactorily meet any of the requirements of the five criteria.

Reviewers were also asked to provide qualitative comments regarding the five criteria, specific strengths and weaknesses of the project, and/or any recommendations relating to the work scope. These scores and comments were placed into a database for easy retrieval and analysis. These comments are summarized in the following sections of this report.

ORGANIZATION OF THE REPORT

The project comments and scores are grouped by Subprogram (i.e., Production and Delivery, Hydrogen Storage, Fuel Cells, Systems Analysis, and Manufacturing) in order to align with DOE Program planning scheme. Each of these sections begins with a brief description of the general type of research being performed. This is followed by the results of the analysis for each of the projects presented at the 2009 Annual Merit Review. A summary of the qualitative comments is provided for each project, as well a graph showing the overall project score and a comparison of how each project aligns with all other projects in its Subprogram area. A sample graph is provided in Figure 1.

The project comparisons illustrated in the report are criteria based. Each rectangular blue bar in the chart represents that project's average score for one of the five designated criteria. Each of these scores (each blue bar) is then compared with the related maximum, minimum, and average score for the same criterion across all projects in the same Subprogram. The black line bars that

overlay the blue rectangular bars represent the maximum, average, and minimum scores for each criterion.

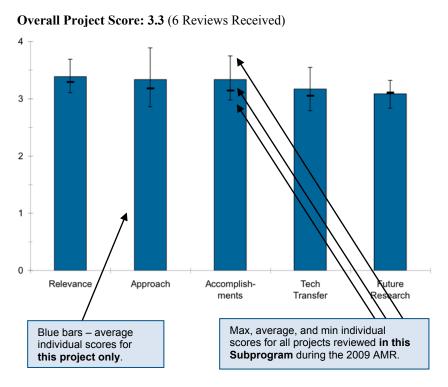


Figure 1: Project Score Graph with Explanation

For clarification, consider a hypothetical review in which only three projects were presented and reviewed in a Subprogram; Table 2 displays the average scores for each of the project's five, rated criteria.

	Relevance (20%)	Approach (20%)	Technical A&P (40%)	Tech Transfer (10%)	Future Research (10%)
Project A	3.4	3.3	3.3	3.2	3.1
Project B	3.1	2.8	2.7	2.7	2.9
Project C	3.0	2.6	2.7	2.8	2.9
Project D	3.4	3.5	3.4	3.2	3.3
Project E	3.6	3.7	3.5	3.4	3.4
Max	3.6	3.7	3.5	3.4	3.4
Average	3.3	3.2	3.1	3.0	3.1
Min	3.0	2.6	2.7	2.7	2.9

Table 2: Sample Project Scores

INTRODUCTION

The Project A chart would contain five, blue rectangular bars to represent the values listed for Project A above. A black line bar indicating the related maximum, minimum, and average values for each criterion would overlay each of the blue bars to facilitate comparison with other projects in the Subprogram. In addition, each project's criterion scores would be weighted and combined to give a final, overall project score that could be meaningfully compared with those of other projects. Below is a sample calculation for the Project A weighted score.

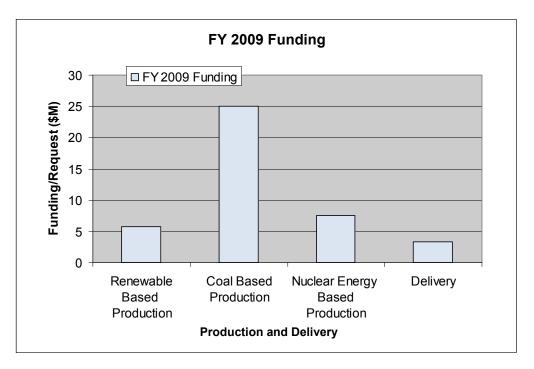
Final Score for Project A = [3.4 x 0.20] + [3.3 x 0.20] + [3.3 x 0.40] + [3.2 x 0.10] + [3.1 x 0.10] = 3.3

Hydrogen Production and Delivery Summary of Annual Merit Review Hydrogen Production and Delivery Subprogram

Summary of Reviewer Comments on Hydrogen Production and Delivery Subprogram:

This review session evaluated hydrogen production and delivery research from all DOE activities working on the President's Hydrogen Fuel and Advanced Energy Initiatives, including: the Offices of Fossil Energy, Nuclear Energy, and Energy Efficiency and Renewable Energy. The production and delivery projects are generally considered to be well aligned with the goals and objectives of the Hydrogen Program.

The production projects include diverse energy sources and technologies for hydrogen production including natural gas reforming, water electrolysis, bioderived renewable liquids reforming, biomass gasification, solar-driven thermochemical cycles, nuclear-driven thermochemical cycles, photoelectrochemical direct water splitting, biological hydrogen production, and hydrogen production from coal. The delivery projects reviewed included the next stage of development of the H2A delivery analysis models and several of the key hydrogen delivery research efforts such as pipeline embrittlement, new fiber reinforced polymer pipeline and linings, and compressor research. Overall, the projects were judged to have made considerable progress in reducing both projected capital and operating costs and in improving material properties. Reviewer concerns and recommendations varied considerably by project and are summarized below.



Hydrogen Production and Delivery Funding by Technology:

Majority of Reviewer Comments and Recommendations:

In general, the reviewer scores for the production and delivery projects were high to average, with scores of 3.9, 3.1 and 1.9 for the highest, average and lowest scores, respectively. The scores are indicative of

the technical progress that has been made over the past year for DOE competitively selected and Congressionally directed projects. Recommendations and major concerns for each project category are summarized below.

Bio-Derived Liquids Reforming: New technology being developed for distributed reforming from bioderived liquids (e.g. ethanol, sugars) will build on distributed reforming from natural gas technology while helping to solve outstanding issues with on-site hydrogen production to reach the bio-derived liquids cost goal of \$3.00/gge by 2017. Two primary recommendations emerged from the reviews. First, the catalyst development tasks must move forward and be successful if the reforming of bioderived liquids is to meet the DOE production cost targets. Second, all projects need to utilize H2A production modeling to provide consistent cost estimates.

Electrolysis: In general, projects in this area were scored favorably. Most of the projects were regarded as well aligned with current program goals and objectives. The projects focused on increasing stack efficiency and decreasing capital cost. Innovative new membranes presented were able to increase the efficiency to above that of the 2012 DOE targets. Advanced manufacturing techniques and new designs were presented that are projected to significantly reduce capital costs. The reviewers noted: 1) long-term durability of the membranes must be tested, 2) the advanced membranes being developed need to be integrated into stacks and tested, and 3) balance-of-plant development is needed to increase system reliability while reducing system cost. The newly started projects will be addressing these important issues.

Biomass Gasification: Two projects in this area were reviewed. Both projects are researching the potential of central plant, low temperature, single step, aqueous phase reforming of hydrolyzed biomass. The project scores ranged from 2.3 to 3.0. Projects scoring higher were noted as having significant technical advancements since last year and to have a focused project plan, which was followed closely.

Solar-Driven High Temperature Thermochemical: Two presentations and two posters were reviewed in this topic area. The projects were favorably rated for their collaborative efforts and technical skills and abilities of the researchers. Recommendations for improvement included ensuring that the calculation of overall system efficiency is consistent for each cycle, completing all material balances, and identifying and resolving waste disposal issues.

Photoelectrochemical Hydrogen Production: The reviewers noted that the teaming approach that was used in some of the projects in this area was effective and necessary to achieve the DOE targets. Several of the projects received high ratings from the reviewers. Nearly all the projects were viewed to be aligned with the program's long-term goals. The projects have achieved good scientific progress in materials research and have established effective collaborations. The reviewers saw the addition of theoretical activities to this area as necessary.

Biological Hydrogen Production: The projects in this area were highly rated and the general conclusion from the reviewers was that the researchers are moving toward the DOE goals in this long-term renewable hydrogen production area. The scientific methods used in the majority of the projects are seen as cutting edge and the collaborations are effective and productive.

Separations: Reviewers commented, similar to prior year reviews, that there is a great need for investigators to test their hydrogen separation and purification membranes using realistic, mixed gas streams and to complete cost analyses. The potential for membrane technology to reduce the on-site hydrogen production footprint (by eliminating the PSA unit) and to reduce capital costs were frequent comments. Overlap with DOE Office of Fossil Energy membrane separations work was noted.

Hydrogen from Coal: The projects reviewed in this area received mostly favorable ratings from the reviewers. Reviewers observed that the projects were in alignment with DOE HFCIT and Hydrogen from Coal Program goals and objectives. The reviewers suggested that the projects need to advance the technology to the point where experiments using actual or close to actual gas streams are being performed. Specifically, the reviewers noted that the membranes need to be tested in the presence of impurities. The membranes also need to go through additional testing to assess long-term durability and stability.

Hydrogen Production Using Nuclear Energy: In general, the projects reviewed in this area were scored favorably. Reviewers approved of the breadth of collaboration for some projects and the well-focused approach of other projects. The projects were judged to be well aligned with the program's goals. As in 2008, reviewers recommended that materials and cost drive research. Specific recommendations were made to understand durability and degradation of the high temperature electrolytic cells.

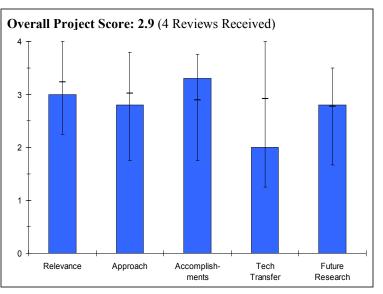
Hydrogen Delivery: The reviewers recognized significant and very relevant progress in the pipeline research. The reviews also complimented the broad spectrum of collaboration across industry, national labs, and universities as well as a good mix of theory, modeling, and experimental work. The reviewers suggested benchmarking results achieved in this program with Technology Validation results or with field installations, e.g. hydrogen embrittlement of existing pipelines. Reviewers also suggested measuring the effect of hydrogen impurities on pipeline and storage system performance and on the cost for purification.

Project # PD-02: Bio-Derived Liquids Reforming

Yong Wang: Pacific Northwest National Laboratory

Brief Summary of Project

The overall objective of this project is to evaluate and develop bio-derived liquid reforming technologies for hydrogen production that can meet DOE's 2017 cost target of <\$3.00/gge. The specific objectives for this project are to 1) identify at least one catalyst having the necessary activity, selectivity, and life at moderate temperatures to justify scale-up; 2) provide input for H2A analyses to determine potential economic viability and provide guidance to the research and development; 3) identify and control the reaction pathways to enhance hydrogen selectivity and productivity as well as catalyst; and 4) provide preliminary data for H2A analyses.



Question 1: Relevance to overall DOE objectives

This project earned a score of **3.0** for its relevance to DOE objectives.

- This project is split into two parts: 1) aqueous phase reforming catalysts and 2) ethanol steam reforming catalysts. Relevance for this project is high in that it directly supports Virent Energy System's aqueous phase reforming project as well as non-precious metal ethanol catalyst work.
- Finding an energy efficient and cost effective way to convert biomass to a useful energy carrier is critical to DOE's mission.
- The project addresses the stated goal of the program.

Question 2: Approach to performing the research and development

This project was rated **2.8** on its approach.

- The project has useful research towards cost reduction, both with regards to capital as well as O&M, but does not necessarily have the most important research.
- The basic catalyst development approaches in the project are strong.
- The use of Pt and Ru as the catalyst for the aqueous-phase reforming (APR) process is questionable when the project itself recognizes the need to identify 'base' metal catalysts as a critical need to meet the cost-effectiveness barrier.
- This project is in contrast to the ethanol stream reforming (ESR) work where a base metal is identified.
- Branch points and go/no-go decisions should be built into the project's approach.
- It is unclear why glycerol is being used instead of one of the sugars produced by hydrolysis. The usage of glycerol will create issues different from those found with using hexoses or pentoses.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated **3.3** based on accomplishments.

- The project shows outstanding progress toward DOE's program and/or project goals.
- The investigation of Re/Pt catalysts on carbon supports is relevant, focused, and a solid achievement.

- Experimental determination of Rh catalyst lifetime at lower space velocity (~20,0000/hr) is an important finding. However, the project cost impact on system needs to be addressed.
- The project's process work is well done. A good start on the economics of the chemical plants is apparent.
- The project team should look at or conduct sensitivity analysis on economics. An EtOH value of \$1.07/gallon is very unrealistic.

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated **2.0** for technology transfer and collaboration.

- The project seems to have work in common with Virent Energy Systems, but nothing as identifiable as collaboration. Virent Energy Systems seem to be disconnected and not part of the development team. The partners in this project do not seem to be integrated and it is not clear if they add substance to the technical development path.
- The project team's interaction with Virent Energy Systems is relevant and productive.
- It appears there is only modest interaction with Ohio State University (OSU).
- The level of collaboration in this project does not make the best use of the DOE complex. The relationship with Virent Energy Systems appears to be mostly one way.
- The project team needs collaboration with commercial entities that have fuels and catalyst/process experience and expertise, i.e., an energy company or catalyst vendor.
- "Collaboration with Ohio State on ethanol steam reforming has been minimal in the past and we have had discussions to specifically increase this interaction" and "Initial discussions were held on collaborative work".
- Regarding the above quoted statements, neither constitutes reasonable progress in a year. Discussions are not considered collaboration.

Question 5: Approach to and relevance of proposed future research

This project was rated 2.8 for proposed future work.

- The project team appears to be addressing late stage commercialization barriers, but it is unclear where the commercialization partner is. Addressing such late stage issues if there is no commercialization plan does not make sense.
- A future plan for this project is solid.
- The project team is looking to find ways to "Improve hydrogen productivity and selectivity by exploring additives that may retard dehydration pathway to acids on Pt-Re/C." This is vital but it would be constructive for the team to provide more specifics on this issue.
- The project's coking mechanisms are well established but knowing them is unlikely to help in coke reduction. Time would be better spent empirically exploring catalyst compositions and process conditions.
- The project team should not work on pressure swing adsorption (PSA) issues. This issue is outside the scope of the project and the expertise of the investigators.
- A systematic investigation of steam:ethanol ratio needs to be conducted.

Strengths and weaknesses

Strengths

• The project team's basic science investigation of new catalyst systems under representative operating conditions is a strength.

Weaknesses

- The project team conducted economic analysis to determine hydrogen cost, but catalyst lifetime assumptions are not defined.
- The lab results in this project indicate that carbon deposition on Co catalyst is substantially higher than on Rh. Lifetime testing is needed to determine real-word effects. Limited Co-based catalyst lifetime has traditionally been a fundamental problem but is not addressed in this project.

- The number of moles of hydrogen produced per each mole of glycerol should have been presented. Selectivity was not defined in this project.
- The project has no real industrial collaboration.

Specific recommendations and additions or deletions to the work scope

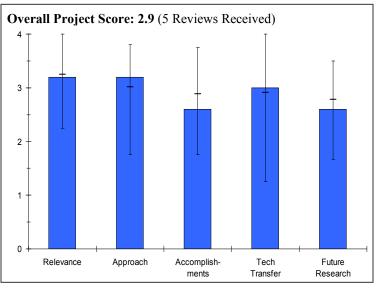
• The project team should consider switching from using glycerol to real sugars.

Project # PD-03: Hydrogen Generation from Biomass-Derived Carbohydrates via the Aqueous-Phase Reforming Process

Bob Rozmiarek; Virent Energy Systems, Inc.

Brief Summary of Project

The overall objectives of this project are to 1) design a generating system that uses lowcost sugars or sugar alcohols that can meet DOE's hydrogen cost target of \$2 to \$3/gge for 2017; and 2) fabricate and operate an integrated 10 kg of H₂/day generating system. The 2009 objectives were to 1) continue fundamental development and analysis to increase the thermal efficiency of the aqueous-phase reforming (APR) system; 2) continue development of the APR catalyst and reactor system that converts glucose to hydrogen; 3) complete hydrogenation fundamental study and interact with PNNL on data exchange and fundamental surface science study; 4) operate reactor development pilot plant



(scale-up testing); 5) develop initial process flow diagram and catalytic reactor design for 10 kg/day demonstration system; and 6) review techno-economic performance of the APR system.

Question 1: Relevance to overall DOE objectives

This project earned a score of **3.2** for its relevance to DOE objectives.

- This project is especially relevant as the team pushes toward less-treated biomass. However, the application of refined biomass has to be questionable versus use of those molecules directly as fuel.
- The project directly targets the objective of low-cost renewable hydrogen. Aqueous reforming is an important pathway for the team to explore.
- This project addresses one of DOE's preferred pathways. Efficient conversion of biomass to hydrogen or other liquid fuel is critical to DOE's mission.
- This project aims at producing hydrogen from a renewable source and has the potential to meet DOE's production target.
- The project team addresses DOE's program goal but uses a convoluted route. A direct cellulose to hydrogen route is preferable to control costs.

Question 2: Approach to performing the research and development

This project was rated **3.2** on its approach.

- The project team had a good identification of barriers they faced in 2008. The team's approach is difficult to judge because of the secrecy.
- This program lends itself to a relatively straight-forward approach. They have clearly articulated a game plan: approach is very good.
- The project team's investigation of basic catalyst science to determine reaction rates and improve catalyst is solid.
- The project team has a good approach as it is important to have a wide range of feedstocks for hydrogen production. The lack of a gas compression step is also useful/productive.
- The project team's fundamentals to improve H₂ yield was a good study.

- The project's approach to address fundamental catalyst issues especially reactor design and system design is good.
- The project team needs to address impurities expected in sugars and their effects on catalyst performance.
- The team needs to address where the \$0.064/pound glucose number comes from. This number seems low.

Ouestion 3: Technical accomplishments and progress toward project and DOE goals

This project was rated **2.6** based on accomplishments.

- The project's gross 10% reduction of cost is a little disappointing (from \$6.50 with a \$3.00 target). The team should have explained how the 10% factors into the 60% needed to reach the target. The secrecy surrounding the project allows only superficial evaluation.
- The team has made significant technical progress. However, more defined metrics are needed regarding their efforts, such as the goal and threshold fuel conversions to meet price goal or the goal and threshold CO₂ and H₂ yields.
- The project has been successful but it has no method in place to evaluate it. The important results are mentioned as "exclusive work-wide licenses, ... multiple new patent applications, ... solid trade secret position." There is a lack of real data in the report.
- If the program has been as successful as claimed, there should be no need for government funding.
- The project's 10% reduction in H₂ costs is not encouraging as the process needs about 50% reduction improvement to meet DOE targets. It is unclear if the low yield is due to catalyst performance or inherent thermodynamics.
- This program is due to end in September 2009. To this date questions remain such as what the status is of 10kg/day reactor? Has it been designed or is it running now? Is it designed for continuous operation? How long has it operated continuously? The team should do a sensitivity analysis on economics to identify critical parameters and examine sensitivity on sugar price.
- The project's reaction network study should be published. This is important information discovered with government funds and needs to be shared with the entire biomass community.

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated **3.0** for technology transfer and collaboration.

- This project seems very well integrated with the University of Wisconsin (UW) Madison folks.
- It is difficult to evaluate the extent of interaction with PNNL and UW. Archer Daniels Midland Company (ADM) is listed as a collaborator but no examples or explanations of contributions are provided.
- ADM is listed as a collaborator but their contribution is not identified. PNNL and the University of Wisconsin appear to be suppliers rather than partners.
- The project has good collaboration with ADM and University of Wisconsin. The project team should consider additional collaborations with a catalyst company and a system design/integrator with expertise in design for manufacturing and assembly (DFMA).
- The project team would benefit from interaction with an entity that has industrial experience/expertise such as an energy company or catalyst vendor.

Question 5: Approach to and relevance of proposed future research

This project was rated **2.6** for proposed future work.

- The approach to and relevance of proposed future research is very superficial due to the project's secrecy. It is unclear how the team plans address the magnitude of the gap. It is also not clear why a larger unit should be built when issues remain for reducing cost to the \$3.00 target.
- This program seems ripe for 50 or 50+% cost share.
- The team should address impurities expected in sugars, especially if the sugars used are produced from lignocellulosic biomass due to their effect on catalyst performance.
- This project closing therefore there is no relevance of proposed future research.

FY 2009 Merit Review and Peer Evaluation Report

Strengths and weaknesses

Strengths

- The project team tried to commercialize something, which is the right place to lead this R&D.
- The project team has a seemingly good coordination of catalyst development theory with test.

Weaknesses

- The project team and the project itself is under secrecy, which makes it difficult to pinpoint weaknesses.
- The project's "bio liquid to hydrogen" concept seems to be a weak approach.
- The team's emphasis seems to be on the hydrogenation reaction. While hydrogenation of glucose to sorbitol is necessary, they also need to examine the actual H₂ production reaction. This concern is not adequately conveyed in the presentation.
- Heat transfer is very important factor in reactor design and needs to be addressed. There is very little information on heat transfer which could be the dominant cost/sizing factor.
- This project needs a space velocity and/or example of reactor size for a given H₂ production rate. The reactor may be very large. It is currently hard to assess its size.

Specific recommendations and additions or deletions to the work scope

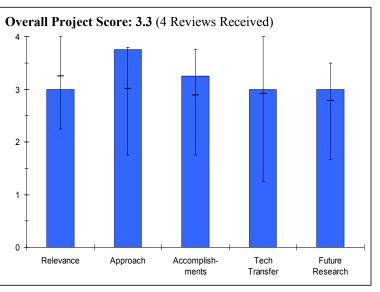
• The project team needs to add intermediate metrics to define targets conversions/yields so that yearly progress may be assessed.

Project # PD-04: Investigation of Reaction Networks and Active Sites in Bio-Ethanol Steam Reforming over Co-based Catalysts

Umit S. Ozkan, Hua Song, Xiaoguang Bao, and I. Ilgaz Soykal; Ohio State University

Brief Summary of Project

The objective for this project is to acquire a fundamental understanding of the reaction networks and active sites in bio-ethanol steam reforming over Co-based catalysts that would lead to 1) development of a precious metal-free catalytic system which would enable low-temperature operation (350°-550°C), high ethanol conversion, high selectivity and yield of hydrogen, high catalyst stability and minimal byproducts such as acetaldehyde, methane, ethylene and acetone; and 2) enabling hydrogen production from renewable sources at low cost. Ohio State has identified the active sites and reaction mechanism and characterized the deactivation mechanism.



Question 1: Relevance to overall DOE objectives

This project earned a score of 3.0 for its relevance to DOE objectives.

- The project's development of non-precious metal catalysts for the ethanol reformation is an enabling technology as it substantially lowers catalyst cost.
- The team's identification of a non-noble metal catalyst is key to providing cost effective electrolysis processes for producing hydrogen. The need for this is evident in many applications of DOE's program.
- This project addresses DOE's program goals well.

Question 2: Approach to performing the research and development

This project was rated **3.8** on its approach.

- This project has very well designed R&D to optimize catalyst.
- The team's description of the systematic approach to catalyst synthesis is very good.
- The project team's interdisciplinary approach is excellent. The amount of analytical data being collected and used is significant.
- It would be helpful to see some formal process to the problem of examining the entire data collection as a whole. It is recognized that this is a difficult challenge.
- This project recognizes the importance of catalyst synthesis to a greater extent than other projects.
- This project also has a good mix of catalyst characterization techniques.
- The team effectively explored the use of diffuse reflectance infrared Fourier transform spectroscopy (DRIFTS), Raman and isotopes.

<u>Ouestion 3: Technical accomplishments and progress toward project and DOE goals</u></u>

This project was rated 3.3 based on accomplishments.

• The team's research is outstanding. The project's progress would also be outstanding if there were numerical benchmarks. For example, what is "high" and what has actually been achieved?

- The project tasks are clearly identified with progress succinctly laid-out. The project's goals should be more clearly identified, e.g., while a target space velocity is shown, lifetime goals and achievements are not listed.
- "One of the best performing catalysts" is listed as Co/CeO₂ hexamethyldisilane (HMDS) in the project. Substantial exploration of dopants, support structure, etc. was conducted by the team, but the "best" catalyst is not defined by it critical attributes. It is described only as generic Co/CeO₂.
- Substantial progress in understanding reaction networks seems to have been achieved.
- The catalyst characterization in this project is very impressive. Linkages of characterization to performance should be strengthened.
- The project uses a flow diagram to illustrate the process. The questions that remain are what are the initial estimates of the cost and what are the cost drivers?
- The slides for this project contained far too much information. It was difficult to follow the presentation because of the overwhelming amount of data presented on each slide.
- The team has a good understanding of mechanism developed. They have a good publication and presentation record.

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated **3.0** for technology transfer and collaboration.

- Collaboration within the team is outstanding, which is clearly an important factor for this effort. Critical insights and contributions coming from partner institutions are not transparent.
- This project has very good partners. The difficulty with explaining collaborations in detail is difficult; however, it would be helpful to see an example of the team building or synergy of the team.
- This project has a good involvement of industry, government labs, and various entities in university.

Question 5: Approach to and relevance of proposed future research

This project was rated **3.0** for proposed future work.

- The project's future work is logical in the micro sense of work progress, but maybe not in big picture. This "understanding" seems way ahead of development. Either this project needs a commercialization partner (if it is commercializable) or it needs a very close linkage with economics to verify that work is addressing the critical issues.
- Future work is detailed and specific for this project. However, longevity studies are the most important element.
- The project's kinetic rate expression determination is of value, but only of the most promising catalyst(s). There was no mention of down-selecting to a top contender for detailed examination.
- The future work plan for the team and project is rational but would be improved by branch points that are driven by discovery.
- More information on effects of varying steam:ethanol ratio is needed. A question that remains is what is the minimum steam ratio?
- The project needs sensitivity analysis to economics. How the decreasing steam ratio effects cost needs to be addressed.

Strengths and weaknesses

Strengths

- Technical catalyst development team activity is superb in this project.
- The team's three-leg approach is well thought-out.
- Each page of the team's presentation contained a very nice and succinct summary of the main message or concept learned.
- The project researcher did a good job of summarizing very complicated results.
- A 3-D yield graph showing various product yields at various temperatures is particularly effective. The team should make this a standard way to portray data.
- The project has good characterization and good work on exploring synthesis space.

Weaknesses

- The project relationship to actual process development needs is not revealed in talks. If there is no process development/commercialization need, this terrific work could be just a waste.
- Regarding the presentation, there were too many graphs on pages which created confusion/clutter without adding meaningful information.
- More focus needs to be placed on lifetime studies. Non-precious metal catalysts are desirable for their lower cost but that cost advantage is erased if the catalyst needs to be frequently replaced due to deactivation.
- More tests should be conducted at higher space velocities and at lower steam:ethanol ratios. Lower steam:ethanol ratios have a beneficial effect on system cost- but only if they do not adversely impact performance/lifetime.

Specific recommendations and additions or deletions to the work scope

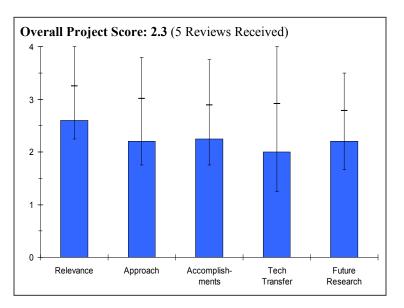
No recommendations were made for this project.

Project # PD-05: Distributed Reforming of Renewable Liquids Using Gas Transport Membranes

U. (Balu) Balachandran, T.H. Lee, C.Y. Park, Y. Lu, J.E. Emerson, J.J. Picciolo, and S.E. Dorris; Argonne National Laboratory

Brief Summary of Project

The overall objective of this project is to develop a compact, dense, ceramic membrane reactor that enables efficient and cost-effective production of hydrogen by reforming bio-derived liquid fuels using pure oxygen formed by water splitting and transported by the membrane. Objectives over the past year were to optimize the performance of the oxygen transport membrane and demonstrate reforming of ethanol. Membrane technology provides the means to attack barriers to the development of small-scale hydrogen production technology.



<u>**Ouestion 1: Relevance to overall DOE**</u> <u>objectives</u>

This project earned a score of 2.6 for its relevance to DOE objectives.

- This project applies to barriers related to low-cost production.
- DOE's FY08 change to ethanol differentiates this project from the work done by Eltron Research.
- The PI is attempting to respond to the needs of the DOE Hydrogen Program, however, this work appears to be an attempt to adapt long term, on-going projects and concepts to fit the goals and objectives of the program. This approach may not be the most practical route to achieve the program goals. DOE and the PI need to consider if these novel approaches have any real benefit over current (or potential future) methods of hydrogen production. A reasonable cost analysis needs to be developed, not simply H2A. If this work is continued, it should be considered a long term fundamental effort, which is appropriate for a national laboratory, However, there should be no expectation that this will be developed in near timeframe (the page 8 schedule is not reasonable).
- This project seems to be using a difficult path (dual membranes) to do something that is nearly commercial today. It is not convincing that the big picture goal (ethanol to hydrogen) makes any sense in the base case.
- Given that the Hydrogen Program has already declared success in methane steam reforming, it is unclear how much benefit is to be gained by this process. A combined two membrane system seems to be complex.
- This project's focus is the use of oxygen transport membrane (OTM) and it appears to be funding long term OTM research with hydrogen money.
- This project's benefits are stated in increased conversion. There is a need to get a third party to assess increased capital cost and complexity and see if there are economic benefits.

Question 2: Approach to performing the research and development

This project was rated 2.2 on its approach.

- This project's economics should be completed on the potential savings prior to experimental program. While this project would reduce reactor size it will not affect the balance of the plant, and thusly only reduce a fraction of the cost of a reformer.
- This PI has suggested an extremely complicated and high-energy approach for the production of hydrogen and it is apparently based on simple ethanol reforming. It is not clear that there is any benefit over standard reforming technology. The proposed design (page 5) incorporates two membrane technologies that are still not

developed and using them in this combined approach is likely not practical. The temperatures required for these materials are too high for any general use. Although not specifically mentioned, there are other numerous material issues (for example seals) that will also be a problem with this approach. Costs were not specifically addressed but, with the exotic materials and complicated engineering approach, it is likely that this approach will never meet the DOE cost targets.

- Work is scattered in this project. The team needs to focus on the proof of concept (POC) experiments and the key data needed for economic evaluation.
- The team's approach is unique and for that reason may be pursued. However, the work on OTM has been extensive at ANL and future work extends quite a way out. This technology may simply be too complex to have a good hope for success.
- Although this project focuses on OTM, hydrogen transport membrane (HTM) is mentioned several times. It needs to be determined whether it is realistic to use two membranes, i.e., whether temperatures, gas compositions, etc. are matched in two membranes. The team needs to model an entire system.
- The project needs to carry out reforming at realistic conditions, i.e., air as oxygen source and varying steam ratios in fuel gas. The team's approach indicates good membrane expertise, but investigators need to learn more about reforming.
- This project ignores seal problems that typically kill membrane applications.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated **2.3** based on accomplishments.

- A technical accomplishment of this program is having/creating stable membranes for up to 1000 hours.
- This project's technical progress since beginning this work in 2005 has been minimal. Flux rates are still minimal and need to be improved. There is no information on the hydrogen membrane at this time. Temperatures are very high and need to be much lower (around 400°C) but, all the tests in this project are still at 700° 900°C. It is likely that the solid membranes will not function at this lower temperature. There has been little work on the reforming reaction. Only a gas phase conversion at high temperature, which produced a variety of products. This tends to suggest that it will probably not be possible to produce an alternate stream of high-purity/high-pressure CO₂, which is also a goal of this approach. The need to add more steam at this point is also a negative aspect that leads to increasing costs. Adding pure oxygen for the reforming. The concept of combining all these processes into one reactor is overly aggressive. In particular, expecting a single section of the reactor to allow oxygen ion recombination, ethanol reforming and hydrogen dissociation is not realistic all occur under different conditions. In addition, the work has not considered the effects of conducting an actual reaction, with heat and volume changes, near and in the OTM. These changes can be significant and result in destruction of the membrane (oxygen separation alone with no reaction is a much simpler system).
- The team's work has identified some minor improvements to the membrane structure.
- The chart on page 7 shows an average of 35% progress- this is troubling. Instead of focusing on the POC and data needed for concept evaluation, researchers seem to be working on improving the membrane.
- Some good progress has been made in improving the performance of the OTM.
- The rest of the project's milestones are far from being met.
- Considering the limited funding of this project, the team has had good progress.
- There needs to be a strategy to reduce byproducts in this project as well as a need to move to realistic reforming conditions as soon as possible.

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated **2.0** for technology transfer and collaboration.

- This project will benefit from collaborations mentioned in their future plans.
- The project has minimal outside collaboration and it is all academic or their sponsor. If this work is to ever get to some kind of scale-up or commercialization, there needs to be some industry perspective, and this is lacking.

- Collaboration does not seem to be the main thrust of this project. The most important collaboration is Directed Technologies, Inc. (DTI) to understand the project's targets and needs, and this collaboration does not appear to be well integrated.
- Collaboration with other institutions appears to be fairly minimal.
- Very little collaboration is seen in this project. The team needs to partner with someone who practices steam/autothermal reforming commercially to identify important issues.
- This project should also partner with sources for scale-up options.

Question 5: Approach to and relevance of proposed future research

This project was rated 2.2 for proposed future work.

- It is not apparent that this project has any clear direction and is primarily Edisonian in nature. The PI needs to establish clear targets, goals and milestones as well as document these accomplishments. In particular, the PI needs to develop a plan to define a reasonable operating target for the process. The temperatures suggested in the presentation for reasonable ethanol reforming are still too high (550°C, page 15) for an acceptable conversion process.
- The team needs to focus on POC and on data needed for economic evaluation.
- The proposed forward plan for the project extends too far to make an assessment.
- The project should have outlines a set of more quantifiable forward milestones.
- The team needs to settle on a membrane and focus on reforming.

Strengths and weaknesses

Strengths

- The team's skills with OTMs are a strength.
- The team's expertise in OTMs is a strength.
- The project has good OTM expertise.

Weaknesses

- The project's target production rate is not included in presentation.
- This project has a lack of focus. There is too much work on advancing OTM and not enough on critical program needs.
- The project has slow progress in other aspects of their work.
- The project is too nascent to provide a good H2A analysis.
- The team needs to focus on seals, reforming, and good modeling.

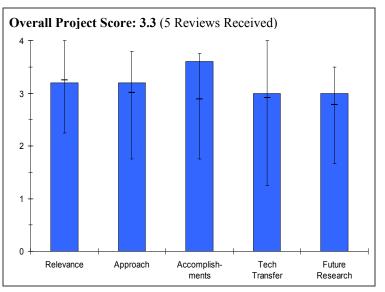
Specific recommendations and additions or deletions to the work scope

- The team needs to address the safety aspect of a failure of OTM resulting in rapid mixing of oxygen stream with ethanol.
- DOE needs to consider this as a fundamental study on solid oxide "oxygen" transport membranes and, if work is to be conducted, the work should focus on improving oxygen flux from air. This work has been ongoing for some time with little advancement. Adding complications such as reforming is not benefiting this development. In addition, DOE should not be expecting any breakthroughs, even minor. in the near future.
- This project feels like it is using technology in search of an application. That is, using the cover of an ethanol to find a hydrogen application because this was and area where funding was available to continue base advancement of the OTM membrane. DOE needs to focus this group on getting the critical data needed to identify if the use of this application makes any sense or choose to advance the membrane for its own sake.
- At some point, module-scale modeling will probably be needed to understand the potential hydrogen pressure that might be achieved.

Project # PD-06: Zeolite Membrane Reactor for Water-Gas-Shift Reaction for Hydrogen Production *Jerry Y.S. Lin, Henk Verweij, Peter Smirniotis, and Junhang Dong; University of Cincinnati*

Brief Summary of Project

The overall objective of this project is a fundamental study for the development of a chemically and thermally stable zeolite membrane reactor for water-gas shift reaction for hydrogen production. The specific project objectives are the 1) synthesis and characterization of chemically and thermally stable silicalite membranes; 2) experimental and theoretical study of gas permeation and separation properties of the silicalite membranes; 3) hydrothermal synthesis of tubular silicalite membranes and gas separation study; and 4) experimental and modeling study of membrane reactor for water-gas shift reaction.



Question 1: Relevance to overall DOE objectives

This project earned a score of 3.2 for its relevance to DOE objectives.

- The project's lower reactor costs support DOE objectives.
- This is a standard zeolite modification project that attempts to develop a hydrogen separation membrane. It is unlikely that this approach will ever meet the DOE purity targets whether separation is based on size or preferential adsorption. In either case the H₂ purity will be low.
- The only concern for this project is that membranes fundamentally give hydrogen at low pressure, which is a poor fit with hydrogen manufacturer (or distribution). However, this project could be a very good fit to a coupled reforming/fuel cell, which could be appealing in power cycles or home combined heat and power (CHP).
- The project's H₂ purification from water-gas shift (WGS) reaction through a membrane is useful technology but not game-changing.

Question 2: Approach to performing the research and development

This project was rated **3.2** on its approach.

- Chemical Vapor Deposition (CVD) of Silica to narrow pores.
- The project is focusing on modifying the exposed surface pore sizes. This may improve separation and it is a reasonable effort for and academic project.
- The team should have a more explicit description of its approach, but its steps to (1) make the membrane work; (2) make the WGS cat work; and then (3) put them together was outstanding.
- It is not clear why sulfur tolerance is required or was tested in this project. Presumably sulfur would have been removed upstream prior to the reformer step.
- This is primarily a membrane development project, which is an appropriate focus but is not broad enough in scope.
- The project's pore decoration approach to tailoring pore size is a good approach.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated **3.6** based on accomplishments.

- Tubular reactor tested for one week.
- The team's work has produced some interesting results. Slide 12 suggests that the purity can be improved (for whatever reason which is not clear). In addition, there appears to be evidence that there is some sulfur tolerance with the catalyst materials being developed. These are all good achievements for a project of this nature.
- The project's objectives are quantitatively stated and achieved.
- It is noted that the quantitation of objectives is taken from page 4, which is not actually described as the target for the project. This should be more explicit.
- It would have been good for the team to show thermodynamic equilibrium of the WGS reaction under the conditions tested (slide 17).
- Progress in membrane improvement through constricting pore opening is a reasonable approach in this project. It would be interesting to know if large scale synthesis if uniform membrane materials is economic.
- The project has great selectivity for zeolite membrane. There is a need to know selectivity for H₂/H₂S in membrane.
- Does the statement "Chemically stable in H₂S, thermally stable at ~400°C" mean that membrane is stable in H₂S at 400°C? The report also mentions a one month stability. Is degradation being seen after one month, or is this just the maximum time tested?

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated **3.0** for technology transfer and collaboration.

- This project's University focus could be improved by increasing collaborations with industries.
- The PI's have put together a well qualified team and have included an industrial perspective for the work (page 19). This is a good collaborative effort between three universities.
- The team's work highlights critical accomplishments by partners (Si CVD of zeolites) on pg 12-13.
- The project seems to have good collaboration with OSU on modifying porosity.
- This is mostly pretty fundamental work.
- More attention to overall energy balances is needed assuming this is a steam methane reforming reaction followed by WGS and membrane.
- Also, partners that provide more of the business possibilities and process sense would be recommended for this project.
- This project needs industrial collaboration to determine if the membrane is commercially feasible and also needs to look at costs.

Question 5: Approach to and relevance of proposed future research

This project was rated **3.0** for proposed future work.

- Benefits of a combined sulfur tolerant catalyst and the separation capability of hydrogen to be demonstrated on long term study is seen in this project.
- The project's future plans are reasonable and appropriate. This project has shown some promise with the recent technical advances and the future work will build on these accomplishments. This is a good project and approach for a collaborative university effort.
- All proposed items by the project team are excellent, however there is a need to focus on: (1) proof of concept which is subsequently needed for combined membrane & catalyst; and (2) advances beyond this proof need to be economically driven. What are the features that need to be improved to make the technology attractive?
- The project appears to have a reasonable technical forward plan. It would be good to know the metrics that are being aimed for in future work and to get an estimate of H₂ delivery costs as well as what assumptions are made to define that cost.
- Why is this project doing disk membranes?
- This project should get an industrial partner (Pall?) to work with regarding cost issues.

Strengths and weaknesses

Strengths

- This project has had some good technical success and provided some interesting gas separation results. This is a project that is worth future funding at a reasonable level.
- This project shows superb collaboration, clear targets, good science and execution.
- This project has a good membrane development team.

Weaknesses

- This project's economics should be completed to determine if this reactor product (~94%) would result in reduced PSA costs for purity required for fuel cell use.
- This project's low WGS pressure as well as uncertainty that comes from the unknowns of combining the WGS with the membrane can be a weakness.
- The team might gain from more catalysis focus and a commercialization partner.

Specific recommendations and additions or deletions to the work scope

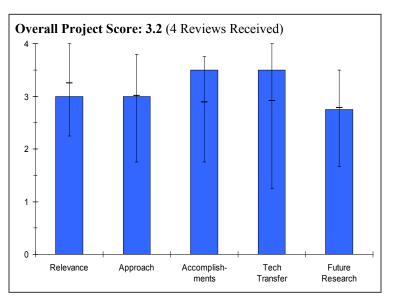
• In this project it would be beneficial to see if the mechanism for separation could be determined. Separation by size is actually very unlikely. These molecules are mostly space and, even though the kinetic diameters appear somewhat different, these molecules are basically the same size. It is not clear if the surface modification changed the adsorption capability of both CO₂ and H₂, but this is a possibility. It does not appear to be simply Knudsen diffusion as the CO₂ permeance appears to go to almost zero. The research has provided a good opportunity to study the mechanism for gas separation in these modified materials which would be a good project for a Ph.D. student.

Project # PD-07: High-Performance, Durable, Palladium Alloy Membrane for Hydrogen Separation and Purification

Jim Acquaviva; Pall Corporation

Brief Summary of Project

The objective of this project is the development, demonstration and economic analysis of a Pd-alloy membrane that enables the production of 99.99% pure hydrogen from reformed natural gas at a cost of \$2-3/gge by 2010. The objectives for the past year were to 1) fabricate a series of membranes covering a specific range of alloy composition and functional layer thickness; 2) optimize the membrane formation process; 3) test the membranes in pure gas streams prior to water-gas shift (WGS) testing; 4) complete the equipment needed for extended WGS testing; 5) obtain initial WGS test results; and 6) initiate the techno-economic modeling as soon as the combined membrane reactor model is available from Directed Technologies.



Question 1: Relevance to overall DOE objectives

This project earned a score of **3.0** for its relevance to DOE objectives.

- This project is very relevant towards the goal of making hydrogen for fuel cells and storage.
- This project is directly addressing the DOE targets for hydrogen production. They are developing supported Pd and Pd alloy membranes on a porous support. This work, and recent work by other researchers, has indicated that this approach can meet the DOE targets (as presented in Slide 5).
- The project aligns with DOE Hydrogen Production element needs by developing and demonstrating a costeffective Pd-based hydrogen separation membrane. The Pall Corporation is well aware of DOE's targets and barriers.

Question 2: Approach to performing the research and development

This project was rated **3.0** on its approach.

- This project has an adequate approach to perform research and development.
- The project's coating method looked good, and alloy choice was okay, but might be too expensive. The project should also attempt to look at membranes with some of the Au replaced by Ag. A membrane with 15% Ag and 5% Au might be expected to have more flux and durability than one with 11% Au and also may cost less. More effort should be put into durability issues like resistance to cycling and start up.
- This project is a standard Pd/Pd alloy membrane development approach. It is a reasonable approach for metallic membrane development. The researchers appear well aware of the standard problems and are working to correct and improve on these issues.
- The team's work has provided a good compact design for a membrane unit capable of producing 100 kg/day hydrogen. This is a big benefit in that scale-up to larger sizes will only require addition of these compact units. Cost estimates appear reasonable and within DOE goals and targets.
- The project and team's approach is sound and straightforward, starting from development of a thin-film Pdbased membrane supported on a substrate, to experimental evaluation of hydrogen separation/purification from reformate gases. In the project objective slide, the program shifts the feedstock from the natural gas reformate

(in 2008 AMR meeting) to the ethanol reformate (this year AMR meeting). Pall should address justification of the change and effects of changes, from the standpoint of the cost of feedstock, compositions of reformates, and impurity on the membrane performance and cost of hydrogen.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated **3.5** based on accomplishments.

- It is hard to evaluate the technical accomplishments in this project because the fundamentals of the process were not presented.
- This project seemed to have achieved most if not all of their goals. They claim to be making progress with quality control, and cycling. More work on these issues is needed. Funding for this project should be kept.
- The team's work has shown some good technical progress. Flux rates are good (200 300 scfh/ft²) and this includes tests with mix gas (including steam). This was the next step in developing these materials (it was time to move beyond pure gas diffusion). The work has had good success and will likely improve in the next year. This project has also demonstrated good stability of the membranes over moderate time frames (slide 19 approximately 100 hours). In addition, the work has demonstrated the ability to produce constant thickness pure and alloy membranes on the 1 3 micron level.
- The Pall Corporation did a great job on reducing the membrane cost while achieving a high H₂ flux goal. Pall also did excellent job on scaling tubes to 12 inches long. The durability test of 100 hours is much shorter than the target of 2 years. It would be much more informative if the project shows the optimum alloy thickness and Au content based on the lab results.

<u>Ouestion 4: Technology transfer/collaborations with industry, universities and other laboratories</u>

This project was rated **3.5** for technology transfer and collaboration.

- The project team has good collaborations with prestigious institutions.
- This team is working with all the right people.
- The research team is adequate and includes a university, national lab and industry entity. The team is well qualified and has the expertise to further develop these membrane materials.
- This project has a good team involving industry and academics.

Question 5: Approach to and relevance of proposed future research

This project was rated 2.8 for proposed future work.

- This project has a good sequence of planned activities.
- The team did not present a particularly clear sense of where they hoped to go next.
- The future direction for this project is reasonable and appears to be following the original work plan. The work appears to be on schedule and within budget. It also appears to be a well managed effort with clear targets and milestones.
- The project work for next year should include testing in the presence of sulfur or other impurities. Impurities could "kill" the membranes and their effect needs to be determined in the near future. Also, additional improvements that are necessary or if the impurity effects are so severe that these membranes will not be able to be used for H₂ separation need to be determined.
- This is a good project worth continuing.
- The project's future work to evaluate the membrane durability, membrane formation process improvement, device operating procedure development, testing matrix, and techno-economic analysis refinement, are very sound. The program should also investigate the effects of feedstock impurity and hydrogen embrittlement of the membrane, and possible solutions.

Strengths and weaknesses

Strengths

- This project has good collaborations and plans.
- This project is relevant, well done and has good results.
- The team has achieved good technical accomplishments during the past year. This appears to be a good project that could meet the DOE targets and is work worth continuing.
- The project has good membrane fabrication capability though the yield rate and thin film quality are unknown.
- Good collaboration among teams is seen.
- This project provides a great means to produce hydrogen with high purity.

Weaknesses

- There is very weak project rationale and the team needs to consider how this could make sense.
- More needs to be done in this project and the team did not present a particularly clear road-map for the future.
- In this project no weaknesses were identified.
- This project lacks study on the feedstock impurity effects on the membrane performance.
- It is unclear if this project is applicable to H₂ central production.
- The lack of information on the hydrogen embrittlement issue and Pd-based alloy coarsening issue after a long period of operation is apparent in this project.

- The team should work with modelers to try to evaluate under what conditions this project would make sense.
- The team should consider looking at membranes with some of the gold replaced by silver. There is a need for more effort to be put into durability issues like resistance to cycling and start up. More work should be done with Doug Way, employing his electrolysis techniques.
- The team needs to address the quality assurance plan for membrane fabrication.
- Membrane durability/life and impurity tolerance are the two key factors to be addressed in this project.

Project # PD-08: Solar Cadmium Hydrogen Production Cycle

Bunsen Wong, Lloyd Brown, and Bob Buckingham; General Atomics Roger Rennels and Yitung Chen; University of Nevada, Las Vegas

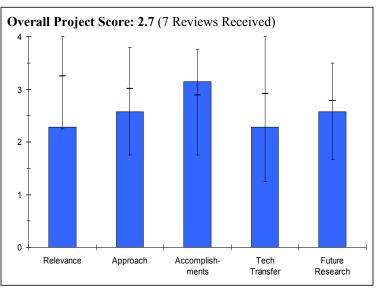
Brief Summary of Project

The overall objective of this project is to demonstrate the feasibility and economics of a solar cadmium hydrogen cycle. Objectives are to 1) validate the key reaction steps with experiments; 2) establish design concepts for process steps based on experimental data; and 3) integrate process design concepts and solar field design into a flowsheet for a solar hydrogen plant.

<u>Question 1: Relevance to overall DOE</u> <u>objectives</u>

This project earned a score of **2.3** for its relevance to DOE objectives.

• This program has taken a different



- direction and this technology is on a different path to the program's goals.
- The objective of this project is to show the feasibility and economics of a solar cadmium cycle for hydrogen production, and therefore, this project supports the Hydrogen Program. There are several (over 140 thermo-chemical cycles investigated since 1955 but the question remains- why this Cd cycle? Is there anything new and exciting here? The uniqueness of this proposed Cd cycle project is not explained. In what way is this cycle better than the 140+ other cycles already investigated?
- The project's big picture "solar to H_2 " is very good.
- A \$3/kg target for H₂ manufacturer out in the middle of the desert is an economic challenge, and this is well above that.
- The project's concept of hydrogen production using solar driven processes pertains to the DOE Fuel Cells Subprogram.
- The project's use of such a dangerous and toxic material in such large volumes may not be feasible. It is not clear that this project would pass an environmental impact review or if the local community would accept it due to toxicity concerns. They should focus on materials with lower toxicity.
- The project addresses renewable hydrogen with solar.
- This project has significant health consequences and challenges of design during scaling up of the design. The project should be evaluated for hazards, and in this reviewer's estimate, it won't be a safe and feasible system. Cadmium has been banned by many nations, as it is a highly toxic and carcinogenic material. This process requires large quantities of the material while using very large, complex and difficult to seal environment.
- This project supports DOE goals for hydrogen production by thermochemical means but because of the high temperature of the main reaction and the need for high-flux solar, it is restricted in its applications.

Question 2: Approach to performing the research and development

This project was rated **2.6** on its approach.

- The project has a good approach.
- CdO decomposition, Cd vapor quenching, and hydrogen production are key steps for hydrogen production. Decomposition of CdO is going to be studied using a number of carrier gases. It is not clear how the decomposition rate is influenced by the carrier gas.
- The project is well focused on proof of concept (POC) demonstration and on key measurements needed to complete H2A guidance.

- The team fails to address a major barrier to this process which is toxicity.
- The team's examination of the reactions rates was effective.
- The project needs more work, perhaps modeling, to validate the rapid quench assumption. This seems to be a critical part of the process and should be further studied.
- The project is very high risk using so many novel, untested technologies.
- There needs to be testing the specific pieces of the scheme at larger scale.
- There is a need for clarification regarding how process steam is generated at night.
- Regarding the solar collector: how do cross beams reduce solar flux and utilization?
- Regarding air use: how does the team plan on handling entrained cadmium in emissions? Nitrogen would be effluent even under stoichiometric conditions.
- Regarding reaction time on CdO regeneration, the team should consider catalyzing this process or using a substrate to improve transport limitations of the process. The reaction appears to be equilibrium or kinetically limited. The team may want to look for promoters or catalysts.
- The project's need for a carrier gas is a handicap that impacts efficiency. The use of air as a carrier gas introduced problems with back reaction. The need for a quench to recover the cadmium is also an inefficiency that effectively eliminates a pathway for heat recovery.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated 3.1 based on accomplishments.

- The project team demonstrated the CdO decomposition at temperatures less than 1150°C. They also studied the effect of carrier gas on decomposition rate and found air is the best carrier gas. The team also demonstrated two pathways to use either molten or solid Cd to produce hydrogen. Progress is being made in modeling of Cd vapor quench.
- The project has done an extensive demonstration of POC.
- The team has acquired key data for economic analysis.
- The team has enabled/completed economic analysis
- The development of the thermogravimetric analyzer (TGA) in this project to measure oxygen reaction rates at the high temperatures was a significant accomplishment which can be applied to other systems.
- The reactor design in this project was very innovative.
- The cost analysis in this project uses unrealistic numbers and still cannot achieve the \$2-3/kg hydrogen cost target. For example, the heliostat costs are much too low.
- The CdO Cycle appears to be well characterized by the team.
- Significant experimental progress has been made in the laboratory especially with regard to producing hydrogen via steam oxidation of molten cadmium. However, yields are low and it is not clear that the introduction of a tumbling reactor filled with ceramic media can be supported by the energy budget. Rotating equipment filled with media are power hogs.

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated **2.3** for technology transfer and collaboration.

- The team is collaborating with the University of Nevada, Las Vegas (UNLV). The required slide explaining the collaboration was not presented or included in the package, and therefore what was done under this collaboration is not clear.
- My belief, from previous exposure, is that their collaboration may be outstanding, but the PI did not highlight who is doing what pieces.
- The working relationship between UNLV and General Atomics seem good.
- No collaborations were listed.
- While collaborations are satisfactory, it is clear that a more practical design is required for the solar reactor. The design showing a fluidized bed at the bottom and Cd vapor recovery via quenching at the top offers too much opportunity for the back reaction to occur. The CdO decomposition step and the quenching step should occur

very close in both space and time. A team member with capabilities to design a simple solar receiver needs to be added. The current design is too complex.

Question 5: Approach to and relevance of proposed future research

This project was rated **2.6** for proposed future work.

- The team may want to redirect work since program goals have changed.
- The project's CdO decomposition using a simulated solar source will be done in the future. The Cd-O₂ reaction is very important and therefore the PI is planning to study the effect of quench rate on recombination reaction.
- Given economics that are well above target, there is a need to engage some kind of limit analysis or process brainstorm to identify what (if anything) could possibly change to enable a step change in the cost. Then focus R&D in those areas in this project.
- The team's future plans should include identifying a critical path for development which will enable the technology to achieve the cost targets. The project does not seem focused. Identifying the critical path will help the PI focus the work to the most important areas.
- In this project, additional work on quenching should be done.
- Questions regarding relative sizing of solar collector vs. thermal storage, i.e., how much thermal storage is there, one day, one week, how does storage size impact collector costs, when system shuts down, and how long and expensive to start up should be considered.
- The team should create an Aspen-like process model including all equipment such as heat exchangers, pumps, etc., and project cost.
- Future work needs to address a simpler less energy intensive method for the hydrogen production step. Future work should also address a simpler design for a solar receiver.

Strengths and weaknesses

Strengths

- The team completed a preliminary flow design for the solar Cd cycle and studied the Cd-O₂ reaction rate. The PI seems to love the thermochemical reaction cycles. General Atomics is well known for its effort in developing thermochemical reaction cycles for hydrogen production.
- This is a beautifully executed program with focus on POC and key data for economic analysis (would hire these guys again in a heartbeat).
- The chemical cycle selected can store the activated Cd enabling 24 hour hydrogen production.
- General Atomics has a great deal of experience in chemical cycles.
- This cycle, relative to the others, has the potential for high efficiency.
- The project's two step reaction is among the greatest strengths. The use of a molten metal in the hydrogen production step is also a plus. The dark color of the CdO at high temperature is also a plus that allows for direct interaction between the solar flux and the reactant.

Weaknesses

- Economic analysis using helium as a carrier gas is questionable when the experiments have shown that air is the best carrier gas. It is wrong to use 1% back reaction rate for the economic analysis when the experiments are showing back reaction rates as high as 30 percent. The question remains: is this done because the economic analysis look good if a 1% back reaction is used? Also, how difficult is to pump liquid Cd and are there pumps to do this job?
- This specific technology in this project is emerging as just too expensive.
- The cadmium is very toxic in this project.
- The team's cost analysis shows the hydrogen cost targets could not be achieved even with the optimistic assumptions.
- Safety practices and assumptions in this project need to be externally verified.
- There is a very serious concern about the safety of this project, and questions of if the risks justify the rewards perceived.
- The high temperature required for the CdO decomposition step limits the available heat sources to high-temperature solar and, as experts in solar receiver design will explain, the higher the temperature of the main

reaction, the less efficient the solar receiver. The use of rotating equipment filled with ceramic media will reduce the overall energy efficiency due to frictional losses.

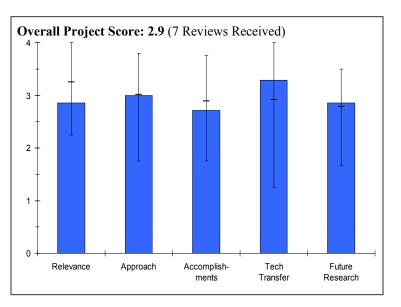
- The team should delete the analysis using He as a carrier gas unless advantages of using He is clearly explained. They should modify the economic analysis using more realistic figures for the back reactions. Questions regarding the toxicity of Cd, in particular Cd vapor, still remain.
- As discussed above, the need to identify if there are potential step-outs that could make step-changes in the economics.
- It is recommended that the team examine a different chemical cycle.
- The team should look at nitrogen as quench gas as it is much cheaper than helium and less prone to leakage. They should go ahead with engineering hazard analysis. With such a complex process involving reducing gases, solid transport, and hydrogen, it's never too early to look for problems.
- The project should place more effort on design of the solar receiver.
- The team should replace the rotating machinery with an alternative approach to producing hydrogen from liquid metal.

Project # PD-09: Solar High-Temperature Water-Splitting Cycle with Quantum Boost

Ali T-Raissi, C. Huang, N.Z. Muradov, S. Fenton, P Choi, D.L. Block, and J. Baik; Florida Solar Energy Center Robin Taylor and Roger Davenport; Science Applications International Corp. David Genders; Electrosynthesis Company, Inc.

Brief Summary of Project

The objectives of this project are to 1) evaluate photo/thermo-chemical water splitting cycles that employ the visible portion of the solar spectrum for production of hydrogen; 2) select a cycle that has the best potential for cost-effective production of hydrogen from water DOE target of \$3.00/kg H2); 3) demonstrate technical feasibility of the selected cycle using solar input in a bench-scale reactor; 4) demonstrate pre-commercial feasibility via a fully integrated pilot-scale solar hydrogen production system; and 5) perform economic analysis of the selected cycle.



Question 1: Relevance to overall DOE objectives

This project earned a score of 2.9 for its relevance to DOE objectives.

- This is a good project.
- The focus of this project is to conduct research on a new sulfur family of thermochemical water splitting cycle for large-scale hydrogen production using solar energy. More specially, the goal of this project is to evaluate the sulfur-ammonia (SA) water splitting cycle. This project is relevant to the DOE Hydrogen Program.
- The project's solar driven thermochemical cycles aligns with the Hydrogen Program RD&D objectives.
- DOE's MYPP indicates that the Solar Program will be reducing heliostat costs. It is unclear why this project is examining that aspect. It seems that improving the chemical process is enough scope.
- This seems like a complex process to produce H₂ to meet the DOE targets. The solar thermochemical cycle proved uneconomic and it is not clear how adding an electrochemical piece will make it cheaper. What assumptions were made to reach that conclusion?
- The researchers have done a very good job at determining the performance and potential economics of this system. However, this does not seem to be in line with the process requirements for the DOE targets.
- The overall goal of producing hydrogen using thermochemical methods is satisfactory in this project. However, as originally conceived, the splitting of the solar beam is too complex to be practical at high throughputs.
- The project fully supports the intent of the Hydrogen Program. The PI acknowledges that the cost objectives will be challenging, but possible, to meet.

Question 2: Approach to performing the research and development

This project was rated **3.0** on its approach.

- The project's approach was not explained clearly. What is RY'09 stand for? RY'09 appears in two slides describing this project's objectives. It is not clear why two schemes (photocatalytic & electrolytic) are evaluated for hydrogen production. Did the PI do a down-selection in previous year to come up with these two schemes?
- The PI exhibited flexibility in changing their approach when it became clear that their original approach would not be able to achieve the cost goals.
- The PI worked on heliostat cost reduction when the Hydrogen Program MYPP indicated that the Solar Program will be working on heliostat cost reduction.

- The project's shift to change from a purely solar driven process to a hybrid process was a good decision.
- The honest comment that the solar cycle approach is unlikely to meet targets and was down-selected was appreciated. Much of the project's work done on the solar thermochemical is now converting to the electrochemical + thermochemical cycle and little data is available to assess its promise.
- The project has a very creative idea for spectrum splitting. The concept appears to make more favorable economics of the design.
- The initial combined photochemical/thermochemical approach, which was novel and interesting, was abandoned in favor of a hybrid thermochemical/electrochemical approach and that was then modified to include a molten salt step. This project has gone off track and now has the flavor of a project aimed at screening different thermochemical cycles. The novel aspect was the combination of a photochemical step and a thermochemical step. Abandoning the photochemical step has placed this cycle in competition with other cycles that are simpler and have been under investigation longer. It is not clear that the latest embodiment has any advantage over what's gone before.
- The presentation delineated all barriers and how they are being addressed. Novel approaches are being utilized to address the most critical barriers in this project.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated 2.7 based on accomplishments.

- The project's technical progress appears to be good but the costs of electrodes may prohibit feasibility.
- The photoreactor system was evaluated in this project. The central receiver system was optimized to deliver energy. The team has completed the half-scale prototype glass reinforced heliostat and demonstrated drive system features and controls.
- The team's work on the electrochemical aspect of the project was appropriate.
- The PI was working on heliostat which the Hydrogen Program MYPP indicates is the responsibility of the Solar Program.
- Changing to potassium from zinc and eliminating the solids was a positive development of this project.
- The team needs to continue decreasing the cell potential of the electrolyzer.
- There has been only fair progress toward meeting goals, given the shift in project focus. Many unanswered questions remain.
- There are problems with 24/7 operation given solar availability.
- Modest progress has been made in this project. However, some barriers appear to have been neglected. In the chemical equations, aqueous ammonium sulfate is shown being produced in one step but solid ammonium sulfate is used in the subsequent step. How did this go from an aqueous solution to solid material? There have been a number of sulfate cycles proposed over the years and every one of them suffered a large energy penalty associated with the recovery of the solid sulfate from an aqueous solution. This was not addressed in the presentation nor the slides and can be a real show stopper if it is necessary to boil off excess water. This needs to be addressed.
- Significant progress has been made on production and efficiency targets, but it is not clear if the cost barrier can be overcome in this project.

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated **3.3** for technology transfer and collaboration.

- The project has used a good variety of partners with diverse interest levels.
- SAIC is the lead in this project. Electrosynthesis Company, Inc is the industrial partner. Their collaborative roles are defined in this project.
- The project appears to have a strong team with good interaction.
- It appears that the project has a reasonable set of collaborators.
- This is a good team collaboration with the solar and electrochemistry experience necessary for the project's success.
- Good collaboration among team members is providing new approaches to solve problems.

FY 2009 Merit Review and Peer Evaluation Report

<u>Ouestion 5: Approach to and relevance of proposed future research</u>

This project was rated 2.9 for proposed future work.

- The project is not slated for future funding, although results so far appear promising.
- The PI had too many slides in his presentation.
- The team is focusing on the important aspects of the process.
- The forward plan for this project is very general and does not seem to specifically address key challenges.
- The project's proposed work is too heavily weighted toward solar receiver development considering the early stage of development of the chemistry. More effort needs to address the electrochemical cell and getting current density up and voltage down. For all practical purposes, this cycle is now in competition with the hybrid sulfur (HyS) cycle and so needs to show equal or better operational parameters for the electrochemical cell, than the HyS electrochemical cell, for this cycle to be considered competitive.
- Barriers are clearly identified and are being addressed by the team.

Strengths and weaknesses

Strengths

- The team members seem to know what they are doing.
- The PI has shown great flexibility in changing their approach in order to reduce cost.
- They have a strong team.
- Project execution is very thorough and clean. This team has done very good work.
- This project has a good team.
- Continued innovation has led to improvements in this project.

Weaknesses

- The efficiency of this process can not be high. It can only be in the range of about 22 percent. The ammonia and sulfur cycle has been well studied for several decades and others have proven that it is a difficult process to optimize and get better efficiency. The question remains: why are these investigators going back to this cycle?
- The PI had too many slides (35 slides) for a 20-minute presentation. The presenter did not have time to explain the collaborations and the future plans. This talk was poorly organized.
- A hybrid cycle requires electricity which will need to be generated on-site or brought in from the grid. In order to achieve 24/7 operation, as the PI indicated was a goal, they will need to be connected to the grid.
- The cost figures assume operation in the desert and therefore underestimate the cost of water and permitting (mostly the water rights cost). It is unlikely that the team would be able to get the water rights for this system in an area which has very little water available.
- This project deals with a complex process with many hurdles remaining. This does not seem to rank at the top of the thermochemical projects.
- The project has too many steps in the cycle requiring a separate reactor.
- The project has too many different chemical reagents needed in its latest embodiment; zinc, potassium, and ammonium sulfates. The HyS cycle uses only one, that being sulfuric acid.
- Much work needs to be done on the electrochemistry of this project.

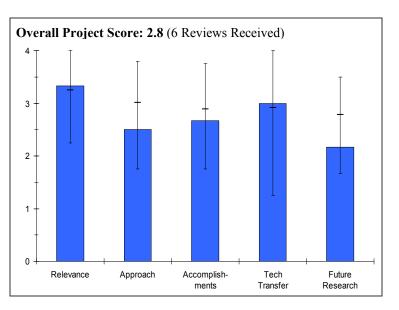
- The sulfur ammonia cycle has been researched for several decades and proven to be difficult to optimize. This project should be dropped.
- The heliostat work is needed, but not sure if this is the right project for it. The Hydrogen Program has very little resources. Those resources should be focused on developing the chemical cycle and not the heliostat. The Solar Program's budget request is very large and they should have enough resources to address the heliostat costs.
- The team should identify the critical path which would enable the technology to become economically as well as technically viable.
- The team should carry out the proposed plan expeditiously. The team should hone down on the real technical challenges.
- The solar receiver work can wait. The team should solve the problems with the electrochemical cell first.

Project # PD-10: Solar-Thermal Ferrite-Based Water Splitting Cycles

Alan W. Weimer, Jonathan Scheffe, and Melinda M. Channel; University of Colorado, Boulder

Brief Summary of Project

The objective of this project is to research and develop a cost effective manganese (III) oxide/ manganese (II) oxide (Mn_2O_3/MnO) solar-thermal thermochemical cycle through theoretical and experimental investigation. Additionally, based on the previous, the University of Colorado will develop a process flow diagram and carry out an economic analysis of the best process option. A reaction mechanism has been hypothesized for Mn_2O_3 dissociation. Mixed manganese oxides have been shown to improve the product recovery steps. Experimental investigation using a mixed manganese oxide is ongoing.



<u>Ouestion 1: Relevance to overall DOE</u> <u>objectives</u>

This project earned a score of 3.3 for its relevance to DOE objectives.

- The project's big picture of solar to H₂ is okay, but concerns about the relevance of a process with a target cost of \$4/kg at plant gate out in the dessert remain.
- The basis of this project being solar driven thermochemical processes is relevant to the DOE Hydrogen Program.
- The project's process attempts to use a potentially low-cost substrate.
- This project is relevant for turning high-temperature heat available from a solar receiver into hydrogen. However, it is not compatible with high-temperature nuclear.
- The project fully supports the Hydrogen Program objectives for solar thermochemical hydrogen production.

Question 2: Approach to performing the research and development

This project was rated **2.5** on its approach.

- If the project's economic basis is unsupported ferrite, then the proof of concept (POC) should be done to measure conversion levels with unsupported ferrite. If materials basis is the atomic layer deposition (ALD) (which is <5% ferrite), then the economics need to be evaluated assuming that all that carrier (95%) is going through the solar furnace absorbing heat. This is a major weakness of the project's approach.
- The team is using less toxic materials than other cycles.
- The project's operating temperature of less than 1300°C has some materials which can work compared to other cycles which require temperatures greater than 1500°C.
- The ALD approach to fabrication may be very expensive considering the quantity that is required for this project.
- The team needs to increase the cycle life testing.
- For this to be economical, the process needs to operate 24/7 which will require activated material storage, without the material deactivating. This needs to be studied and should be prominent in the scope of the project.
- The project's ferrite cycle appears promising.
- The project calls for hundreds (thousands?) of cycles to assure particle integrity.
- Was thermal storage for night operation considered in economics calculations? Project costs need a more detailed break down.

- Energy storage is not addressed in this project. The question remains: how does this process work around the clock?
- Is 1200°-1400°C a realistic temperature range for this project? Has this been demonstrated or projected from a laboratory project?
- The project's approach is good with respect to using a small number of steps to accomplish hydrogen production. It is handicapped, however, in that it requires the transport and handling of solid materials, as opposed to liquids and gases as are typical of other cycles. It also is limited by the need to remove oxygen under vacuum.
- The project focused on a narrow scope of materials science objectives.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated 2.7 based on accomplishments.

- The team's description of the objectives is superficial at best, therefore measurement against objectives is nearly impossible. Furthermore, if there is a general need is for some POC within an economic framework, then there is a total disconnect here as the economic guidance materials are different from research materials in a way that is critical to the analysis.
- For the economic analysis the team should not assume that an oxygen credit and the capital cost seems too low (especially for the heliostats). This analysis should be re-done.
- Initial tests in this project are well done.
- This project requires more cycle and lifetime tests are needed, especially for the ALD coated substrates.
- Good work was done by the team in evaluating ferrites.
- ALD shows improved kinetics in this project.
- ZrO₂ is not addressed in the ASPEN model. The team should show how substrate thermal cycling affects the process.
- What is the degradation mechanism or hypothesis of what is causing the degradation in this project. What can be done to address this degradation?
- Good technical progress is shown in this project but more thought should be placed in the design of a solar receiver able to do large scale throughput. A relatively simple design for a solar receiver was shown, suitable for proof of concept but not a design conducive for high throughput in this project.
- Progress is being made in addressing materials and cost barriers for this project. The solar field design appears to be specified but not validated.

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated **3.0** for technology transfer and collaboration.

- The project team's collaborations are mentioned at the end of the presentation but there is no indication of how they fit into the critical progress of the program.
- The project team has strong interactions both nationally and internationally.
- The team has good publications regarding this project.
- This project can improve by including an engineering partner with experience with large projects to better estimate costs.
- This is a good team but needs U.S. collaborators.
- This is a good team and strong collaborations are evident.

Question 5: Approach to and relevance of proposed future research

This project was rated **2.2** for proposed future work.

• All the project plans are ALD, but all the economics are based on unsupported ferrite and require high (35%) conversion. This is a total mismatch because the solar field is a key cost, and ALD materials require solar energy to be wasted heating the >95% carrier. The project should not continue until this mismatch is resolved.

- The team needs to increase the cycle life studies.
- The PI needs to include work on how the team will enable 24 hour operation. This can be achieved by thermal storage or activated material storage. This should be a major focus of the work. Without 24 hour operation it is extremely unlikely that the process will be able to achieve the DOE cost targets.
- The project should concentrate on stability of materials upon multiple cycling.
- The team should include attrition testing for moving bed work.
- Proposed work with zinc looks promising in this project.
- It is not clear how future work identified is aimed at overcoming barriers.

Strengths and weaknesses

Strengths

- This project has a cycle that contains and uses less expensive materials and less toxic materials compared to other cycles.
- This project may be able to operate 24/7, but the project team needs to verify this claim.
- This project uses simple chemistry and has well defined reactions.

Weaknesses

- The ALD is not just an issue of particle cost and needs to be addressed.
- High utilization of solar flux is critical for this project because the heliostat field is very expensive. The use of solar flux to heat carrier must be included in the economics. Proposing high-carrier solids while doing economics on zero-carrier solids is not unacceptable for this project.
- The cost assumptions in this project presume that cheap water is available in the desert. The water rights and water cost in arid regions are much more difficult and expensive to attain than what is assumed in the economic models.
- The team needs to demonstrate that their coated substrates will not disintegrate.
- The assumption that ALD can be economical at the scale of production that is required needs to be validated by the team.
- The team has not included enough studies on 24/7 operation.
- The team has not presented a critical path which leads to achieve the technical and economic DOE targets.
- The project and team needs a support for the ferrite to make this work well.

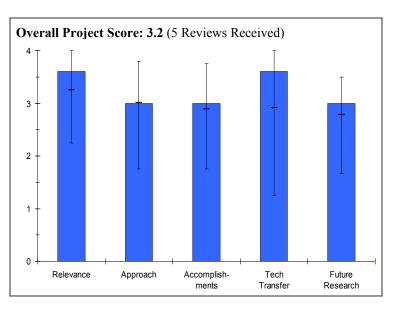
- This project needs cycle life testing to validate that the team can use the supported material.
- The team needs to identify a critical path which will enable the pathway to meet the technical and economic DOE Targets.
- Further work in this project is recommended to addresses how the proposed reaction can be accomplished in a high throughput reactor.

Project # PD-11: R&D Status for the Cu-Cl Thermochemical Cycle

Michele Lewis; Argonne National Laboratory

Brief Summary of Project

The objective of this project is to develop a commercially viable process for producing hydrogen based on a thermochemical cycle that meets the DOE cost and efficiency targets. The Cu-Cl cycle was chosen and the current Aspen flowsheet indicates that it is possible to meet the targets if assumptions can be validated. Features that promote meeting targets include: 1) the 550°C maximum temperature reduces demands on materials; 2) yields near 100% in hydrolysis and oxychloride decomposition without catalysts (no recycle streams in these reactions); 3) conceptual process design uses commercially practiced processes; and 4) preliminary H2A analysis indicates H₂ production costs are within range of 2025 target if assumptions validated.



Question 1: Relevance to overall DOE objectives

This project earned a score of **3.6** for its relevance to DOE objectives.

- This project has both nuclear and solar sources of heat that are relevant to DOE's program goals.
- The project's thermochemical water splitting aspect supports the Fuel Cells Subprogram objectives.
- This is another thermochemical cycle-based project co-funded by DOE, EERE and the Office of Nuclear Energy (NE). It appears to have the potential to meet targets by 2025 but may require some real breakthroughs.
- ANL scientists have been developing the Hybrid Copper-Chlorine Cycle for thermochemical production of hydrogen for a number of years.
- The project's temperature range of this process matches up well with medium and high-temperature advanced nuclear reactors and could also be adapted to moderate temperature solar, which make this almost a universal cycle.

<u>Ouestion 2: Approach to performing the research and development</u>

This project was rated **3.0** on its approach.

- The project has a good approach to adapt commercially available solutions to unit operations.
- The minimization of copper (Cu) crossover is dependent on anion exchange membrane, which may have a lifetime issue.
- The thermochemical cycle in this project requires low temperature (550°C).
- The project team is focusing on the correct areas.
- The team should develop a credible critical pathway to achieve DOE's cost and technology targets in a timely manner.
- The approach to work on the separate reactions seems appropriate in this project. The use of the ultrasonic nebulizer seems to have helped progress. Numerous breakthrough technologies seem to be required to make this a viable process. This project must still be considered in its early stages despite several years of work.
- The overall approach of this project is good. However, the report does not clearly state how the different steps of the process, such as hydrolysis, oxychloride decomposition, electrolysis, and separation will be completed

with appropriate modeling, design, process control, construction and testing. Some of the unit operations are shown as conceptual designs of the process. A more definitive approach needs to be presented.

• The cycle this project uses has several material handling problems. The approach is well focused on solving those problems but suffers due to the use of non-standard methods. In particular the use of an ultrasonic nozzle does not bode well for a scale-up to high throughputs.

<u>Ouestion 3: Technical accomplishments and progress toward project and DOE goals</u></u>

This project was rated **3.0** based on accomplishments.

- Good progress has been made on many of the technical issues in this project. Progress on the electrochemical step appears to be slowing as the team has pushed end date forward.
- The team has created a conceptual design based on many industrial processes.
- The cost estimate of this project was based on the conceptual design and it did not achieve the \$2-3/kg H₂ cost target. It is highly likely that the cost will increase more so as the process gets refined.
- No analysis was completed to identify what the project needed to implement or do to achieve the cost goals.
- The project team needs to significantly improve the electrochemical step to achieve reasonable life and decrease costs.
- The team needs to demonstrate that the particles will not sinter, aggregate, etc. over time under the high-temperature conditions. They need to do a cycle life / durability test.
- It is hard to assess how much technical progress has actually been made, and how much is relying on future developments in this project.
- The primary focus of this project is on hydrolysis with modeling and demonstration of high yield and free flowing Cu₂OCl₂ powder. Yet, no model has been presented on how to optimize (1) the particle size distribution of the powder; (2) heat and mass transfer rates; and (3) process parameters for both high yield and good flow properties. It is anticipated that as the size of the droplets produced by ultrasonic nebulizer is decreased, the hydrolysis reaction yield will be improved with the increasing surface area but the fine powder produced in this way will be cohesive as a dry powder.
- Excellent progress has been made in defining the chemistry and developing approaches to mitigate side reactions in this project. The development of a membrane to prevent copper ion crossover is a significant achievement.

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated **3.6** for technology transfer and collaboration.

- The project has a good cross-border program including a multitude of universities. It is well leveraged with other programs using their own funding.
- The project team's collaboration with partners, other than Atomic Energy of Canada, Ltd., is good.
- The collaboration with Atomic Energy of Canada, Ltd. was important to the success of the project. The lack of cooperation has impacted the project significantly by slowing the progress.
- The list of collaborators seems strong and appropriate in this project. It is not known, however, how well the PI is managing all the collaborations.
- The complexity of this multi-stage process requires a strong collaborative approach and the authors are giving their best efforts in maximizing the DOE investments by jointly working on the problem with other groups. However, the details of the collaborative efforts are not sufficiently presented. The team needs to show how the current technological barriers in each of these processes will be solved by the different groups working on the Cu-Cl cycle.
- This project has an excellent international team.

Question 5: Approach to and relevance of proposed future research

This project was rated **3.0** for proposed future work.

• This project has a great unknown of future funding.

- Back up plans in case of the project's failure, such as not being able to find a stable anion exchange membrane, should be identified.
- Titanium is not stable in HCl unless it is used in combination with Pd to create an alloy, Ti-Pd. As an alternative the project team should look at De Nora Tech, an Italy-based company that has a branch in Ohio that can coat titanium with RuOx, which is stable to HCl.
- The project team needs to consider cycle life and integrated experiments.
- The team needs to identify a critical path and show that it is possible to achieve the cost targets.
- The project's forward plan is reasonable, but many good things need to happen.
- The team provided a good general description of the future work plan, but the objectives are not stated with specifics.
- Proposed work in this project will continue to address issues with chemistry and separations. However, the project should also begin looking at scale-ups to larger sizes.

Strengths and weaknesses

Strengths

- The project has a very good team to address the problems in bringing about this technology.
- This project is well managed.
- The project implements and uses a low temperature process.
- A potentially strong team is heading this project.
- This project has a good team.
- The authors have an excellent track record in this field. The proposed Cu-Cl cycle is one of the most promising processes for hydrogen conversion at a moderate temperature (435° 500°C). Their collaborative efforts with Atomic Energy of Canada Ltd. and Nuclear Energy Research Initiative Consortium (NERI-C) have a good chance for success.
- The international team of investigators is this project is its greatest strength. Also, the fact that all the reactions can be performed at temperatures below 600°C is a very big plus.

Weaknesses

- The project's anion exchange membranes are not nearly as stable as cation or Nafion® type membranes. What is the back up plan in case these do not work? What data supports the anion exchange membrane reducing crossover?
- The materials used in this project are very caustic.
- The team has not identified a critical path to achieve the cost goals.
- The project has had relatively slow progress and many remaining hurdles.
- The report lacks some the specifics on (1) the technical barriers being solved; (2) modeling studies; (3) process optimization; (4) material engineering components related to heat exchangers, corrosion resistance, and mixing; and (5) cost reduction steps.
- Side reactions, particularly the production of chlorine, are a problem that still needs to be addressed in this project. The need to remove water to concentrate products is also a weakness although the use of electrodialysis is a step forward.

- The project should consider increasing membrane efforts.
- The project teams should have a back up plan if no me membrane becomes available. For example, can you use electrode cycling to remove Cu build-up?
- The project teams should consider putting more effort on materials compatible with a very corrosive environment.
- As part of the close out, the team should identify a critical path that would enable them to achieve the target costs. If a reasonable path cannot be identified then that should be noted.
- The team needs to demonstrate cycle life of the materials.
- The authors should submit specific objectives for their proposed studies. This project merits further funding.
- This project needs to begin addressing scale-up to large sizes and throughputs. In particular, what will production scale equipment look like?

Project # PD-12: Sulfur-Iodine Thermochemical Cycle

Paul Pickard; Sandia National Laboratories Ben Russ; General Atomics

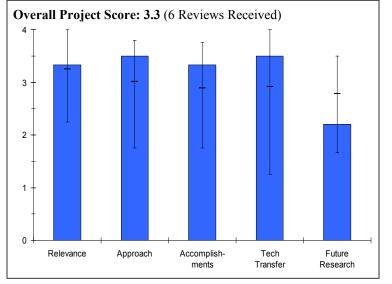
Brief Summary of Project

The objective of this project is to evaluate the potential of the S-I cycle for hydrogen production using nuclear energy. Sulfur cycles have the potential for high efficiency. The approach of the project is to construct and operate an Integrated Lab Scale experiment to investigate the key technical issues. This will provide a basis for nuclear hydrogen technology decisions.

<u>Question 1: Relevance to overall DOE</u> <u>objectives</u>

This project earned a score of **3.3** for its relevance to DOE objectives.

This project addresses the big picture of



- H_2 from nuclear or solar, but a concern remains about the project's relevance when cost targets are so high for H_2 at the plant gate.
- This project is aimed at DOE EERE and NE objectives. Cost targets should have been mentioned.
- The S-I cycle is one of the most promising methods for producing hydrogen. This is due to the rate of hydrogen production as well as the efficiency of production can compete with the currently used steam methane reforming (SMR) process but with no carbon footprint. Once the material engineering issues are resolved, the project has a strong potential to reach DOE goals on producing hydrogen in a commercially viable process.
- This project fully supports DOE's objectives but is not necessarily critical since there are other approaches to both sulfur (S) and iodine (I).
- This project addresses hydrogen production in particular and thermochemical hydrogen production in general. Until credible and reviewed production costs of this process are available, it will not be possible to assert whether or not this is critical to the Hydrogen Program.
- The project's cycle is a good match with both the Nuclear Program and the Solar Program.

Question 2: Approach to performing the research and development

This project was rated **3.5** on its approach.

- The absence of a sulfur scrubber, which prevented fully integrated operation, seems like a flaw in the project's approach.
- The project's approach appears to be reasonable. This is a very challenging project to manage all three reactions safely.
- The project's interface unit allows separate operation which lowers coupling between unit operations.
- The success of the S-I cycle using its fluid-based "closed loop" process depends upon overcoming the current technological barriers involved in the decomposition of H₂SO₄ and HI in a highly corrosive chemical environments at a high temperature. Fabrication of appropriate materials that are both chemically and thermally stable is needed for reaching the DOE goals. The approach of this project is targeted in overcoming this challenge at a reasonable cost.
- The focus of the research for this project has been on the development of lab scale experimental setups for each of the three reactors and on testing their performance both separately and after integration of the three units.
- The project's integrated laboratory scale (ILS) should be essential to planning for pilot scale and would permit adequate data to support pilot design and decision-making whether or not to proceed to pilot. Production rate of

100 I/hr is barely adequate to support design and decision to move from ILS to pilot scale-up. The Bunsen reactor design performance is inadequate to provide feed to HI reactor. The project's testing regime is inadequate to demonstrate Bunsen reactor performance.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated **3.3** based on accomplishments.

- The project would have been "outstanding" if the objectives had been detailed in the discussion. Objectives are not stated in enough detail to enable more than a "ran ILS" check mark. Nonetheless, there has been a lot of work accomplished.
- Some major enabling accomplishments in this project appear to have been made over this period.
- The Bayonet reactor design is enabling for H_2SO_4 to SO_2+O_2
- The Bunsen reaction is most challenging but appears to have been resolved in this project.
- In this project, no control feedback is seen between stages as of yet.
- Given that the project is complete, it would have been appropriate for the team to give some estimation of the hydrogen delivery cost with this technology.
- Significant progress has been made in this project on each of the three reactor operations and their interconnection for producing hydrogen according to the integrated lab scale units design. Both corrosion and separation problems have been addressed; however, more emphasis is needed in these two areas with respect to the scaling up process for industrial application. For example, stability of the glass lined stainless steel (SS) during thermal cycling in a highly corrosive environment could be a serious problem in large scale installations. Availability and cost of these components for installations and plant maintenance may determine the overall success for commercial application.
- Is hydrogen is not detected in HI decomposer? Is the hydrogen infusing with the reactor vessel?
- This project has a very good subsystem integration process.
- The project's progress is excellent. The full integration of the test section was never achieved. This shortfall requires that either the current ILS facility be "upgraded" or retrofitted to permit truly integrated operation or another integrated test system be constructed and run.
- Much good work has been accomplished in this project but significant progress has not been made in overcoming many of the materials issues associated with corrosion. The process of extractive distilling HI from phosphoric acid is a handicap that saps efficiency.

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated **3.5** for technology transfer and collaboration.

- In this project three partners build skids, which are all then integrated at General Atomics. This is evidence of a good collaborative effort.
- The collaboration between General Atomic and Sandia National Laboratory is a good one.
- The project work reflects an exemplary cooperation between different organizations. The authors could explore possible cooperative studies with the Japanese Atomic Energy Research Institute since this institute is in the process of building a large scale plant using the S-I cycle for hydrogen production.
- Three institutions were in close coordination to achieve the ILS construction and operation. Nevertheless, there appeared to be inadequacies in overall supervision and decision-making authority to deal with both institutional and international issues. Adequate centralized supervision and decision-making authority would likely have resulted in better progress and more useful operational information.
- This project has an excellent international team.

Question 5: Approach to and relevance of proposed future research

This project was rated 2.2 for proposed future work.

- This project's future research was not identified even as a speculative next stage.
- This project is complete.

- The current project has been successfully completed. While further research will be continued, no specific plan for future research has been presented.
- This project is complete.
- No proposed future work was provided. If the ILS accomplishments had been sufficient to move to the next phase, perhaps no proposed future work would be necessary in light of the planned Nuclear Hydrogen Initiative (NHI) down-select this summer. It is likely that there will be insufficient information to effect a down-select among the three candidates and the ILS effort has significant deficiencies so additional work would appear appropriate.
- Reactive distillation may be a good solution for the problem of HI concentration in this project. Also, control systems need to be addressed and operation of all sections simultaneously should be addressed. More attention needs to be paid to cross contamination.

Strengths and weaknesses

Strengths

- This project has a competent team.
- Both General Atomics and Sandia National Laboratory have been doing pioneering research in this field since the invention of the S-I cycle by General Atomics. The project has been well planned and executed. The results are impressive and the presentation was excellent.
- This team has done excellent process integration work.
- The Sulfur Iodine thermochemical cycle is the most studied thermochemical hydrogen production cycle. This feature should serve to help identify priority and focus in the production enterprise. The process shares a similar high temperature step with the hybrid sulfur process, permitting resource sharing. Finally, the process is susceptible to operating with both solar and nuclear thermal sources, allowing some flexibility in future operation.
- This project has a good team with much experience.
- The chemistry in this project is well understood.
- The maximum temperature below 1100°C in this project makes for a good match with several advanced heat sources.
- The S-I Cycle can be easily scaled to large sizes and throughputs.

Weaknesses

- There are ongoing technical challenges. This is a difficult project.
- The project has no economics provided.
- Specific recommendations along with a cost analysis have not been provided for nuclear hydrogen technology decisions. An alternative application of solar radiation concentrators was not considered for the S-I cycle.
- ILS proved insufficient to answer many questions, especially with regard to truly integrated operation that would assist in pilot plant design and, instead, would answer many questions regarding the actual chemical process costs that are important to understanding true hydrogen cost at the gate. Reduced time and money makes this process vulnerable to premature down-selection.
- This project has three chemical reactions and one difficult physical separation in cycle requiring significant process equipment.
- This project has corrosion caused by HI which is a materials issue that is expensive to overcome.

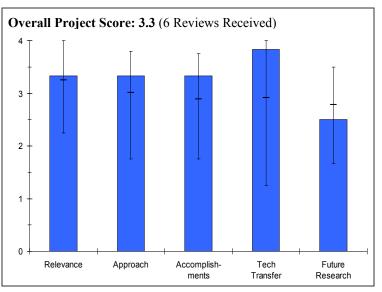
- Funding for this project should continue for studies on large scale design, catalysis, separation of the reaction products, removal of the product gases, stability of the candidate materials, and a comprehensive cost analysis.
- From the perspective of the EERE R&D program, renewed effort in operating the ILS or modifying the ILS to permit fully integrated study of the cycle would be essential before further investments in the cycle implementation under solar power would be justified.
- This project should have continued funding.

Project # PD-13: Hybrid Sulfur Thermochemical Cycle

William A. Summers; Savannah River National Laboratory

Brief Summary of Project

The overall objective of this project is to develop and demonstrate the hybrid sulfur thermochemical process as a viable option for large-scale hydrogen production using nuclear energy. The objectives for fiscal year 2009 are focused on improving performance and operating lifetime of the SO₂-depolarized electrolyzer using a proton exchange membrane-type cell. Hightemperature portions of HyS Cycle are common with Sulfur Iodine Cycle and are being developed in parallel with this project. System design and economics have been performed in conjunction with industry to ensure relevance and to establish realistic performance and cost goals.



Question 1: Relevance to overall DOE objectives

This project earned a score of 3.3 for its relevance to DOE objectives.

- In this project, if the heat can be driven with solar heat, the electrolysis system efficiency would be good for not only fuel cells but industrial H₂ customers.
- Regarding the big picture of this project, H₂ from solar/nuclear is good. However concerns about relevance of this program deal with costs. This project has H₂ cost of \$5/kg at plant gate which are far from market.
- This project has a novel approach. However, the team's approach to DOE cost targets is an issue. These cost targets should have been mentioned in the presentation.
- The project's hybrid thermochemical process has a strong potential for large scale hydrogen generation with efficiency close to 40% or better.
- The project is fully supportive of DOE program objectives, but not necessarily critical because there are other thermochemical cycles that could provide solar-powered hydrogen production. As cost projections become more firmly grounded in data, the essential nature of the project will be clarified.
- This particular thermochemical cycle has elements that are common to several other alternative cycles and progress made here may have applications beyond this Hydrogen Program.

Question 2: Approach to performing the research and development

This project was rated **3.3** on its approach.

- This program is indeed highly focused, but only on the SO₂-depolarized electrolyzer using a proton exchange membrane (PEM) type cell, and in particular crossover. No or little work has been done on integration into a prototype of breadboard system in this project.
- This project has an excellent focus on proof of concept (POC) issues and on data needed for economics.
- It is not clear what the DOE targets are for H₂ costs, but they should have been included in the presentation. This information would be needed to compare costs with economics proved in end of packet slide.
- The project team's overall approach on the development of the process in collaboration with other federal laboratories, universities, and industrial partners is very good. Specific objects are well planned in some areas. While the sulfur crossover problem has been has been given the needed attention, corrosion problems due to the presence of high concentration of H₂SO₄ (close to 50%) have not been addressed adequately.

- The project's SO₂-depolarized electrolyzer (SDE) reactor formed the focus of the work during the past year. The project also included the use of SNL Bayonet design permitted essential program focus on SDE. The project plan is comprehensive and permits high visibility for management purposes. The question that always remains is whether additional external expertise in electrolyzer design and tests would accelerate progress and reduce costs.
- The project has identified key barriers to efficient electrochemical cell operation and has designed approaches to overcome the barriers. Progress is being made through innovative electrochemical cell design.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated 3.3 based on accomplishments.

- This project provides a very innovative solution for sulfur crossover. Instead of relying on material advances (membrane or electrode) they have identified conditions that allow minimum crossover.
- The project has well defined goals and is nearly accomplishment all of them.
- It is unclear what the durability of the system and membrane under an extended run time.
- Regarding slide 10, was the reversible potential reduced by 87% or was the 87% referring to the water case?
- The project's accomplishments toward overcoming some of the major barriers suggest the overall feasibility of the process used. More integrated laboratory scale investigations are needed for solving the remaining technical problems and for scaling up studies.
- The project's apparent resolution of sulfur crossover is a major step forward. How good the solution actually is remains to be seen. Additional testing will be required before the electrolyzer is selected for integrated testing.
- Durability testing for this project remains as an outstanding requirement before transition to ILS testing would be appropriate.
- The project has shown success in reducing sulfur crossover from anode to cathode and their approach was successfully demonstrated in 200 hours of testing. These cells demonstrated no sulfur buildup in the separator which was a failure mechanism in previous work. This, by itself was a great accomplishment. However, there is still concern about the small amount of sulfur dioxide that is still getting through the membrane separator to form hydrogen sulfide in the cathode. Hydrogen sulfide in the hydrogen exhaust stream should be a concern even at levels of a few hundred parts per million and should not be taken lightly.

<u>Ouestion 4: Technology transfer/collaborations with industry, universities and other laboratories</u>

This project was rated **3.8** for technology transfer and collaboration.

- The project team holding a workshop amongst the various and highly diverse (government, university, industry) partners is commendable.
- This project has many collaborations. Some are "core" collaborations without whom progress could not have been made and are well recognized in the presentation. Some more peripheral collaborations are also acknowledged.
- This project seems to have a good combination of partners.
- The project's collaboration is excellent.
- The project has an excellent team of collaborators. In particular, teaming with Giner for electrochemical cell design was a good move.

Question 5: Approach to and relevance of proposed future research

This project was rated 2.5 for proposed future work.

- Strongly endorse running an integrated system.
- The project team had a fairly superficial description of future plans which is perhaps due to fitting the situation of waiting for a down-select decision.
- The project's future plans should include extended durability tests at a reasonable scale.
- The project's overall approach for future research is stated without sufficient details.

- Future plans are hostage to program continuation, but the program has taken steps to plan for them eventually. Electrolyzer selection should be the level 1 milestone so that all the button testing can terminate and resources can be directed to integrated lab scale testing.
- There are issues that still need to be addressed in this project at a fundamental level. Two of these are the cell voltage and the small levels of sulfur crossover that is still occurring. These are passed over as being only minor annoyances but they may become significant issues as the system is scaled up.
- The program needs to demonstrate long term durability of the electrolyte membrane.

Strengths and weaknesses

Strengths

- The project's use of electrolysis to depolarize SO₂ is a good one.
- The team has come up with a clever solution to minimize crossover.
- The project has a strong team of diverse backgrounds.
- The project appears to have a competent team focusing uniquely on a combination of thermal and electrochemical approaches. Good progress is shown.
- The project work is undertaken by a team of well qualified engineers and scientists and the progress to date shows a strong potential for success.
- The project's process is susceptible to operation with both solar and nuclear thermal power sources and shows promise of meeting DOE cost goals. The process is similar in its high-temperature step with regards to the sulfur iodine process so that resources are partially process-shared.
- The project has only two chemical steps in the cycle.
- The project's sulfuric acid decomposition is well developed and presents no serious materials problems.
- The electrochemical cell development leverages advancements being made in PEM fuel cells.

Weaknesses

- It is unknown if the special operating conditions can hold over the 40k hour target for lifetime. No data were given on preliminary outcomes, or whether small amounts of crossover are still occurring after, for example, 1,000 hours.
- There is no correlation between level of sulfur impurity and lifetime.
- Issues regarding durability of the system and whether 50 hours without sulfur buildup is adequate are significant.
- The overall feasibility of a commercially viable hybrid process for producing hydrogen needs to be established by comparing the hybrid cycle with other processes of hydrogen generation.
- The electrolyzer design, extended testing and costing remain as critical elements for assessing utility of this process relative to competitors. Time and money are running out so that there is a possibility of premature down-select in this project.
- The use of an electrochemical cell limits the cost savings that can be realized by scale-up to industrial size equipment. Increasing the cell size by a factor of 10 increases costs by a factor of 10, unlike the cost savings that might be realized by scaling up chemical reactors.
- The need for concentrated acid coming from the electrochemical and going into the acid decomposition reactor has a significant impact on efficiency.

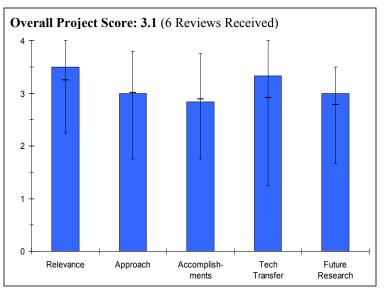
- The project team should work with Pickard of SNL/GA/CEA team on integrating into a full system.
- The team needs to determine what happens during an uncontrolled shutdown of the electrolyzer (gas feed on, loss of power to electrolyzer). Is the effect reversible or permanent?
- Durability testing needs to be done in this project.
- The project is innovative and deserves additional funding unless a comparative cost analysis does not support further advancements.
- The addition of long term durability tests to the program is recommended.

Project # PD-14: High Temperature Electrolysis System

Steve Herring; Idaho National Laboratory

Brief Summary of Project

The overall objectives of this project are to 1) develop an economical method for the CO₂-free production of hydrogen in centralized facilities; and 2) configure the plant for the integration of heat and electricity from a nuclear reactor and for interactions with the grid to accept or supply power as wind/solar sources vary. The objectives for the past year were the 1) construction and operation of the threemodule Integrated Laboratory Scale (ILS) experiment for long-duration (>1,000 hrs); 2) organization and sponsorship of a workshop on solid oxide electrolysis cell (SOEC) degradation with experts from the solid oxide fuel cell/SOEC community; 3) characterization of degraded cells to



determine silicon/chromium transport, delamination and destabilization of electrolyte; 4) tests of short stacks and button cells of other designs and from other manufacturers; and 5) building of capability to simultaneously run five small tests.

Question 1: Relevance to overall DOE objectives

This project earned a score of 3.5 for its relevance to DOE objectives.

- The overall objective of this project is to develop an economical method for the CO₂-free production of hydrogen in a centralized facility. This project supports the DOE Hydrogen plan (nuclear hydrogen initiative).
- Ability to switch H₂ production to aid in grid stability is a good feature of this project.
- The solar-thermal is a good fringe benefit.
- The general project concept is responsive to the Hydrogen Program. The work is attempting to develop a hightemperature process and ILS for hydrogen production using nuclear (or solar) heat/power. The PI understands the goals and objectives of the program and is working to attain those goals/targets. The project appears to be following the agreed upon work scope by DOE and INL.
- This is an ongoing project for generating hydrogen from steam by using high-temperature SOECs in stack formation. The team of researchers lead by the PI at INL has been working on this process for more than six years and the project has reached a stage for pilot plant development with a goal for producing hydrogen with optimized efficiency, cost and durability. The project is very relevant in reaching the goals of DOE for hydrogen production.
- This project fully supports program objectives, but other electrolytic processes are possible with which to produce hydrogen. Cost and operational issues will need to be resolved before the level of critical support to program objectives can be assessed.
- Although funded through the Nuclear Hydrogen Initiative, this work has a much broader appeal. Large-scale, high-efficiency water electrolysis can have applications in intermittent and renewable energy storage as well as hydrogen production.

Question 2: Approach to performing the research and development

This project was rated **3.0** on its approach.

- The approach of this project is to develop energy-efficient, high-temperature SOECs for hydrogen production from steam. Nuclear heat will be used. The approach is to increase the SOEC stack durability but unfortunately the performance of the stack degrades too fast. Twenty percent per 1000 hr is a high rate. This project is not making good progress.
- The team's use of solid oxide electrolyzers could significantly reduce the capital costs for the production of H₂.
- The project has a very good approach with regard to building test systems and analysis of failure mechanisms.
- The project's approach is based on a relatively old principle (25+ years) that has been researched by numerous investigators over the years. The principle may be applicable in some small scale applications (e.g., oxygen sensors) but expansion to a relatively large scale may be extremely difficult. Ceramic materials are inherently difficult to deal with (fabrication, sealing, etc.) and these problems are compounded exponentially with multiple stack units. The investigator appears aware of the issues and is taking steps to address them. The approach is acceptable for identifying and solving the necessary issues. Another issue concerning the approach is the incomplete conversion of the water/steam feed which will require additional separation and polishing. This could be a major cost issue in and overall larger system. The presenter failed to discuss this issue and simply stated that the membrane separation will be employed. This is not an answer and will not to work well at this time either. Condensing the stream may be an approach; however, it is not clear how much conditioning will be required for the water reactant which may become another cost issue.
- A comprehensive approach is presented both in terms of overall goal and specific objectives. The goals for efficiency, cost, and durability are not expressed in quantitative terms. The aims are to design and construct a 200 kW pilot plant for producing hydrogen in a commercial scale. This will be a major breakthrough in CO₂-free hydrogen generation if successful.
- The project plan seems adequately focused on the discovery of an acceptable cell design. However, it appears that inadequate design practices are applied to cell test stand configuration. Test stands should be designable before construction and implementation.
- The approach for this project is satisfactory and is addresses many barriers simultaneously. However, the jump to a multi-kilowatt size demonstration may have been premature since there are still some materials issues that have not been solved.

Ouestion 3: Technical accomplishments and progress toward project and DOE goals

This project was rated 2.8 based on accomplishments.

- The project demonstrates hydrogen production rates up to 5.6 Nm³/hr in the ILS facility. Long-term cell degradation is a serious issue. Degradation has been characterized well but the approach to over come the degradation is not clear.
- The project team has had very good progress with actual skid system on meeting goals with respect to production of hydrogen.
- The project's lifetime/degradation appears to limit impressive initial outputs compared to other, far more complex technologies.
- The project has been ongoing since 2003 and the technical progress is somewhat limited. The work does demonstrate some hydrogen production (slide 9) although still at moderate levels. Of major concern are the materials issues (element transfer, delamination, etc,- see slide 10 for example). These are well know problems, and this work does not appear to have made any significant advancements in solving these problems. Until these issues are properly addressed, building larger scale test units has no purpose. In addition to the problems specifically mentioned, seals will be a major problem. The PI and team should consider a revised approach to address these problems before attempting to demonstrate a scaled up unit.
- The project has accomplished several milestones. One of their integrated lab scale production unit was able to produce 0.5 kg H₂/hr for 1000+ hours. Previously experienced corrosion-related problems were solved. SOEC stacks were designed and tested. While these major advancements have been made, a serious problem with respect to long term durability of the cells was noticed. Extensive tests and analysis were performed to identify the problem for developing an appropriate solution.
- However, in view of the team's focus mainly on the cell degradation problem, many of their stated objectives were not addressed. Analysis with respect to efficiency and cost were not presented. Safety analysis was not addressed.

- Testing regimen for long periods exceeds the regimens for both HS and sulfur iodide SI. However, more time should be spent exploring detailed causes of cell degradation and establishing fixes to assure an operational concept in support of down-select. Until then, less time should be spent in long term durability testing.
- Excellent progress has been made in this project especially regarding the production of 1/2 kilogram of hydrogen per hour from it's demonstration stacks is noteworthy. Although the degradation rate is at least an order of magnitude too high, these barriers have been overcome by the solid oxide fuel cell developers using similar materials and technology and need only be addressed by the current program to be solved as well for the electrolysis cell.

<u>Ouestion 4: Technology transfer/collaborations with industry, universities and other laboratories</u>

This project was rated **3.3** for technology transfer and collaboration.

- The project has very good collaboration (see slide 12). The presenter explained the contributions and roles of these collaborators. Good to see collaborations with NERI projects.
- It is not clear in the presentation which team member contributed various results or segments of the program.
- INL has assembled a diverse and talented team with good experience in this particular area however, INL needs to better utilize this group to solve the fundamental problems associated with this approach rather than spending money on multiple test units. Based on the presentation, INL seems to have neglected the expertise of Ceramatec, who has a good track record with high-temperature ceramics development. They need to more fully incorporate this knowledge and experience into the materials development effort.
- The team work in this project is very impressive. The authors presented how the different components of the project were investigated by respective team members from national laboratories, academic institutions, and private enterprises.
- Broad collaboration exists in the project. However, reliance on only Ceramatec might prove to be a weakness. It was not made apparent that parametric requirements were established and industrial RFP sought. There could be a reason for this "sole source", but, if so, it was not made apparent.
- The partners are well coordinated. The inclusion of Ceramatec as a partner is good since it allows the program to tap into solid oxide fuel cell expertise.

Question 5: Approach to and relevance of proposed future research

This project was rated **3.0** for proposed future work.

- How is the project team going to solve the degradation problem(s)? The project's future plan does not address this important issue. It is mentioned that the PI is going to collaborate with SECA SOFC manufacturers. SECA program has been talking about the degradation issues for very long time yet there seems to be no solution is in sight.
- The team's roadmap for degradation is relevant.
- If one or all of these mechanisms in the project are confirmed, what are possible solutions?
- Which of these potential mechanisms are show-stoppers?
- This category is not relevant for this project. Continuation depends on a down-selection. However, the PI should recognize the need to solve the materials issues rather than focusing on building a larger scale ILS.
- The team's future work is described clearly and appears to be well planed for the project goal.
- Too many options are left open for future work on this project, even given continuation beyond down-select.
- Future plans of this project are focused on overcoming materials issues that limit lifetime and reduce performance. Should this work continue to be funded, it is suggested that the participants survey one or more of the other SOFC developers. Several claim high-temperature electrolysis cells based on SOFC designs with much better durability that reported by the current program. It would be advantageous to shorten development time by bring the best of them on board this program.

Strengths and weaknesses

Strengths

• This project has a very strong team as well as a long list of publications & presentations.

- This project team provides a very simple and elegant way to produce low-cost H₂.
- This project has had great initial output.
- The project's thermal balance is easy to maintain, aiding scale-up.
- The PI and the team members are highly experienced and qualified to complete the project. The project appears to be close to demonstrating a commercially viable hydrogen production process.
- This project has some similarities to previous NHI approaches but high-temperature electrolysis (HTE) should be simpler. It is also, however, apparent that both operational management of electrolyzers and scale-up issues are different between hybrid sulfur and HTE.
- The project's demonstration of multi-kilowatt stacks is a strength.
- The technology/processes described in this project have performed well enough to operate at the thermal neutral voltage.
- This project has a good team with much experience in developing similar technology.

Weaknesses

- This project neither shows nor offers a clear approach to solve the degradation problem.
- The team faces the basic weakness of SOFC -- interconnects and durability applies to SOEC.
- The accelerated degradation rate of SOEC compared to SOFC is worrisome, implying either extreme conditions for current known SOFC failure modes, or some yet to be discovered failure mode not common with SOFC.
- The project's approach has major materials issues.
- The team's lack of cost analysis and operational features along with the project's durability problem are of major concern.
- The believed simplicity and reduced potentials for HTE relative to conventional electrolysis was not emphasized in the process description; such was also not evident in the work presented.
- Performance degradation is this project's main weakness. The team is attributing performance degradation to materials issues such as chromium diffusion into the electrodes, strontium migration into the electrolyte, delamination at or near the electrode/electrolyte interface, and silicon migration from the seals. These should have been addressed before moving to multi-kilowatt stacks. These are issues that plagued the SOFC developers several years ago that they seem to have overcome using sub-kilowatt, bench-scale experiments before moving on to multi-kilowatt demonstrations.

- Issues relating to drastic degradation of cell performance must be addressed before moving forward.
- Agree with large focus on durability.
- The work needs to focus on addressing the materials problems in a logical method. Stop all production tests and address the real development problems which are mainly the materials.
- The project should receive continued funding if the team members clearly establish that they could resolve the durability and other materials-related problems and reach their goals in terms of efficiency, cost of production, and scale-up design.
- The team needs to address the materials and performance degradation issues. This should be the main focus of the research going forward.

Project # PD-15: Technoeconomic Boundary Analysis of Photobiological Hydrogen Producing Systems *Brian D. James, George Baum, Julie Perez, and Kevin Baum; Directed Technologies, Inc.*

Brief Summary of Project

Directed Technologies conducted a technoeconomic boundary analysis and defined and evaluated four different H₂ production approaches: 1) photosynthesis with algae and bacteria; 2) water algae fermentation; 3) lignocellulose fermentation; and 4) microbial electrolysis. These approached included multiple system embodiments and system integrations. Concept feasibility, performance and cost and resultant \$/kgH₂ were estimated.

<u>Question 1: Relevance to overall DOE</u> <u>objectives</u>

Overall Project Score: 3.4 (3 Reviews Received)

This project earned a score of **3.7** for its relevance to DOE objectives.

- Longer-term renewable methods for hydrogen production are critical if this energy carrier is to succeed in the market. Photobiological hydrogen production has been assessed many times over the last 15 years. However, there is only limited bench scale data for many of the systems identified in this analysis. It would have been of value if error bars had been provided on the costs to determine the relative accuracy of the analysis.
- This project has a critical need in the field. Although, without an economic basis it is very hard to focus the team's research efforts.
- This project aligns well with DOE's goals to develop a cost-effective system for biological hydrogen production.

Question 2: Approach to performing the research and development

This project was rated **3.7** on its approach.

- Better discussions on how this team's work influences the research approach were needed especially regarding whether to set priorities or eliminate research pathways.
- The project team looked at both a series of different organisms and a set of different approaches for growing these organisms. The set of both organisms and reactor systems seemed comprehensive. Sizes were appropriately normalized for comparison in terms of the amount of hydrogen produced. The team took into account cycling times for some of the batch reactors vs. continuous growth. They also considered the issues associated with mixed gases (hydrogen and oxygen). The project team considered the reactor design, the materials and amounts of materials required. They also considered the mixing and flowing issues. They also constructed a bill of materials for each case.
- The team's approach is logical and appropriate. Systems used in this project for technoeconomic boundary analysis were carefully designed.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated **3.3** based on accomplishments.

• The team has a reasonable systems analysis approach for this project. An improvement would have been to use a previous study conducted 5 years ago and assess if the technology and costs have been reduced as a result of government support. It would also be beneficial to determine if the high-priority barriers with the greatest cost impact had been included in the research funding.

- The project team was able to compare costs for each of the systems. The oxygen tolerant systems were cheapest but these result in gas mixtures. The amounts of hydrogen that can be created using each of the system dramatically changes. The algal system has a rather low amount of output. The cellulose systems were better. The microbial electrolysis cell (MEC) was the best option but requires energy input and needs acetate as an input. Overall costs for this project were dominated by infrastructure. There was no apparent benefit for using integrated systems. A key issue is that the lignocellulose system was much higher in total costs than the other systems.
- Progress for this project has been very good. Although the three integrated systems studied did not reduce the cost of biological hydrogen production, they provided guidance for designing better integrated systems in the future.

<u>Ouestion 4: Technology transfer/collaborations with industry, universities and other laboratories</u>

This project was rated **3.7** for technology transfer and collaboration.

- Excellent investigators are involved in the work, but more discussion could have been presented on roles, responsibilities and if issues arose over cost or technical factors. Light could have been shed on how the team resolved these issues due to limited amounts of quantified data.
- The project team had some of the major groups in this area providing information about the algal and fermentation systems.
- The investigator collaborated closely with the Bio-hydrogen Working Group and other university investigators, resulting in a successful project.

Question 5: Approach to and relevance of proposed future research

This project was rated 2.5 for proposed future work.

- The team's future research included the validation of costs, however, this should have been discussed in the initial work and any additional systems analysis should refine or reduce the assumptions. The project team could have benefited from using consultants with waste water treatment experience and algal producers for high-value food additives. This would allow them to perform and independent validation of the approach and then use their assessment to determine where this work should focus.
- This team has shown no future work. The project is essentially completed.
- The project's proposed future work is appropriate.

Strengths and weaknesses

Strengths

- This project has a good team of knowledgeable experts.
- The project uses reasonable technologies to bracket potential concepts.
- This project addresses a critical question that should drive much of the science.
- The team considered both a range of organisms and a range of bioreactor types.
- This project shows strong teamwork.

Weaknesses

- This project lacks sufficient information on assumptions.
- There is not enough information on the range of outputs, plus or minus 50%, 100% or more in this project.
- The project has had no outside independent review.
- There are undoubtedly additional factors in this project that need to be considered, particularly in terms of some of the inputs like water into the system, but this is an excellent initial model that can be expanded.
- There were too many assumptions used for the boundary analysis in this project.

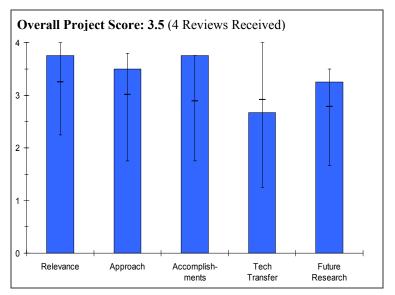
Specific recommendations and additions or deletions to the work scope

• The cost for waste algae fermentation is too high in this project. This approach should be abandoned.

Project # PD-16: Maximizing Light Utilization Efficiency and Hydrogen Production in Microalgal Cultures *Tasios Melis; University of California, Berkeley*

Brief Summary of Project

The objectives of this project are to 1) minimize the chlorophyll (Chl) antenna size of photosynthesis to maximize solar conversion efficiency in green algae; 2) identify and characterize genes that regulate the Chl antenna size in the model green alga Chlamydomonas reinhardtii; and 3) apply these genes to other green algae as needed. The approach is to 1) interfere with the molecular mechanism for the regulation of the chlorophyll antenna size; and 2) employ deoxyribonucleic acid insertional mutagenesis and high-throughput screening to isolate tagged green algae with a smaller Chl antenna size.



<u>**Ouestion 1: Relevance to overall DOE**</u> <u>objectives</u>

This project earned a score of 3.8 for its relevance to DOE objectives.

- The project goals are well aligned with DOE's program targets for maximizing light utilization efficiency and hydrogen production in microalgal cultures.
- The project's focus on minimizing chlorophyll antenna size to maximize solar conversion efficiency is relevant to improve solar to hydrogen conversion efficiency.
- The success of this project is instrumental in feasibility of photobiological hydrogen production.
- Findings from this research can potentially be applied to other phototrophs to develop efficient photobiological hydrogen production.
- The work in this project aligns well with the need for a longer-term renewable hydrogen production technology, and photobiological hydrogen production that has been hampered by light sensitivity.
- A key issue in large-scale growth of algal cultures is going to focus on the penetration of light into the culture. While this can be remedied by mixing or simply by using a smaller thickness of growth culture, these approaches have disadvantages in terms of energy consumption and the distribution of energy to different organisms in the culture.
- The project aligns well with DOE's efforts to develop a cost-effective system for photobiological hydrogen production.

Question 2: Approach to performing the research and development

This project was rated **3.5** on its approach.

- The project has a very good approach, using a random mutagenesis technique and high throughput screening method to obtain mutants with truncated antenna size and with increased rate of photosynthetic activity (O₂ evolution).
- Systematically obtaining mutants with reduced levels of antenna size and increased light utilization efficiency validates the effectiveness of this project's approach.
- Both the tla1 and tla2 genes are important in regulating chlorophyll antenna size. The homology comparison suggested that other phototrophs may use the same strategy. This approach therefore has immense applications expanding beyond the current organism used in this study.

- In the accomplishments summary, the PI focused on plans instead of accomplishments, specifically with the down regulation of the tla1 gene. The PI also indicated the team had advanced the biochemical and biophysical analyses but had difficulty with the molecular analysis. There was however, insufficient information on the effectiveness of this work.
- The team's approach is standard but effective. They are looking at random mutagenesis of the organism and isolating mutations that decrease the antenna size. The team has a rather unique ability to make these measurements.
- Random mutagenesis combined with high throughput screening was employed in this project to identify green algae mutants with a smaller Chl antenna size. The approach is well-focused on specific technical barriers and it is very effective.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated **3.8** based on accomplishments.

- The progress toward the project's goals is excellent.
- The team systematically demonstrated the truncation of antenna size which has potential to meet the 2010 target
- The project's accomplishments included the cloning of the tla1 gene and determined that tla1 is a hydrophilic protein. Work is underway to determine a sub cellular localization of the protein, which is a novel discovery.
- The team managed to overcome the complication that antibody raised against Tla1 also cross-reacted with D2 protein. The team has also since identified the C-terminus of D2 protein displaying antigenecity toward the tla1 antibody. This is verified by using mutants deficient in D2 protein.
- The project team has cloned the tla2 gene and work is underway to characterize the protein to gain a more indepth understanding as to its role in regulating antenna size in Chlamydomonas.
- This is the first demonstration of two different genes that regulate the chlorophyll antenna size in photosynthesis, which signifies the importance of the team's work.
- This is a 5-year research project and, based on the data, the team has successfully accomplished a significant reduction of antenna size and light sensitivity. However, the PI stated that it made the DOE target for utilization efficiency of solar light, however all the information presented is on the original mutant tla1 and nothing on tla_x or tla_{new} except for the two graphs.
- The project team has isolated three mutations that greatly decrease the antenna size which is evidence of achieving the goals set by the team. The first mutation has been characterized in some detail. This was complicated by the fact that, as it turns out, D2 of PSII has a common epitope with the gene product of the gene that was mutated. The team has worked through this and understood the cross reactivity of the antibody in detail. They are currently in the process of characterizing the second mutation and will move to the third. The team has demonstrated that the decreased antenna size increases the photosynthetic conversion efficiency and decreases the sensitivity to photoinhibition.
- The team has made good progress in FY08. The tla2 gene was cloned and the tla1 immunoblot problem was solved. The project has reached the DOE target beyond 2015.

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated 2.7 for technology transfer and collaboration.

- Very little collaboration is shown in this project. Coordination amongst different partners may have and can potentially expedite the research progress.
- Technology transfer was initiated in this project with UC Berkeley's Office of Technology issuing a nonexclusive license for the commercial use of tla1 gene.
- The team does not appear to have much collaboration on this work.
- There were no collaborations on this project but none were necessary to satisfy the scope of work.
- This project is a sole source effort.

Question 5: Approach to and relevance of proposed future research

This project was rated **3.3** for proposed future work.

- The project's sub-cellular localization of the tla1 protein is underway.
- A clear plan is laid out for future research in this project, including characterization of the tla2 gene.
- The next step in this project is to characterize genes conferring the phenotype in tlaR strain.
- Most of the team's proposed work is focused on whether tla_{new} is stable and can be replicated to demonstrated repeated results with 25% efficiency.
- The project team will continue to characterize the second and third mutations that they have discovered.
- Proposed work for cloning genes from the tlaR strain is appropriate. However, the investigator did not propose further plans to study biological functions of tla1 and tla2 proteins.

Strengths and weaknesses

Strengths

- The investigator has demonstrated superior progress toward well-defined goals.
- The investigator has a collection of mutant organisms with truncated antenna sizes and, based on these mutants, novel genes were identified. The outcomes reveal how chlorophyll antenna sizes are regulated for the first time in Chlamydomonas.
- The team's research is very valuable in guiding the design of other phototrophs with improved light conversion efficiency via down-regulating of antenna size.
- The investigator's laboratory is well equipped to determine chlorophyll antenna size.
- The team has a good PI and demonstrated accomplishments.
- This project has a well defined problem to solve which is directly applicable to large scale growth.
- The project team has demonstrated that mutations that result in decreased antenna size can be found and can also improve photosynthetic efficiency and stability to high light levels.
- The investigator is an expert in photosynthetic systems of Chlamydomonas.

Weaknesses

- Even though mutants with truncated antenna sizes displayed higher photoconversion efficiency (O_2 evolution), it is not yet determined if hydrogen production is similarly improved, especially at high light intensity.
- The truncated antenna mutants would be less competitive compared to the wild type and therefore pose an issue with contamination when scaling up.
- The project has insufficient data and descriptions on advanced mutants.
- Ultimately, this project needs to be coupled to hydrogen production values in order to be critically evaluated.
- In this project, no data was presented to show increased hydrogen production in the tla1, tla2, and tlaR mutants.
- The investigator did not address the questions about the proposed biological functions of tla1 and tla2 proteins from previous reviews. A biological function study is essential to reveal regulation mechanisms of the Chl Antenna Size, which may lead to a rational design of better algae mutants.

Specific recommendations and additions or deletions to the work scope

No specific recommendations were provided for this project.

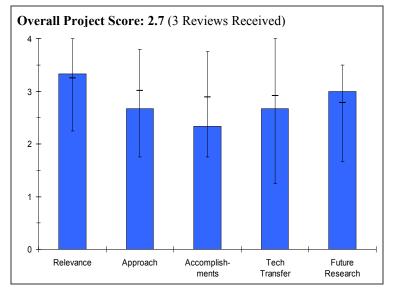
Project # PD-17: Biological Systems for Hydrogen Photoproduction

Maria L. Ghirardi; National Renewable Energy Laboratory

Brief Summary of Project

The overall objectives of this project are to 1) develop and optimize aerobic photobiological systems for the production of hydrogen from water; 2) utilize the sulfur-deprivation platform to address biochemical and engineering issues related to photobiological hydrogen production; and 3) integrate photobiological with fermentative organisms to more efficiently utilize the solar spectrum and the substrates/products from each reaction.

<u>Question 1: Relevance to overall DOE</u> <u>objectives</u>



This project earned a score of **3.3** for its relevance to DOE objectives.

- This project, which is based on biological hydrogen, supports DOE's RD&D objectives.
- This project is relevant because it creates an integrated photobiological/fermentative system.
- Key issues in this project are oxygen tolerance ability to optimize the sulfur deprivation system and the integration with the fermentation system. In principle, this could become an important approach to generating biomass from biomass derived from photosynthetic microbes.

Question 2: Approach to performing the research and development

This project was rated 2.7 on its approach.

- The team's approach was clearly presented as logical stepwise steps.
- The project's milestones should be better defined.
- The project team is trying to improve oxygen tolerance via a rational design of the enzyme or by expressing heterologous hydrogenases or through random mutagenesis. The rational mutagenesis relied on finding the pathway that oxygen uses to reach the cofactors. However the hydrogenases appear to be heterogeneous in their oxygen effects, making this hard to evaluate. They are also introducing bacterial hydrogenases in algae and looking at the stability of these to oxygen.
- The project team is currently looking at sulfur deprived organisms and their ability to convert light. They have been looking recently at immobilized systems in films. It is not clear how relevant this is to scaled systems, though it provides some fundamental understanding of the system

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated 2.3 based on accomplishments.

- The team is proceeding in a stepwise manner.
- With the considerable funding for this project, more progress was expected.
- The team has been developing the high-volume throughput screening tests since 2007. More details on their progress are needed.
- The team's antenna and sulfur deprivation work seem very similar to what was done by Professor Melis at UC Berkeley.

- Initial project work on integrating the fermentative and algal systems was interesting. The team needs to include information on any treatments made to the algal biomass/water mixture prior to feeding it to the fermentative system. Purified proteins and algal lipids seem like an expensive fuel.
- Results of using fermentation products for feed in a photosynthetic system were encouraging, but more details about pretreatments, etc. are needed.
- The team has had difficulty analyzing the rational mutagenesis results because of the heterogeneous hydrogenase issues. They have not yet been able to assay the other approaches for improving oxygen sensitivity.
- The project's sulfur deprivation of immobilized algae in films shows 1% conversion efficiency. Hydrogen production takes place in the presence of oxygen because the film protects the hydrogenase. ATPase mutants improve the hydrogen production, which is an interesting observation.
- For the integrated system, first the team looked at whether the spent algal biomass can be used by fermentative system. They see increased hydrogen production when algal biomass is provided. Both the lipid and protein are fermented and utilized for hydrogen production. At the moment, the team is working at very small scale.

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated 2.7 for technology transfer and collaboration.

- It appears that the team has had collaboration between partners.
- The PI should identify areas that the partners collaborated more clearly. It is difficult to determine what was done by partners and what was done by NREL.
- The project team has a set of collaborators with expertise in the different tasks.

Question 5: Approach to and relevance of proposed future research

This project was rated **3.0** for proposed future work.

- The project team's future plans are the same as in previous years. Since progress has been made, it would seem reasonable to adjust the plans.
- The project has continued work on the same issues. Basic research with long term goals have been accomplished however, this project is not going to reach production scales any time soon.

Strengths and weaknesses

Strengths

- This is a long-term project that is well funded and has many partners.
- The project team is exploring the fundamental understanding of hydrogenase structure and function, particularly with regard to oxygen tolerance.
- The team is also characterizing the conditions that allow hydrogen production, particularly when some oxygen is present.

Weaknesses

- Progress in this project seems slow or at least unclear. For example, they have been working on developing high-volume throughput screening tests for several years and it is not clear what progress has been made. The challenges and progress should be better identified.
- The near term milestones are inadequate for this project. "Test the performance of immobilized ATPase mutants" does not seem very ambitious. The milestones should include some performance targets as well as "testing" a number of organisms. There are no milestones for the high-volume screening process development, which has been identified for the last several years as an important component of this program. Milestones should be added.
- There is no indication, at this point, how this work could be scaled and no real understanding of how to increase the hydrogen production to a point that will be useful at scale.
- This project is early stage exploratory work, which is not a weakness, but it makes extrapolation to any kind of useful system essentially impossible.

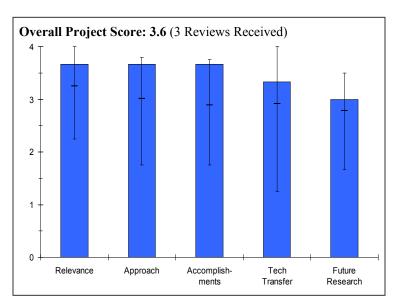
- The PI has reported making an impressive number of presentations 19. This is over one conference a month, which is a lot of travel. Their resources and time would be better utilized if they limited their conference attendance to only the premiere conferences.
- The project team's milestones need to be focused on achieving technical targets. "Testing an organism" is a weak milestone.

Project # PD-18: Fermentative and Electrohydrogenic Approaches to Hydrogen Production

Pin-Ching Maness; National Renewable Energy Laboratory Bruce Logan; Pennsylvania State University

Brief Summary of Project

The long-term objective of this project is to develop direct fermentation technologies to convert renewable lignocellulosic biomass resources to hydrogen. The near-term objectives of this project are to 1) optimize bioreactor performance for the cellulosedegrading bacterium Clostridium thermocellum; 2) identify key metabolic pathways to guide generic engineering to improve hydrogen molar yield; and 3) integrate microbial electrolysis cell (formerly BEAMR: bio-electrochemically assisted microbial reactor) process to improve hydrogen molar yield.



<u>Ouestion 1: Relevance to overall DOE</u> <u>objectives</u>

This project earned a score of 3.7 for its relevance to DOE objectives.

- This project aligns to DOE's Hydrogen Program.
- The project team is trying to convert lignocellulose directly to hydrogen without going through sugar. This is much simpler than going through a monomeric sugar. They are also coupling this to a microbial electrolysis cell (MEC) step that uses the byproducts of the fermentation. If economic ways of using biomass have to be made then this is probably required.

Question 2: Approach to performing the research and development

This project was rated 3.7 on its approach.

- The project team has a step-wise approach.
- The team is using a single bacterium for the degradation of cellulose. This bug can use cellulose as a carbon source and it also works at high temperature. The byproducts of the fermentation are used in an MEC which seems like a well thought through approach.

Ouestion 3: Technical accomplishments and progress toward project and DOE goals

This project was rated 3.7 based on accomplishments.

- The project team has made good progress towards the DOE targets.
- The team's integrated system surpasses the DOE hydrogen production targets.
- Comparing the project's MEC efficiency based on electricity to water electrolysis is not a fair comparison since the MEC is decomposing an organic compound and the electrolyzer is decomposing water. Electrolyzers that decompose organic compounds use much less power to produce hydrogen than the process of water electrolysis does. To be consistent with other technologies, the only efficiency number of merit is the one that includes the lower heating value of the organic material.
- The hydrogen production rate in this project is very slow and needs to be increased dramatically in order for this technology to be viable.

- The project team is observing hydrogen production using corn-Stover, and they are able to see greater H₂ production than CO₂. They have looked at the effects of metabolic pathway inhibitors to see if blocking certain pathways will increase hydrogen production. This aspect points to the use of metabolic engineering at the points that the inhibitors work. They have looked at several inhibitors and can see the predicted increases in hydrogen production. The team is in the process of developing the genetic system for this work.
- For the MEC system, the project team has looked at a synthetic mixture of byproducts, and optimized the system for the individual substrates and then combined the organisms. They are now getting more hydrogen energy out than the electrical energy they are putting in.
- Overall, the project is getting almost 10 moles of hydrogen per hexose. This is more than twice the goal.

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated **3.3** for technology transfer and collaboration.

- There appears to be good collaboration between the partners in this project.
- The team has developed new collaborations with Oakridge to work towards the metabolic engineering. The fundamental collaboration between the fermentation work and the MEC is excellent.

Question 5: Approach to and relevance of proposed future research

This project was rated **3.0** for proposed future work.

- The team's proposed future work should also consider ways to increase the production rate (kg H₂/day and kg H₂/ volume).
- The project team's focus is on metabolic engineering based upon the inhibitor studies. They will continue to improve the efficiency of the MEC output, which seems like an excellent approach.

Strengths and weaknesses

Strengths

- This project has a strong team with good communication.
- The team has meaningful milestones, which indicate substantial thought being put into the process. As a result, the team has developed a plan to achieve its goals.
- The project's integrated process better utilizes the feedstock.
- This project has a very good combination of novel fermentation with MEC technology.
- The systematic inhibitor study to help guide the metabolic engineering was excellent in this project.
- The project results in terms of molar yields are quite impressive.

Weaknesses

- This project requires a relatively expensive feedstock.
- Maintaining the feed mixtures will be a significant challenge for this team.
- Hydrogen gas produced is not pure; therefore purification technologies will be required in this project. Unless the project team can produce the hydrogen under pressure, which is difficult, the compression costs will be high.
- It would be good for the team to start working on predicting the effects of scaling output and considering the roadblocks involved in the scaling process.

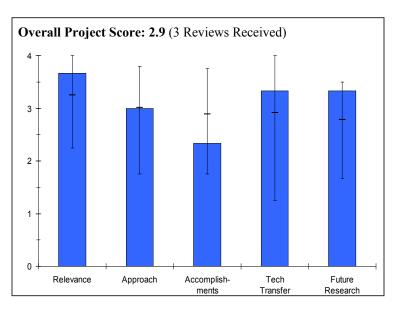
Specific recommendations and additions or deletions to the work scope

• Over the past year the team presented on 11 occasions, which would consume a significant amount of time and resources. It is recommended that they limit their conference attendance to the most prestigious conferences in order to better utilize their funds and time.

Project # PD-19: Development of Water Splitting Catalysts Using a Novel Molecular Evolution Approach Neal Woodbury, Arman Ghodousi, Trent Northen, Matt Greving, Pallav Kumar, Bharath Takulapalli, Nicolas Yakubchak, James Allen, JoAnn Williams, Trevor Thornton, Stephen Johnston, and Zhan-Gong Zhao; Arizona State University

Brief Summary of Project

The objectives of this project are to 1) develop a novel approach to creating molecular catalysts for redox reactions based on high throughput synthesis on electrodes; 2) mimic nature's approach to water splitting; and 3) reduce the overpotential by 30%. Specific objectives for fiscal year 2009 are to 1) optimize high throughput peptide synthesis on CombiMatrix Arrays; 2) optimize the multielectrode measurements of water splitting on the CombiMatrix Arrays; and 3) demonstrate several rounds of optimization for catalytic activity.



Question 1: Relevance to overall DOE objectives

This project earned a score of 3.7 for its relevance to DOE objectives.

- While this project is relevant to renewable hydrogen production, it implements and uses very fundamental research and it is not certain that it should belong in Basic Energy Sciences (BES).
- This project is critical to DOE's objective of improving efficiency of hydrogen production through improved catalysts.
- This project addresses the viability of direct renewable hydrogen production.

Question 2: Approach to performing the research and development

This project was rated **3.0** on its approach.

- It appears this project has a trial-and-error approach and a more systematic approach might be needed. Quite a bit of optimization is needed to yield of peptide synthesis and to prevent/minimize effects of side chain protecting groups during synthesis. It is unclear what the technical targets are.
- The project's approach is developing a broad range of catalysts using a peptide synthesizer. This involves a large amount of trial and error to see which formulations will work.
- The project's selection of the CombiMatrix as basis for evaluation is good approach.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated **2.3** based on accomplishments.

- This project does not show any significant breakthroughs from previous to this year. The research needs to be more focused on addressing key issues.
- Much progress has been made in producing and testing numerous formulations in this project. Automation allows mass throughput.
- The team faces difficulty in overcoming noise in results and is limiting. No specific results were shown and preferred catalysts were presented.

<u>Ouestion 4: Technology transfer/collaborations with industry, universities and other laboratories</u>

This project was rated **3.3** for technology transfer and collaboration.

- The project team had good collaborations with CombiMatrix and others.
- Coordination with CombiMatrix as equipment supplier has been good for the project.
- A strong industry partner has been good for this project.

Question 5: Approach to and relevance of proposed future research

This project was rated **3.3** for proposed future work.

- The project team needs to focus on addressing key issues and addressing key targets.
- The remaining work on this project intends to close-out research performed to date.

Strengths and weaknesses

Strengths

• This project has strong industry partners and a good technical approach.

Weaknesses

• The team needs to overcome the problem of noise in results in order to differentiate between peptides.

Specific recommendations and additions or deletions to the work scope

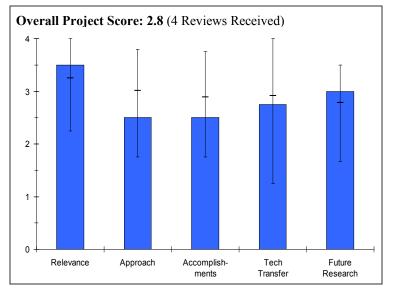
No specific recommendations were provided for this project.

Project # PD-20: High-Capacity, High Pressure Electrolysis System with Renewable Power Sources *Martin Shimko; Avalence LLC.*

Brief Summary of Project

The electrolyzer development project goals are to 1) achieve at least a 15x increase in the gas production rate of a single highpressure production cell; 2) demonstrate the high-pressure cell composite wrap which enables significant weight reduction; 3) build and test a 1/10th scale pilot plant; and 4) perform an economic assessment for a full scale plant (300 kg/day, 750 kW) that meets the 2017 DOE cost target of \$3.00/gge.

<u>Question 1: Relevance to overall DOE</u> <u>objectives</u>



This project earned a score of **3.5** for its relevance to DOE objectives.

- This project takes a very unique (but very challenging) approach to high-pressure hydrogen production. When successful, downstream mechanical compression stages will be reduced and possibly eliminated to help reduce the cost of delivered hydrogen gas.
- This project focuses on high-pressure electrolysis from potentially renewable sources for cost effective hydrogen generation.
- The electrolysis of water is a currently available hydrogen production technology. The challenge for the project to meet the Hydrogen Program and DOE energy goals is to develop the technology for it to produce hydrogen at a cost such that a hydrogen fuel cell vehicle could be competitive with a gasoline-based vehicle. The cost of electricity accounts for 50-75% of the cost of the hydrogen from electrolysis. It is doubtful that the cost of electricity can be substantially reduced. Therefore the only way to meet the DOE cost targets is for substantial electrolyzer capital cost reduction. It is, at best, unclear that the Avalence, LLC's technology approach can achieve the required capital cost reduction.
- In order for electrolysis to be a low greenhouse gas (GHG) emitting technology, the electricity used must be produced predominantly from renewable or non-carbon emitting technology. This could be realized in a large located at a central electrolysis facility near or at a wind-farm or other low GHG emitting electricity production facility. The Avalence technology seems to be targeted for distributed production and appears to be not well suited to large central scale production. For distributed electrolysis to use low GHG emitting electricity, the U.S. grid would need to use predominantly renewable or other low GHG emitting electricity production. This is a goal of DOE but, practically, will take a very long time to achieve.
- This project focuses on improving efficiency and cost of high-pressure electrolysis systems.

Question 2: Approach to performing the research and development

This project was rated **2.5** on its approach.

- It is good to see that the 2008 goal of 6500 psi wrapped cell demonstration has been reduced to 2500 psi in 2009. In this project, many of the same design challenges still exist a year later. This seems to indicate that the project may need additional resources to overcome these barriers.
- This project appears to be mostly engineering and optimization and not much innovative and novel approach. The 2500 psig is still not a high enough pressure where a hydrogen compressor can be eliminated. It is important that work needs to concentrate on 6500 psig system for H₂ fueling applications for vehicles.

- Nowhere in the project goals is cost reduction nor a cost target specifically mentioned. This is the key goal for electrolysis-based hydrogen production for the DOE Hydrogen Program. The project milestones include a "go/no-go" decision 2 years into this 4.5-year project, based on electrolyzer performance and cost but there is no quantification of these targets.
- The project goals state that a full-scale production unit would produce only 300 kg H₂/day. DOE expects distributed forecourt refueling station hydrogen production units to need to produce 1500 kg/day. It would take five 300 kg/day units to achieve this. The costs would thus scale linearly rather than a single 1000 or 1500 kg/day full-scale unit that would have an economy of scale advantage and thus have a better chance of meeting the DOE cost targets. For large central scale hydrogen production, the larger the base electrolyzer unit the lower its cost based on the same economy of scale argument. The Avalence technology by nature is difficult to scale-up to large base electrolyzer units.
- The approach of using multiple concentric tubular "cells" to obtain some advantage for high-pressure operations is novel but very challenging.
- There are four slides in the presentation devoted to discussing using hydrogen as an energy storage system that includes an electrolyzer and fuel cell. Although this is an interesting concept worth pursuing, it is not part of this Avalence project.
- The project focused on addressing engineering challenges of the high-pressure system.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated **2.5** based on accomplishments.

- The project drawings of the various options for the 1000 psi single cell are encouraging but no evidence was provided that construction of the actual test cell has begun (other than the valving control panel). One question raised on slide 14 was to settle on a design pressure (2500 vs. 6500). A staged approach is recommended where starting at lower pressures would first be achieved before moving on. The identification, testing, tube forming and joining of sheet membrane materials are listed as two accomplishments. Details surrounding that work would strengthen the presentation and should have been shared.
- This project appears to be mostly for practical engineering design activities and more progress towards a scalable 6500 psig system should be seen. Also, work on how the system can be integrated with renewable sources and manage supply and demand should be shown.
- Not enough progress is observed with this project in working towards meeting DOE's cost target.
- This is a relatively new project. It was initiated in May 2008 and is currently on track vs. its planned schedule of accomplishments.
- The project has identified membrane materials; shown that it can be formed into tubes; seam sealed and has initiated the construction of a test cell.
- Steady progress has been made toward objectives of this project.

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated **2.8** for technology transfer and collaboration.

- A team member from MIT was not shown in this year's partner list. Has their collaborative work been completed or was some other conflict keeping them from assisting with the two-phase fluid design? It was unclear from the slides and presentation how any particular partner was assisting to overcome the project barriers.
- Not much collaboration with other institutions was observed in this project.
- Avalence is partnering with HyperComp, which is experienced in high-pressure wrapped composite vessels. This is a good collaboration. The project team is also partnering with the Hydrogen Energy Center and MaineOxy but it is not clear what these collaborations offer.
- It would seem that there would be other very fruitful collaborations that could add to the capabilities of Avalence to increase the probability of a successful project.
- The project has good coordination and interaction amongst its partners.

<u>Ouestion 5: Approach to and relevance of proposed future research</u>

This project was rated **3.0** for proposed future work.

- There seems to be a couple of options with regard to the single cell design and the design pressure of this project. It is unclear what criteria will be used to select a winner, unless both designs are going to be fabricated and tested against each other. It is suggested that the team throw a couple simple IV curves up at different pressures.
- The team needs to also address any potential challenges associated with the 6500 psig system (other than the hose leaking issue observed so far).
- The project's current system is looking at around 300 kg/day. There is a need to focus more attention on addressing any potential scale-up issues (to 1500 kg/day for forecourt and larger for central production).
- There is no slide that is titled Future Work Plan, but the Project Technical Objectives and Program Schedule do provide an overall work plan that is well organized.
- More detailed information on the work plan for the next 12 -18 months leading to the "go/no-go" decision point would be very helpful for this project.
- Future work continues current activities in this project.

Strengths and weaknesses

Strengths

- The project's unique design is a plus but there seems to be up-coming challenges. The electrochemical (high) pressure goals will be valuable in reducing mechanical compression stages downstream.
- This is a relatively new project. It was initiated in May 2008 and is currently on track vs. its planned schedule of accomplishments.
- This project has identified membrane material; shown it can be formed into tubes; seam sealed and has initiated the construction of a test cell.
- There is no slide that is titled Future Work Plan but the Project Technical Objectives and Program Schedule do provide an overall work plan that is well organized.

Weaknesses

- The team should provide a clearer indication of where the project is with regards to objectives and timeline. Regrettably very few details are provided on the year's accomplishments.
- It is unclear that the Avalence technology approach can achieve the required capital cost reduction targeted by the DOE Hydrogen Program. The basic tubular design is well suited for high-pressure operation but this design and operating pressure are relatively expensive. This design is also not well suited for scale-up to a large base (>1000 kg-H₂/day) electrolyzer. Thus, the project could lose the potential capital cost savings resulting from economy of scale to meet the production quantities sought by the DOE program.
- In order for electrolysis to be a low GHG emitting technology, the electricity used must be produced predominantly from renewable or non-carbon emitting technology. This could be realized in a large central location at an electrolysis facility near or at a wind-farm or other low GHG emitting electricity production facility. The Avalence technology seems to be targeted for distributed production and appears to be not well suited to large central scale production. For distributed electrolysis to use low GHG emitting electricity, the U.S. grid would need to use predominantly renewable or other low GHG emitting electricity production. This is a goal of DOE but practically will take a very long time to achieve.
- Nowhere in the project goals is cost reduction nor a cost target specifically mentioned. This is the key goal for electrolysis-based hydrogen production for the DOE Hydrogen Program. The project milestones include a "go/no-go" decision 2 years into this 4.5-year project, based on electrolyzer performance and cost but there is no quantification of these targets.
- It would seem that there would be other very fruitful collaborations that could add to the capabilities of Avalence to increase the probability of success of this project.

Specific recommendations and additions or deletions to the work scope

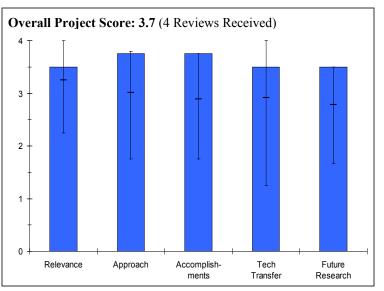
- Cell degradation was discussed during the Q&A with an answer of "No cell degradation". This seems impossible. Running the cell over 5,000 50,000 hours will degrade the cell in some manner, so perhaps more sensitive voltage measurements should be made to quantify.
- This project should develop a detailed cost estimate assuming success of their design. This should be compared with the DOE cost targets for Distributed and Central Production to determine if this electrolysis technology approach should be pursued.

Project # PD-21: PEM Electrolyzer Incorporating an Advanced Low Cost Membrane

Monjid Hamdan; Giner Electrochemical Systems, LLC

Brief Summary of Project

The overall project objective is to develop and demonstrate an advanced low-cost, moderate-pressure proton exchange membrane (PEM) water electrolyzer system to meet DOE targets for distributed electrolysis, by developing a 1) highefficiency, low-cost membrane; 2) long-life cell-separator; 3) lower-cost prototype electrolyzer stack and system; and 4) prototype electrolyzer system at the National Renewable Energy Laboratory. Objectives for fiscal year 2008-2009 are to 1) develop a low-cost, high-efficiency, highstrength membrane with electrochemical performance comparable to thin Nafion® (N1135) and high strength to allow operation at 300 psig and 80-90°C; 2)



initiate cell-separator development; and 3) complete preliminary system design and development of lower-cost components.

Question 1: Relevance to overall DOE objectives

This project earned a score of **3.5** for its relevance to DOE objectives.

- Improving capital cost and system efficiency of PEM electrolysis is vital to bring reliable and low-tech electrolyzers to distributed/home fueling stations.
- This project's focus on hydrogen production helps in addressing issues with capital cost and system efficiency.
- This project has clearly defined targets.
- Electrolysis of water is a currently available hydrogen production technology. The challenge for this project is to develop technology to produce hydrogen at a cost such that a hydrogen fuel cell vehicle could be competitive with a gasoline-based vehicle. The cost of electricity accounts for 50-75% of the cost of the hydrogen from electrolysis. It is doubtful that the cost of electricity can be substantially reduced. Therefore the only way to meet the DOE cost targets is for substantial electrolyzer capital cost reduction and to improve the electrolyzer efficiency. The approach that Giner Electrochemical Systems, LLC. (GES) is taking has the opportunity to substantially reduce electrolysis capital costs and improve efficiency.
- In order for electrolysis to be a low GHG emitting technology, the electricity used must be produced predominantly from renewable or non-carbon emitting technology. This could be realized in a large central electrolysis facility located near or at a wind-farm or other low GHG emitting electricity production facility. The Giner PEM technology could be scaled to reasonably large base electrolysis units suited for this purpose. For distributed electrolysis to use low GHG emitting electricity, the U.S. grid would need to use predominantly renewable or other low GHG emitting electricity production. This is a goal of DOE but practically will take a very long time to achieve.
- Project addresses several key objectives in the area of electrolysis improvement.

Question 2: Approach to performing the research and development

This project was rated **3.8** on its approach.

- This project has a strong technical team and partnerships working to overcome the project challenges. After demonstrating ~1200 psi without a pressure dome why is it required for a 'mere' 300 psi stack? The O&M impact of the N₂ purge and frequency of the dome will be interesting to ask about next year.
- The team is addressing the low-cost membrane, durability and high efficiency of their project technology.
- This project is addressing key issues, which are durability with Dimension stable membrane (DSM) and cost with Bi Phenel Sulfone, H form (BPSH).
- This project lays out a logical approach to targets (from inside out) membrane to stack to integrated system.
- Given the fact that the stack pressure is relatively low, going with a round design might not be a best fit in terms of system layout (the system is in a rectangular box).
- The Giner research is targeted to: develop a high-efficiency low-cost membrane, a long life lower cost cell separator, and to reduce the cost and improve the efficiency of the BOP. These are exactly the improvements needed for PEM-based electrolysis to meet the DOE Hydrogen Program cost targets.
- Giner has and continues to do detailed cost estimates to ensure their approach can lead to achieving the DOE cost targets. Initial economic analysis results are promising.
- Giner could increase their probability of success of achieving the DOE cost targets if they put some more thought and effort into trying to target larger and larger cell/base electrolyzer sizes.
- This is a well-focused project aimed at reducing cost and improving efficiency of PEM water electrolyzer systems.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated 3.8 based on accomplishments.

- The team appears to be making steady progress towards an alternative membrane for their stacks. While the slope of the cell voltage on slide 10 appears to be 'zero' there has to be some cell degradation. Extrapolating from 1000 hours (milestone met) to 50,000 hours seems a bit of a stretch. As new lower cost BOP materials are selected it will be interesting to see if GES can also drive the temperature range from 50°C towards the 90°C to take advantage of the efficiency boost.
- This project has a good durability testing progress 1,000 hrs at 80°C without degradation (DSM). They also have a 71 75% stack efficiency lower heating value (LHV).
- Good progress has been made in addressing safety, durability and costs in this project.
- Giner has successfully developed a Dimensionally Stable Membrane (DSM) based on a novel design incorporating perfluorosulfonic acid (PFSA) ionomer in an engineering plastic support. Lab testing has demonstrated improved performance over Nafion membranes and projects to >45,000 hour lifetime. They also have initial promising results on a Bi-Phenyl-Sulfone-based membrane. Both these membranes can be substantially lower cost than Nafion.
- Giner has developed a lower cost cell separator that looks promising in initial lab tests and is in progress on working with vendors to reduce the cost and improve the efficiency of the BOP.
- The project team is making excellent progress toward stated objectives of project.

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated **3.5** for technology transfer and collaboration.

- The Parker Hannifin Corporation and Virginia Polytechnic Institute and State University (VT) seem to be strong partnerships for the project's targeted tasks.
- The project has good collaborations with Virginia Tech for low-cost membrane development and Parker Hannifin Corp. for system and component development.
- Giner is collaborating with Virginia Tech University on new polymer membranes and with Parker Hannifin Corp. on the BOP issues. These are key additions to Giner's in-house capabilities for success in this project.
- There could be additional collaborations that would further enable this project.
- Good collaboration with industry and university partners to take advantage of strengths available for incorporation into project.

<u>Ouestion 5: Approach to and relevance of proposed future research</u>

This project was rated **3.5** for proposed future work.

- The project team's focus on hydrogen drying is an excellent area for cost and efficiency improvement. Stack/BOP would ideally handle higher temps 80-90°C. Next year it would be interesting to hear more about how the hydrogen drier has been improved and how the 97% efficiency was determined. More information should be shared on any new deionized (DI) water level sensing process or device in the phase separator.
- The project team should focus some efforts on system integration, power electronics and testing to address durability and operational issues.
- The team should consider leveraging parallel fuel cell MEA development for synergies.
- The future work plan for this project is brief but clear. A more detailed work plan would be helpful.
- Future work is well planned to continue current excellent progress to address electrolyzer costs and efficiency issues.

Strengths and weaknesses

Strengths

- The project's strong technical teams and partnerships are making progress. The PI did an excellent job highlighting the technical accomplishments.
- The Giner research is targeted to: developing a high-efficiency, low-cost membrane, a long life lower cost cell separator, and reducing the cost and improving the efficiency of the BOP. These are exactly the improvements needed for PEM-based electrolysis to meet the DOE Hydrogen Program cost targets.
- Giner has and continues to do detailed cost estimates to ensure their approach can lead to achieving the DOE cost targets. Initial economic analysis results are promising.
- Giner has successfully developed a Dimensionally Stable Membrane (DSM) based on a novel design incorporating PFSA ionomer in an engineering plastic support. Lab testing has demonstrated improved performance over Nafion membranes and projects to >45,000 hour lifetime. They also have initial promising results on a Bi-Phenyl-Sulfone-based membrane. Both these membranes can be substantially lower cost than Nafion.
- Giner has developed a lower cost cell separator that looks promising in initial lab tests and is in progress on working with vendors to reduce the cost and improve the efficiency of the BOP.

<u>Weaknesses</u>

- Why is the dome used in this project? The team needs to present a better answer to stack degradation rather than saying it is "low."
- Giner could increase their probability of success of achieving the DOE cost targets if they put some more thought and effort into trying to target larger and larger cell/base electrolyzer sizes.

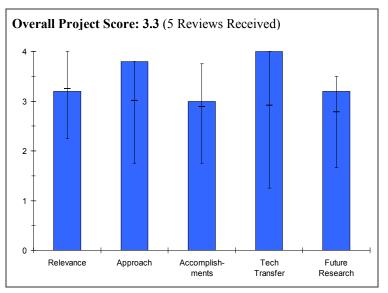
Specific recommendations and additions or deletions to the work scope

No specific recommendations were provided for this project.

Project # PD-22: Photoelectrochemical Hydrogen Production: DOE PEC Working Group Overview *Eric L. Miller; University of Hawaii at Manoa*

Brief Summary of Project

The primary objective of the DOE Photoelectrochemical (PEC) Working Group is to develop practical solar hydrogen-producing technology using innovative semiconductor materials and devices research and development to foster the needed scientific breakthroughs. The objectives of the DOE-solar hydrogen generation research PEC are to 1) identify and develop PEC thin-film materials systems compatible with high-efficiency, low-cost hydrogen production devices; 2) demonstrate a functional multi-junction device incorporating best-available PEC film materials; 3) develop collaborative avenues (national and international) integrating the best theoretical, synthesis



and analytical techniques, for optimizing future PEC materials and devices; and 4) explore avenues toward manufacture-scaled devices and systems.

Question 1: Relevance to overall DOE objectives

This project earned a score of **3.2** for its relevance to DOE objectives.

- DOE's PEC working group is playing a critical role in accelerating the developing of the PEC technology, which is one of the key pathways in DOE's renewable hydrogen production goals.
- PEC is a potentially long-term hydrogen producer and therefore does very little to bring down cost of hydrogen in the next 10-15 years to meet the overall DOE objectives. However, the potential impact of PEC is very high.
- The working group is effectively coordinating theoretical, modeling, and experimental efforts directed towards meeting the DOE multi-year PEC hydrogen production targets.
- This group multiplies the effectiveness of this technology development by increased information flow between teams, thus allowing a wide search of materials without overlap of efforts.
- The high-risk/high-payoff search for the Holy Grail, providing direct storage of solar energy in a transportable hydrogen energy carrier is fully supportive of program objectives. Establishing cost effectiveness remains to be done in order to assess level of importance of the process to program objectives.

<u>Ouestion 2: Approach to performing the research and development</u>

This project was rated **3.8** on its approach.

- The PEC working group approach to problem solving is outstanding. Their combination of theory, experiment and analysis is what will be needed to solve this challenging problem.
- The close coordination between various team members is helping accelerate the development and avoiding repetition.
- Lessons learned and development of the material library will be critical to development of this project in the long term.
- White papers approach is pretty good for current and future developments of this project.
- This summary of PEC work showed a good cross-section of the working being conducted. The standardized test protocol is a valuable tool at this (early) point in the project.

- The presentation should provide information on the budget for managing/administrating the PEC Working Group. The use of White Papers to document current research status is good, but it is unclear what the status/availability of the white papers is from the presentation, or what kind of collaboration is being achieved within each task force. The development of standardized testing and reporting protocols is critical, so it is very good that progress is being made here.
- The project's integrated feedback loop using all technical tools available with tight inclusion of the technical experts is characteristic of this project. No other material development project has integrated the levels of sophistication and depth of inquiry than this project. Flow charting of critical parameters assessment to permit "go/no-go" decisions is superior for this project. This feature is partly characteristic of the process physics and partly due to highly interactive management of distributed work.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated **3.0** based on accomplishments.

- The team needs to look at the progress of the whole group in a structured format, rather than a list. For example, divide the work into class of materials (similar to hydrogen storage) program with "go/no-go" decision points and/or conditions identified to allow the group to move on from something that is non-practical.
- Generally, this group has made steady progress on materials and developing capabilities.
- Steady progress is being made to identify and characterize candidate materials in this project.
- The team's rate of progress is partially hampered by budget and partially by the broad scope of materials under consideration. Future down-selection efforts may help speed progress on most promising materials.
- The project appears to continue to pursue incremental improvements of inadequate materials even though dramatic changes are essential to meeting cost performance metrics. It's always hard to move people away from things they know into unknown, and it's impossible to demand instant invention of new materials that would surely be better than current materials.

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated **4.0** for technology transfer and collaboration.

- This project is an outstanding example of collaboration to deliver on common goals. Perhaps a good addition would be to get an industry entity involved for a different perspective.
- It is good to see a growing number of domestic and (more recently) international researchers involved in this project. Are there companies out there with brilliant materials people (GE, 3M?) that would be interested in collaborating on this?
- The purpose of this project is to foster collaboration on PEC hydrogen production R&D. All DOE-funded PEC projects are actively participating in the working group to share information and develop common testing and reporting protocols, and international collaboration is being achieved through the International Energy Agency (IEA).
- This project has every individual and every institution with the interest and skills related to the task have been invited to an open community for discussion of optional paths forward and decisions regarding focused funding and effort.

Question 5: Approach to and relevance of proposed future research

This project was rated **3.2** for proposed future work.

- The team's future work should also include an element on system development and cost estimation.
- The project's 'tool chest' is getting full enough that large amounts of material characterizations can be processed in the coming year. Perhaps the team should highlight any benchmarking the PEC Working Group has conducted with international community.
- Strong working relationships have been built in the PEC working group and good plans are in place to continue that work in the future. Future focus continues to be on coordinating efforts to develop and apply the PEC "tool

chest," to develop and apply screening protocols and test procedures, and to make down-selection decisions that will focus R&D on the most promising materials classes.

• Future work did not achieve "outstanding" category simply because a plan had not been developed that establishes a clear path toward different approach to discovering truly promising and revolutionary materials. Modeling and simulation remains about as difficult as synthesis and characterization so that more rapid screening of complex materials is still elusive. Planning might be improved by focusing effort on work-arounds for inadequate aspects of otherwise promising concepts. More effort should be implemented in developing theoretical screening of advanced materials. This is partly a DOE responsibility to provide more funding and partly a project responsibility to properly apply such funds.

Strengths and weaknesses

Strengths

- This project has good collaboration between outstanding researchers.
- Growing domestic and international collaboration for this project is promising.
- Collaboration and coordination between various stakeholder groups is a highlight of this project. The team's work is directed towards meeting DOE PEC targets.
- The direct conversion of solar energy to transportable stored energy is a strength reflected only in direct electrolysis. PEC is presumed to be more efficient and cost effective than direct electrolysis. Progress in PEC is also directly interesting to improved photovoltaics, so that there could be presumed spin-off benefits of the effort.

Weaknesses

- The project needs to get an industry view.
- Can DOE lure any material scientists from corporate America to help?
- Many years of this project's research efforts have been spent without notable progress toward adequate performance. This weakness might be turned into a strength through the project re-orientation to an integrated feedback loop between materials modeling/simulation, synthesis and characterization.

Specific recommendations and additions or deletions to the work scope

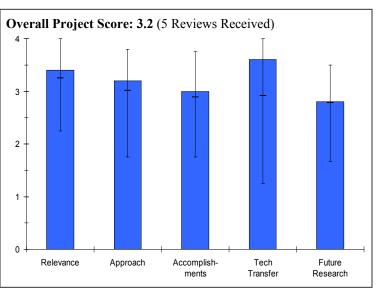
No specific recommendations were provided for this project.

Project # PD-23: Technoeconomic Boundary Analysis of Photoelectrochemical (PEC) Hydrogen Producing Systems

Brian James; Directed Technologies, Inc.

Brief Summary of Project

The objectives for this project are to 1) perform economic and technical analysis of H_2 producing systems including PEC H_2 production conceptual system designs and hydrogen cost calculations; and 2) identify key factors affecting cost estimates. Design features include 1) advancing implementation of new technology by designing physical systems tailored to PEC materials; 2) design of gas collection system for continuous operation; and 3) design of solar collection for maximum sunlight conversion.



Question 1: Relevance to overall DOE <u>objectives</u>

This project earned a score of 3.4 for its relevance to DOE objectives.

- The project team involved the cost estimates at an early stage to assess how close or far their approach was from being practical and competitive.
- For the team's progress to be measured towards hydrogen production cost targets, a cost basis must be established through modeling of current PEC "state-of-the art" systems. This modeling effort is essential for showing progress towards DOE cost goals and for identifying high-cost components that can be targeted with R&D.
- This project's analysis is critical to guiding researchers toward a feasible system application.
- The team's work is highly relevant to DOE program goals to establish "go/no-go" decision frameworks for the broad suite of possible activities. However, the foundation of the work is far more assumption-driven than fact-driven so that decisions based on this work are not yet possible.

Question 2: Approach to performing the research and development

This project was rated **3.2** on its approach.

- The team's approach to do economic analysis is fair; however a lot of assumptions were made about cost, system design and footprint possibilities.
- The team needs to involve an industry representative for feedback and input into the cost estimation process.
- The team needs to pay more attention to land use and site preparation costs. It should be a major component in the cost breakdown.
- The technoeconomic model is well designed in this project. Because these systems are still only conceptual, it is appropriate that the focus has been on two of the simpler material applications. The design effort included expert input at multiple steps.
- The process that was followed places limits on the scope of costs that may be associated with this technology.
- The project's approach framework is essentially what is needed, but the data essential to its useful application remains elusive. Consequently, more work is warranted until such time as real data becomes available.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated **3.0** based on accomplishments.

- The project team achieved the goal of estimated produced cost from hydrogen after making certain design, system and cost assumptions.
- Regarding the 1 tonne per day (TPD) system, would this require many pumps because it includes a slurry mixing system? The only pump listed on the BOM is for water make-up. When the question was asked of where the slurry mixing pumps cost is captured, the response was essentially: "Included somewhere else." The sum of all of the costs on slide 7 (BOM) reaches the \$2,080,963 value, making it unclear how the pumps could have been added in to the capital cost of the 1 TPD system somewhere else,. The cost/operation of these pumps are not trivial based on 43 acres of slurry in bags.
- The project has an excellent first modeling of the economics of PEC systems. Results from the modeling should be helpful in future cost reduction efforts for hydrogen from PEC generation.
- While performing an outstanding analysis of concepts, half the project's concepts implemented have not been brought through a feasibility first (suspended colloids). Colloids have not shown ability to produce hydrogen or oxygen bubbles in any arrangement, and should not be considered for scale-up. Only spectrum adsorption appears to be operating in this technology embodiment. Electrochemistry and transport processes do not provide for a feasible scale-up in this reviewer's experience.
- The project's technical accomplishments in formulating the model framework and its general implementation are outstanding. Nevertheless, more data is necessary before barriers to useful application are surmounted. Some design options can be shown either inadequate or perhaps better than others, but all such decisions are premature until active materials are discovered.

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated **3.6** for technology transfer and collaboration.

- Good collaboration has been provided by the PEC group. They, however, need to involve an (energy) industry member.
- It is unclear how the partners contributed to the project's results.
- The project team has excellent collaboration through their work with the PEC Working Group. They directly drew status information and system design concepts from researchers in the PEC Working Group and included them in their models.
- This project has effectively involved the group of researchers associated with it.
- The task leaders were open to input and collaboration with concept leaders.

Question 5: Approach to and relevance of proposed future research

This project was rated 2.8 for proposed future work.

- The project has a fair list of proposed work for completion as it is in the early stages of work.
- This BOP work seems premature without having at least one strong candidate material.
- The project is nearing completion, so preparation of a final report is the next step in their current contract. Future work to include new materials systems and fabrication methods as well as exploring new system concepts would be valuable additions to the techno-economic modeling of PEC systems.
- The work proposed by the team is reasonable.
- Incorporation of new data and some new processes can continue to support program planning for this project.

Strengths and weaknesses

Strengths

- The project has a strong background in H2A type economic analysis.
- This project will help measure progress towards and potential for meeting the DOE cost targets. The methodology was systematic and included good collaboration with outside experts.
- This project provides a decision framework to implement "go/no-go" directions.

Weaknesses

- The project team lacks an industrial background.
- Imagining what the 'winning' PEC material will look like is difficult enough without guessing what type of BOP/process will be required to take advantage of its unique properties.
- There is no validation effort on this model.
- The project is too heavily leaning on unproven technology (colloids). Among the PEC consortium, there appears to be significant disagreement that this is a remotely viable pathway.
- The following is not a problem for the analysis project, but a problem for the implementation of analysis findings: the team's effort should become more focused on discovering slurry particulates that would permit actual operation of the dual bed slurry concept.

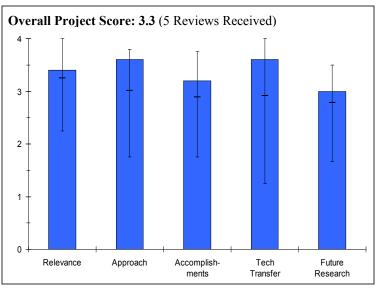
Specific recommendations and additions or deletions to the work scope

No specific recommendations were provided for this project.

Project # PD-24: Characterization of Materials for Photoelectrochemical Hydrogen Production (PEC) *Clemens Heske; University of Nevada, Las Vegas*

Brief Summary of Project

The goals of this project are to 1) develop standardized testing and reporting protocols for PEC material/interfaces evaluation; and 2) publish the standardized PEC characterization techniques in a peerreviewed journal to reach a maximum number of people. The purpose and scope of the project is to 1) properly define the efficiencies (solar-to-hydrogen) that should be used for wide-scale reporting vs. efficiencies (incident photon conversion efficiency) that are useful for scientific, diagnostic purposes only; 2) describe proper PEC procedures for characterizing planar photoelectrode materials; 3) focus on single band gap absorber material only; and 4) describe the techniques, the knowledge



gained, the experimental set-up and procedure, the data analysis, and the potential pitfalls and limitations.

Question 1: Relevance to overall DOE objectives

This project earned a score of 3.4 for its relevance to DOE objectives.

- This project supplies a critical tool chest for the PEC development. The project is instrumental for analysis of PEC materials.
- The project is well aligned with the program goals of achieving system efficiency and life targets.
- Characterization of electrochemical properties is essential for hydrogen generation employing photoelectrochemical (PEC) electrolysis of water. The PEC process is the most direct method for producing hydrogen from water with no carbon footprint. Unlike the other CO₂-free hydrogen production processes, such as S-I cycle, Cu-Cl Cycle, hybrid cycle, and high-temperature SOEC electrolysis, where hydrogen production takes place in a highly corrosive chemical environment. The PEC process is relatively simple with respect to materials handling. The characterization of the photochemical electrodes for splitting water with only sunlight is of major importance in hydrogen generation.
- This project is a workhorse for the technology, and has done admirably to characterize and promote the understanding of the technology's inner workings.

Question 2: Approach to performing the research and development

This project was rated **3.6** on its approach.

- This project has a good approach to use a standardized characterization method set to disseminate it to the community.
- This project has good experimental capabilities and very powerful analysis toolkits.
- The project team should use well-established flow chart symbols for easier understanding of decision points versus other process steps. Glad to see that there seems to be a process/tracking for calibration of all the sensors.
- The team's approach is innovative and appears to be sufficient for achieving the desired results.
- The project has a comprehensive approach for characterizing the electrochemical properties of candidate materials is described.
- The project's technical approach is very reasonable.

<u>Ouestion 3: Technical accomplishments and progress toward project and DOE goals</u></u>

This project was rated 3.2 based on accomplishments.

- The project's progress was presented against milestones. There was no cost extension for another year requested which may represent some delay in timeline.
- The project appears to be successfully applying and developing state-of-the art measurement techniques and equipment to achieve the required experimental results.
- The project has shown good experimental results that can be explained fundamentally.
- The accomplishment reports analysis on candidate materials is an example of technical achievements made. A table showing the properties of the most promising materials analyzed, including metal oxides and compound semiconductors, would have been more useful.
- No details are given by the PI regarding the characterization of the chemical stability of the materials. This is one of the major issues in the PEC process.
- The progress report illustrates the experimental facilities available at UNLV with pictures. However, no details are given and contributions from other team members on experimental or theoretical analysis, such as density functional theory (DFT) calculations, are not discussed.
- The project's *in situ* characterization process is not elucidated.
- The team's analysis has been modified to fit PEC material characterization needs. Additional modifications are proposed to increase surface chemistry understanding.

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated **3.6** for technology transfer and collaboration.

- This project has very good collaborations between this group and rest of the PEC team, as also seen live during a previous UNLV visit.
- Are there any other places in the world conducting characterization testing on PEC material? If so, as this testing is still in the early phases, what have the researchers done to benchmark or reproduce work being conducted at other institutions?
- Collaboration appears to be excellent with all partners in this project.
- The collaboration is impressive but no specific details regarding how the characterization is performed as a team and how the each member of the team interacts with one another. The standardized PEC evaluation process should have been described cited as a reference.
- The project collaboration is admirable. This team has collaborated and improved fundamental understanding for the entire consortium.

Question 5: Approach to and relevance of proposed future research

This project was rated **3.0** for proposed future work.

- The teams should continue doing more of the same alongside developing new techniques, which is needed.
- The team's proposed future work looks reasonable and in line with program objectives.
- A future plan is included without any details on how researchers could have candidate material evaluated with guidance from the project team using the standardized test method developed under the project.
- The team will continue the excellent work they are already doing, plus adding ability to further understand surface chemistry of the PEC.

Strengths and weaknesses

Strengths

- The team, especially the group leader, has used powerful analytical techniques and technical expertise in this project.
- This project is providing a lot of feedback to the Standardized Test Protocol project.
- The project is well aligned with the program goals of achieving system efficiency and life targets.

- The team's approach is innovative and appears to be sufficient for achieving the desired results.
- The project appears to be successfully applying and developing state-of-the art measurement techniques and equipment to achieve the required experimental results.
- The project has shown good experimental results that can be explained fundamentally.
- Collaboration appears to be excellent with all partners.
- The PI is a highly competent researcher in material characterization related to the PEC process with an excellent track record in publication and presentations. Availability of a standardized test method for PEC material evaluation would be immensely valuable.

Weaknesses

- The project team's lab safety is a concern.
- The report lacks many specifics.

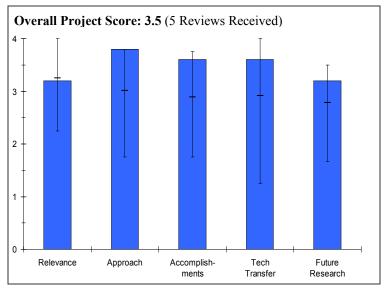
Specific recommendations and additions or deletions to the work scope

• The project team should clean up the lab area (papers, cardboard boxes, etc.) shown on slides 18 and 19. There are reports on top of devices obstructing device cooling/air flow (slide 18).

Project # PD-25: Nanostructured MoS₂ and WS₂ for the Solar Production of Hydrogen *Thomas F. Jaramillo; Stanford University*

Brief Summary of Project

The main objective of the project is to develop new photoelectrode materials with new properties that can potentially meet DOE targets (2013 and 2018) for usable semiconductor band gap, chemical conversion process efficiency, and durability. To date, there are no known materials that simultaneously meet these DOE targets. The project aims to quantum confine semiconductors through nanostructure to tailor their bulk and surface properties for photoelectrochemical cells. By synthesizing ~ 5 nm diameter MoS₂ nanoparticles, Stanford has tuned the band gap from 1.2 eV to 1.7 eV, a value very close to DOE's 2013 and 2018 targets of 2.3 eV and 2.0 eV, respectively.



Question 1: Relevance to overall DOE objectives

This project earned a score of **3.2** for its relevance to DOE objectives.

- The PEC materials development in this project is a key to PEC pathway success for hydrogen production.
- This project is well aligned with DOE's program goals of achieving high efficiency and durability at low cost.
- This work expands understanding of PEC base material behavior. The work done here is expanding the ability to find solutions to the PEC systems.
- This project is fully supportive of program objectives. Its approach is critical to for future success of photoelectrochemical hydrogen production enterprise. The project's exploration of alternative approaches to band gap and band edge modification in the search for appropriate configurations for efficient and inexpensive hydrogen production is crucial.

Question 2: Approach to performing the research and development

This project was rated **3.8** on its approach.

- The project's approach of quantum confinement is novel, unique and a distinct way to address the solution to search of right PEC material. In theory this should all work but the team needs to practically demonstrate it.
- The team appears to have a unique approach to solving some of the numerous PEC barriers.
- The team's approach is innovative and shows potential to be able to tailor material properties to achieve high efficiency and low cost (i.e., do not need Nobel metals). Durability was not addressed in this project.
- This is a very creative approach. This reviewer is interested in the handling and robustness of the system. Surface damage seems to be significant due to handling and exposure. This early in the project however, this should not be a huge concern. This technology may very well find application in a different area as well.
- The assessment of outstanding is certainly dependent on successful implementation of the project's approach.
- The study of alternative approaches to doping and alloying that modify band gap and band edge alignment while retaining intrinsic materials performance is an innovative and possibly important approach to acquiring dramatic improvements in poorly performing materials. "Outstanding" award in this project is dependent on additional assessment of the retention of quantum confinement effects for the various structural options presented. Some theoretical/analytic evidence of quantum confinement should be sought before moving to the synthesis/characterization phase in this project.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated 3.6 based on accomplishments.

- This project is a good demonstration of success in achieving the band gap with quantum confinement.
- Demonstration of success in various stages of the final process step by step is shown in this project. The project team now needs to do it all together and show the right behavior at the PEC level.
- The project has had good progress towards DOE's goals from the opposite direction.
- This project is showing significant progress towards meeting goal of 2.0 eV band gap for photo cathodes.
- There are a number of fundamental questions that still need to be answered (e.g., molecular nanowire orientation), but the project appears to be poised to answer most, if not all of them.
- The team has done very good work in the time and budget allocated.
- The project's synthesis of samples has been successful. MoS nanoparticles extended the MoS band gap from 1.2 eV to 1.7 eV. .Further development indicates band gap extension to over 2 eV. Developed AlO₃ frameworks for nanowires and demonstrated data essential to assuring electrochemical deposition of MoS₂ as nanowires inside AlO₃ framework. Nevertheless, it is not clear from analysis that nanowire configuration will retain quantum confinement effects.

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated **3.6** for technology transfer and collaboration.

- The PEC group has outstanding collaboration and approach for working together.
- More collaboration will be needed as this project progresses.
- This project appears to be very open in sharing both techniques and fundamental understandings of findings.
- The PI is a strong contributor to collaborative work and is one of the most articulate members of the working group.

Question 5: Approach to and relevance of proposed future research

This project was rated **3.2** for proposed future work.

- The team needs to demonstrate the success in terms of photoelectrochemical behavior of the synthesized materials.
- This is an ambitious project that would probably benefit from more time and funding.
- The project team should engage the theoretical group in assessing energetic isolation of nanowire building blocks to assess retention of quantum confinement. Such theoretical studies might identify either materials or processing particulars to assure such retention. The proposed future work did not address this feature.

Strengths and weaknesses

Strengths

- This project shows a different approach allowing much better control of material properties.
- This project is well aligned with DOE's program goals of achieving high efficiency and durability at low cost.
- The project's approach is innovative and shows potential to be able to tailor material properties to achieve high efficiency and low cost (i.e. do not need Nobel metals).
- This project is showing significant progress towards meeting goal of 2.0 eV band gap for photo cathodes.
- Absent miraculous discovery of a new material that meets all the requirements for band gap, band edge alignment, charge carrier generation, survivability and mobility, approaches such as promoted in this project will be essential to improving specific materials properties to improve overall material performance.

Weaknesses

• This project may construct and implement materials that are extremely expensive to manufacture by bulk techniques.

- Durability was not addressed in this project.
- There are a number of fundamental questions that still need to be answered (e.g., molecular nanowire orientation), but the project appears to be poised to answer most, if not all of them.
- More collaboration will be needed as the project progresses.
- The work presented suffers from a lack of theoretical performance modeling and molecular dynamics assessments of stable configurations of materials under nano-configurations. Virtually all planning has been based on observation of gross properties for nano-scale configurations. Such macro-scale properties do not assure the retention of other properties essential to performance.

Specific recommendations and additions or deletions to the work scope

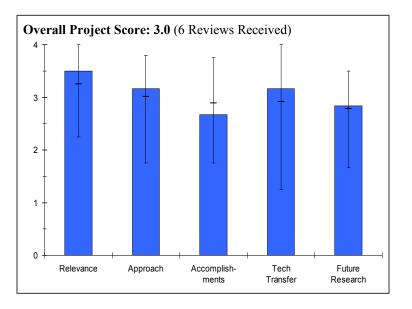
- This is an ambitious project that would probably benefit from more time and funding.
- This project may benefit from modeling of light adsorption and bulk characteristics. Optical absorption rates would determine thickness of nano-materials required, and mechanical property of this layer would be of concern. Mechanical considerations should be accounted for.

Project # PD-26: Development of Hydrogen Selective Membranes/Modules as Reactors/Separators for Distributed Hydrogen Production

Paul KT Liu; Media and Process Technology Inc.

Brief Summary of Project

The objectives of this project are to 1) develop, fabricate and demonstrate field implementable hydrogen selective membranes/modules; 2) achieve process intensification of conventional hydrogen production; and 3) reduce cost for distributed hydrogen production. Specific objectives for fiscal year 2008-2009 are to 1) perform economic analysis; 2) conduct tests using the process development unit (PDU) testing facility at the University of Southern California and pilot testing unit at Media and Process Tech; and 3) fabricate field implemental membranes/modules for field testing by end users.



Question 1: Relevance to overall DOE objectives

This project earned a score of **3.5** for its relevance to DOE objectives.

- This project's objectives align with the Hydrogen Program RD&D mission goals.
- The PI is aware of the DOE technical goals and targets and the timeframe to achieve these targets. In particular, the PI has modified the direction to address the required purity targets that could not be achieved with the prior carbon molecular sieve (CMS) membranes.
- The project studies of separation purity and H₂ recovery are directly applicable to the DOE objectives.
- This program is aligned with DOE objectives but does not seem to provide any game changing technology.
- Development and evaluation of H₂ selective membranes and their evaluation are critically important in hydrogen production and delivery processes.
- This technology has potential to significantly reduce steam methane reforming (SMR) and gasification system complexity and cost.

Question 2: Approach to performing the research and development

This project was rated **3.2** on its approach.

- The project follows an engineering development path suitable for scale-up. The project in its development path has identified barriers and attempted to overcome the barriers.
- Some of the project's assumptions are ideal. Palladium is a well-known hydrogen transport material, but phase change and stability are issues that the project has not addressed.
- The PI should present the flux data in the DOE recommended unit, SCFH/f² at 100 psi trans-membrane ΔP at DOE-recommended operating temperature and pressure.
- Regarding the actual presentation, the different unit(s) presented only confuses the readers and presenting a ratio instead of independent performance data is further confusing.
- The PI is addressing a process intensification approach that involves incorporating both water gas shift and hydrogen separation. This is a preferred approach that could include cost reductions due to combining engineering process elements. In addition, the work is attempting to utilize a commercial membrane bundle as the Pd support. The bundle has already been demonstrated in other commercial applications. However, the use

of Pd has already been extensively researched and demonstrated limited separation/flux efficiencies and the use of a pure precious metal may have severe commercial limitations.

- The major improvement in this project is based on delivering super atmospheric pressure H₂ on the delivery side of the membrane. It is not clear what the innovation is exactly coating on a ceramic rather than metallic substrate?
- Design, fabrication, evaluation and economic analysis of H₂ selective membranes are the main objectives of the project. The specific approach taken to reach commercially viable processes is well presented. Process simulation, optimization, and field-testing methods are sufficiently described.

Ouestion 3: Technical accomplishments and progress toward project and DOE goals

This project was rated 2.7 based on accomplishments.

- The major technical accomplishment of the project is supplying a module to the Ballard Corporation.
- It is not clear what membrane the project recommends, say for scale-up. Would the team use just the CMS or Pd-coated CMS.
- The project's experimental and economic studies are conducted on both types of membranes and presented interchangeably in a lumped mode and, thus, not readily comprehensible to the reader.
- How the technology can achieve high-pressure permeate stream without additional compression is unclear in this project. What the additional cost for high-P permeate stream is not discussed.
- Technically, the hydrogen flux rates are well below an acceptable limit for Pd membranes (slide 11). There have been numerous other investigations that show much higher flux rates (with both pure and mixed gases). In addition, these prior efforts have also addressed seals and leaks, which this work has not clearly considered (slide 13 suggests a poor H₂/N₂ ratio). The PI suggests a Pd level of 1 micron (on slide 13) but this is an unreasonable thickness because a defect free coating will not be achieved. There will be a significant error if cost estimates are based on this assumption (see chart 1, slide 11).
- The PI made good performance over the year. The team's achievement fell short in terms of permeance but they defend that since the cost much lower than the target, that the system meets the intent of the DOE objectives.
- The team's claim that they "need optimization" suggests that the results are not that much better than the competition. However, with fine-tuning, it can be better. There was no compelling reason for this technology to provide great improvement.
- The project accomplishments show successful separation performance of the relatively low-cost Pd membranes developed and evaluated in pilot scale units. Some of the barriers in reaching economic production of the membranes have been resolved. Field-testing appears promising. Cost analysis shows how the production costs can be minimized.
- What causes the CO₂ permeation and what is the CO breakthrough? Does this device need a further downstream clean up to provide transportation-grade hydrogen?

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated **3.2** for technology transfer and collaboration.

- The project team consists of the University of Southern California, Chevron ETC, a catalyst manufacturer (Johnson Matthey), and the Ballard Corporation. These collaborations provide the best opportunity to move the R&D product to market readiness.
- The project involves collaboration with both academics and industrial partners. During the past year, the PI has added the involvement of Ballard, which provides additional insight from an industrial fuel processing end user. The identified partners are well qualified to scale up and commercialize this technology if the larger scale pilot tests are successful.
- The project has good collaboration with industry and academia. It is not clear if all the pieces are being fully addressed by the partners.
- Collaborative efforts with academic faculty members and industrial professionals are well planned in this project.
- This project could benefit from a wider industry exposure. The team can possibly collaborate with European hydrogen production companies.

Question 5: Approach to and relevance of proposed future research

This project was rated 2.8 for proposed future work.

- The project is 95% complete, and ended June 30, 2008. The proposed future work, especially how it is funded, is not evident.
- The team's future work involves membrane/module fabrication for field test. This would be a good success story.
- The project's future work plan is acceptable. A pilot scale test is necessary; however, it is questionable if this membrane will have an acceptable flux level and function in a mixed gas environment.
- The project's future work seems reasonable especially the aim for commercialization.
- The team presented excellent plans for further development of the membranes, testing, and field evaluations.
- This project should consider impurities impact. For example breakthrough of sulfur species if any, effect of CO diffusion and H₂O permeation. What is the scaled-up expected reliability? At a small scale, good performance can be expected, but at scaled-up level, defects can be significant factor.

Strengths and weaknesses

Strengths

- The project's actual test data, collecting permeance and purity information and projecting into system context, is exactly what is needed.
- Apparently a good team is working together in this project.
- The project is on schedule and shows a strong possibility for successful completion.

Weaknesses

- The project's pressure/temperature cycling of bundles was conducted at 220°C rather than 350°C.
- Permeate not 100% H₂.
- The PI had a weak explanation of permeate pressures as well as how the steam purge is implemented.
- The quantification and explanation of electrical energy savings is poorly conveyed by the team.
- The diagrams on slide 17 do not appear correct: individual stage pressures do not add up to permeate pressure.
- The explanation of systems penalty due to added compressors was not clearly spelled out.
- The project had a lack of convincing data that DOE's targets can be achieved.
- Palladium-based membranes are relatively more expensive than carbon-based membranes under development by the project team.

Specific recommendations and additions or deletions to the work scope

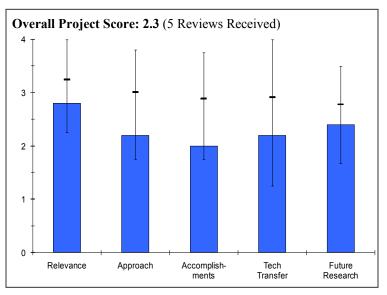
- The team should report membrane performance in units consistent with DOE requirements.
- It is not clear that this project has demonstrated adequate technical targets to proceed to larger pilot scale testing. Larger scale testing may not be worth the cost.

Project # PD-28: A Novel Slurry Based Biomass Reforming Process

T.H. Vanderspurt, S.C. Emerson, R. Willigan, T. Davis, A. Peles, Y. She, J. MacLeod, G. Marigliani, and S. Seiser; United Technologies Research Center

Brief Summary of Project

The objectives of this project are to 1) illustrate through an initial feasibility analysis on a 2,000 ton/day (dry) biomass plant design that there is a viable technoeconomical path towards the DOE 2012 efficiency target (43% lower heating value) and assess the requirements for meeting the DOE's cost target (\$1.60/kg hydrogen); 2) demonstrate through preliminary results that an acid tolerant model sugar solution reforming catalyst with acceptable kinetics has been synthesized and that a viable technical path for scale up (mass production) of this catalyst in a costeffective way exists; 3) identify hydrolysis conditions for a simulated biomass system and viable techno-economic path towards



the achievement of the hydrolysis of the real biomass system; and 4) demonstrate through extensive test results an acid tolerant, long life, cost-effective biomass hydrolysis product reforming catalyst.

Question 1: Relevance to overall DOE objectives

This project earned a score of 2.8 for its relevance to DOE objectives.

- This project supports the overall DOE Hydrogen technology R&D program goal and the biomass utilization focus area.
- The team's work is attempting to produce hydrogen from a biomass source, which is a goal of the Hydrogen Program. The PI appears aware of the DOE technical and cost targets.
- The production of hydrogen is relevant however; parts of the project such as operating conditions and residence time seem risky.
- The development of a commercially viable process for the conversion of biomass to hydrogen is one of the DOE goals of hydrogen production.

Question 2: Approach to performing the research and development

This project was rated **2.2** on its approach.

- Hopefully, the project's proposed proof-of-principle approach will work and be scalable. A 2,000 psig titanium liquid phase reactor is cost-prohibitive and operationally difficult. If it is assumed that a scaled-up practical unit will be operated by steam hydrolysis, then the pressure of saturated steam at 310°C is approx 1,400 psi. Additional slurry compression is highly energy intensive.
- The project team's approach is weak and vague. There does not appear to be any clear direction to this project. Since the last review, the investigators seem to have decided that their approach should be a base digestion of biomass coupled with high-pressure reforming (with the subsequent hydrogen separation that was not addressed). The work appears to be a laboratory scale curiosity due to it requiring a high pH base to digest a small amount of biomass (1%). This will not be practical at any scale outside the laboratory. In order to run this process, reasonably exotic materials will be necessary and this will likely be costly. The environment is so corrosive that it even destroys the catalyst and Ti basket (slide 11). Overall, the entire approach does not seem practical and likely has little chance to achieve any of the DOE targets and goals.

- The approach is novel and the results seem too good to be true. The project needs an independent assessment.
- A comprehensive approach is taken for developing an economic process for biomass reforming along with a cost analysis that includes the required initial investments. The objective is to produce hydrogen using a carbon-neutral gasification/reforming process followed by Pd-based membrane separation. Specific objectives are well described.
- This process calls for an extremely high-pressure high-temperature reactor, with 300°C water and reaction time on the order of 2-3 hours. This makes for an extremely expensive design. Construction methods would resemble steam turbines, where similar pressure and temperature are used, but at orders of magnitude larger scale. Cost projections are questionable. Effluent stream is not characterized in the liquid phase. Neither water usage of this process nor recycling strategy is addressed. The catalyst used does not appear to be reusable, and would be a consumable. Safety aspects of the reactor have not been addressed.

Ouestion 3: Technical accomplishments and progress toward project and DOE goals

This project was rated 2.0 based on accomplishments.

- The project's claimed accomplishments are based on efficient and cost-effective separation of hydrogen by a hydrogen transport membrane(s) (HTM). But the selectivity, flux and cost performance of the United Technologies Research Center (UTRC) advanced concept HTM is unknown. Thus, the presented results are speculative. Delivering hydrogen at the claimed cost should be further examined by experiments and system analysis.
- The order of magnitude lower membrane cost and nearly order of magnitude lower capital claims are speculative, because the team has not provided experimental data or system analysis data.
- There appears to be little accomplishment on this project in the past year. The total results appear to be two experiments: 1) the reaction of 1 wt% yellow poplar and 2) the use of approximately 1.7 wt% ethanol. This is minimal work for a project of this size (\$3 million). The only results appear to be a picture of a clear liquid, that evidently represents complete conversion of the biomass into four products: H₂, CH₄, C₂H₆, and C₃H₈. This does not seem realistic from a chemical standpoint considering the complicated organic structure of the biomass. When questioned, the PI was unable to provide any comment on the overall material balance. This is a basic chemical principle and not being able to address this concept in some way is unacceptable technique. The only real data appears to be a plot on page 11, which provides little solid information. The work also advises some cost suggestions however, it is not clear what these are based on. These costs are mainly general assumptions with no clear technical basis and it is unclear that these have any real meaning. The presentation continues to mention modeling efforts (e.g., slides 6, 14 and 24) but modeling is worthless unless clear experimental results are obtained.
- This project is really a 3.5 rating, but a 4 was given based on full faith in the results described. The predicted H₂ selling price is well below targets and is outstanding if it can be achieved. However, the full conversion of even the lignin fraction of the wood is questionable. The pretreatment of some biomass sources might be required and an overall mass balance be carried out and described.
- The range of predictions on H₂ delivery capital costs, etc., suggest there are many unknowns still to be determined in this project.
- It is surprising that a ceria-zirconia-based catalyst will have the durability under aqueous base conditions.
- It was not clear how dilute the system was how much biomass per volume liquid.
- Technical accomplishments in this project include the establishment of proof-of-principle methods, economic analysis, design of new reactors and their performance assessments. Kinetic models of the reformers have been developed to demonstrate the feasibility of the methods proposed. Cost analysis results are very attractive for reaching the DOE goals much ahead of the DOE time schedule.
- Sufficient technical accomplishments to account for the funding level were not presented.

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated **2.2** for technology transfer and collaboration.

• UTRC is the prime on the project and the University of North Dakota Environment Energy Research Center (UND-EERC) is conducting the experiments and cost analysis studies.

- In the presentation, slide 16 suggests two direct collaborations in this project UND-EERC and an unidentified catalyst vendor. Neither seems to have any clear involvement in this work. In addition, the slide suggests leverage from another high-cost DOE project but neither appears to have provided any added value to this work. UTRC needs to actively involve other participants if this project is to have any success.
- Collaborations on hydrolysis studies and membrane development and vendor involvement are all good in this project.
- Collaboration with the UND-EERC is shown with their specific roles and project outcomes.
- This project seems to be working in a vacuum, only tapping into University of North Dakota.

Question 5: Approach to and relevance of proposed future research

This project was rated 2.4 for proposed future work.

- For this project there has been, thus far, no FY09 funding and out-year funding is also unknown. Future work has been proposed including a 1 kWe demonstration unit for Phase 2.
- UTRC has demonstrated little success thus far, therefore, the future plans to simply continue on with the work seems to make no sense. In addition, it is not clear that there is any correlation to the established statement of work or work plan which should be the guiding document for the project. At a project of this size more effective project management from both UTRC and DOE is an absolute necessity.
- This project is good but uses a very aggressive plan to technology transfer.
- Future research plans are presented in detail for this project.
- No future work has been proposed.

Strengths and weaknesses

Strengths

- This project has a novel concept and surprisingly good results. This could be a game changer.
- The PI and the research team members are exceptionally qualified to reach the project goals.

Weaknesses

- This project demonstrates no clear strengths.
- The project data is sparse and accomplishment claims are speculative.
- There is a severe lack of project direction and management. The project has produced minimal results and a relatively high cost.
- At this point the project certainly raises eyebrows as no one has seen such results before. Project operation at such high temperature and pressure make aqueous base conditions dangerous.
- Because of the complexity of the economic assessment involving biomass conversion, the cost analysis should be rechecked by an independent source in collaboration with the project team. Biomass projects have significant concerns related to their actual efficiency and socio-economic impacts.
- No sufficient detail was given in order to determine that this is a feasible technology. This is a relatively simple proposed system, and for the funding and time allotted, should have been able to demonstrate better understanding of the process.

Specific recommendations and additions or deletions to the work scope

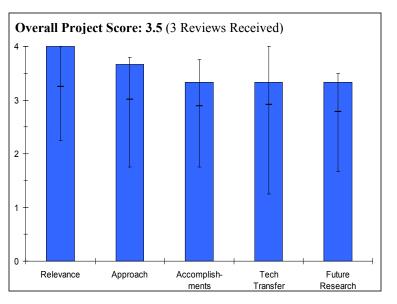
- The experimental result on the 100% conversion of yellow poplar to gas needs to be duplicated, a few times, using designed parametric experiments. The advanced concept HTM must be developed and proven first before making the hydrogen delivery price claims.
- DOE needs to seriously consider terminating this project immediately.
- The project team should get independent confirmation of overall mass balance and quantify reactor productivity in a flow system.
- Capital outlay and operational cost analysis and future plans merit further funding of the proposed studies.

Project # PD-30: Hydrogen Delivery Infrastructure Analysis

Marianne Mintz; Argonne National Laboratory

Brief Summary of Project

The objectives of this project are to 1) refine technical and cost data in the H2A Delivery Models (H2A Hydrogen Delivery Components Model and H2A Hydrogen Delivery Scenario Analysis Model, (HDSAM) by incorporating industry inputs and evolving technologies (revised data and analysis, enhanced model capabilities and user options, improved consideration of storage and component sizing, carrier analyses); 2) explore options to reduce hydrogen delivery cost, including storage optimization and novel carriers; and 3) develop enhanced models to assist in program planning and development.



<u>**Ouestion 1: Relevance to overall DOE**</u> <u>**objectives**</u>

This project earned a score of 4.0 for its relevance to DOE objectives.

- This is a critical program. This project provides the ability to evaluate new developments in the total context of the program.
- The project and project tools are effectively used to evaluate numerous hydrogen delivery technologies as well as determine their costs and investigate least-cost pathways which directly supports many of the DOE program goals and objectives.
- The Hydrogen Delivery Scenario Analysis Model (HDSAM) has proven to be a very useful tool in estimating the costs and benefits of alternative delivery pathways and system configurations. Continued updates to the model are needed to incorporate new data, evolving technology improvements or operating strategies, and new technology options. The model permits analysis of options and trade-offs and can help to identify an optimized delivery infrastructure that can meet DOE cost targets.

Question 2: Approach to performing the research and development

This project was rated **3.7** on its approach.

- The project is well designed and does a good job addressing economic barriers, although it was not clear how rigorous the technical review was based on the presentation.
- In general it would have been nice to see more of the overall economic and technical barriers, although presentation time was very limited.
- The project team continues to work closely with industry to incorporate new data and reporting features that enhance the usefulness of the model and its ability to guide and inform the R&D efforts. The model documentation is excellent, assuring that all assumptions are transparent.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated 3.3 based on accomplishments.

• The project team's technical accomplishments this year were very good and the overall tool appears to be very useful to help answer key program questions concerning cost.

- It might have been possible to evaluate additional pathways if HDSAM were designed to be easier to modify or manipulate data (e.g., Excel is a very challenging tool to use for such a large data set).
- The project team's FY09 progress was strong, and the presenter clearly described the updates to the model since the last merit review. Inclusion of three new delivery pathways (700 bar fueling, cryo-compressed fueling, and high-pressure tube trailer) and station polishing steps was essential for modeling of current potential delivery pathway options.

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated **3.3** for technology transfer and collaboration.

- Overall, the project collaboration looks good, but it was not clear how well the project is coordinated with the Delivery Components Model work.
- The H2A modeling team continues to make strong use of outside collaborations for data gathering and QA, including the technical teams, industry members, researchers, Technology Validation Subprogram data, and others.

<u>Ouestion 5: Approach to and relevance of proposed future research</u>

This project was rated **3.3** for proposed future work.

- It would be nice to see chemical hydrides added to the list of delivery technologies being evaluated next year.
- Next steps for this project are reasonably well defined and seem in line with programmatic goals. How necessary is the fuel station footprint size analysis? The footprint makes little difference in the total delivery cost of hydrogen. The plan to allow for multiple markets, on the other hand, could greatly reduce the cost for delivery by reducing the seasonal storage needs. Releasing Version 2.1 of HDSAM (and corresponding documentation) which includes the updates made in the last year is important.

Strengths and weaknesses

Strengths

- The project has good continuity throughout.
- The project is well designed and does a good job addressing economic barriers.
- The technical accomplishments in this project this year were very good and the overall tool appears to be very useful to help answer key program questions concerning cost.
- Overall, the project collaboration looks good.

Weaknesses

- The project team should clarify how rigorous the technical review was based on the presentation.
- In general, it would have been nice to see more of the overall economic and technical barriers, although presentation time was very limited.
- It might have been possible to evaluate additional pathways if HDSAM were designed to be easier to modify and manipulate (e.g., Excel is a very challenging tool to use for such a large data set).
- The project team should clarify how well the project is coordinated with the Delivery Components Model work.

Specific recommendations and additions or deletions to the work scope

• Chemical hydrides should be added to the list of delivery technologies being evaluated next year.

Project # PD-31: H2A Delivery Components Mode

Olga Sozinova; National Renewable Energy Laboratory

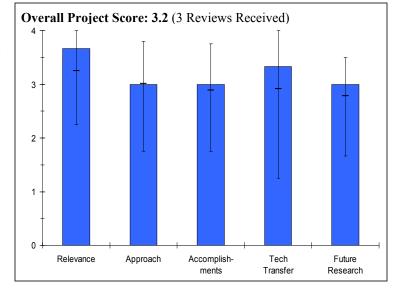
Brief Summary of Project

The objectives of this project are to 1) update and maintain the Components Model of the H2A Computer Model; 2) support other models and analysis that include delivery costs; and 3) expand the Components Model by designing new components. Activities included the development of the H2A Delivery Components and Scenario Models.

<u>Ouestion 1: Relevance to overall DOE</u> <u>objectives</u>

This project earned a score of **3.7** for its relevance to DOE objectives.

• This is a good program.



- The Hydrogen Delivery Components Model has become a well-used tool by the hydrogen community and is essential for cost analysis of hydrogen delivery components and systems on the basis of common and transparent assumptions. Continued updates to the model are needed to incorporate new data, evolving technology improvements or operating strategies, and new components. The components model also provides important cost data for use in systems-level and scenario analysis models.
- H2A Delivery components model has been critical to identify to key areas for R&D investment in the Delivery Technical Team program.

Question 2: Approach to performing the research and development

This project was rated **3.0** on its approach.

- The project approach appears to be on track with program's goals.
- The project approach seemed strong, although somewhat poorly communicated in the presentation.
- The team's approach of the modeling effort is good. Expansion of the model to correspond to new needs and developments in the program is aligned.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated **3.0** based on accomplishments.

- The project team appears to have good progress and has caught H2A glitches. The PI's notes at the back of the presentation with assumptions were appreciated.
- The project had significant progress in the last year, the most important of which was allowing for multiple runs through scripting in MATLAB. Progress on new hydrogen delivery options and components, including the addition of a refueling station tab for H2A Production; addition of cost data for rail delivery and 700-bar refueling; and cost analysis for short-distance, urban delivery pathways is important.
- The creation of an automated way to run HDSAM was very important for understanding the impact of many parameters and to more easily perform sensitivity analysis on those parameters.
- The project's technology accomplishments have been steady. The investigation into rail options is interesting but not particularly advantageous in terms of economics. It was confusing as to why 100,000's of model runs were needed for HyDS-ME. Is this project trying to use a model output to make a database for another model and, if so, why? Why not feed one model's results into the following model?

<u>Ouestion 4: Technology transfer/collaborations with industry, universities and other laboratories</u>

This project was rated **3.3** for technology transfer and collaboration.

- This project has a good use of partners. The team should consider having a rail company involved.
- The project has good collaboration with the H2A modeling team (ANL, NREL, PNNL, etc.). Regarding the railroad analysis, no railroad companies were included in discussions. The design of the train station could likely have been improved through interactions with railroad experts.
- There is good cooperation among the national labs and researchers and industry on getting the data together to build and calibrate this model.
- This project is our best product of the U.S. DOE Delivery Technical Team.

Question 5: Approach to and relevance of proposed future research

This project was rated **3.0** for proposed future work.

- The presenters should have access to and should use a laser pointer for presenting.
- The project's next steps seem logical and would be good for the Hydrogen Program. Continued refinement (and industry vetting) of the railroad delivery cost components are needed, as is the addition of cost components for cryo-compressed refueling and applications involving the "combined heat, hydrogen and power" pathway.
- The future work here is primarily driven by other projects areas that need modeling as they are developed. The cut in proposed funding will end progress.

Strengths and weaknesses

Strengths

• This project model allows H₂ Delivery Technical Team to focus resources on areas needing development and breakthroughs.

Weaknesses

• This project model needs calibration with actual installation costs to verify accuracy of predictions.

Specific recommendations and additions or deletions to the work scope

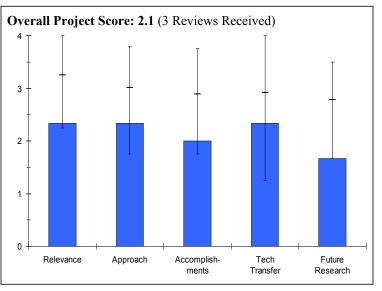
No specific recommendations were provided for this project.

Project # PD-32: Hydrogen Energy Station Analysis in Northeastern US and Hydrogen Sensors for Infrastructure

Eileen Schmura; Concurrent Technologies Corporation

Brief Summary of Project

The objectives of this project are to 1) investigate the potential dual use options, developing a hydrogen infrastructure; 2) analyze early market Hydrogen Energy Station (HES) fuel cell applications; 3) focus on the initial transition to a hydrogen economy, where less than one percent of vehicles will use hydrogen; 4) explore the indigenous energy with an emphasis on renewable feedstocks for hydrogen; and 5) identify the market readiness of the technologies and processes associated with HES biogas/fuel cell systems.



Question 1: Relevance to overall DOE objectives

This project earned a score of 2.3 for its relevance to DOE objectives.

- The majority of this presentation focused on HES analysis of stationary fuel cell sites powered by biogas (landfill and di-ester gas) in the northeastern U.S. corridor for combined heat and power (CHP) and combined heat, hydrogen, and power (CHHP). The secondary topic was on proposed evaluation of hydrogen sensors. It is hard to see the relevance of the two topics.
- The CHHP study is a very useful examination and it is very relevant to understanding the role of CHHP systems. The relevance rating for this project is good.
- Rationale or need for the H₂ sensor development is not clear. The relevance rating for this part is poor to fair.

Question 2: Approach to performing the research and development

This project was rated **2.3** on its approach.

- The project has no comparison of target or metrics of hydrogen sensor work for the currently available technology.
- The project has good cost analysis of CHP and CHHP approaches and the payback time for different classes of sites (biogas sites, big box/industrial sites, and coke gas production) and locations (from state to state).
- The project's hydrogen sensor studies appear to focus on evaluation of commercial sensor technology. It is unclear how will advance sensor technology.
- The project has a logical approach and is well laid-out.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated 2.0 based on accomplishments.

- This project confirms the government incentives required for hydrogen energy stations (HES).
- The project team has shown good progress on HES citing analysis but little or no progress on hydrogen sensor studies.
- The project's cost benefit analysis assumptions are unclear: \$7/kg or \$4/kg H₂, \$0.149/kWh or \$0.075/kWh electricity?

- This project's analysis seems to include free land fill gas. This is not accurate as the gas can be sold and therefore should have a cost to the CHHP system.
- The payback period is a simplified method of semi-quantitatively assessing the economics of a project but a discounted cash flow analysis should be conducted.
- It should be pointed out that the systems only look attractive because of the federal/state capital cost subsidies. A case should have been presented to show the economics without subsidies.
- The cost breakdown of HES & H₂ infrastructure equipment should be given by the project team.
- Benchmarks and goals for the H₂ sensor are not given. This is perhaps due to time constraints in the presentation. The PI did not adequate convey the progress of system and no mention was made of sensor cost which is critical. Discussions of why specific listed features are even needed were not included.

<u>Ouestion 4: Technology transfer/collaborations with industry, universities and other laboratories</u>

This project was rated **2.3** for technology transfer and collaboration.

- Roles of collaborators are unclear in this project.
- This project has good collaboration regarding HES analyses. There is little or no collaboration in sensor work aside from what appears to a commercial off-the-shelf sensor.
- A list of collaborators is given but it is difficult or impossible to measure level of their interaction.

Question 5: Approach to and relevance of proposed future research

This project was rated 1.7 for proposed future work.

- The project's funding is complete.
- No plans for future activities were presented.
- No future plans were discussed.

Strengths and weaknesses

<u>Strengths</u> No strengths were provided for this project.

Weaknesses

• This project has had little or no progress on sensor evaluation.

Specific recommendations and additions or deletions to the work scope

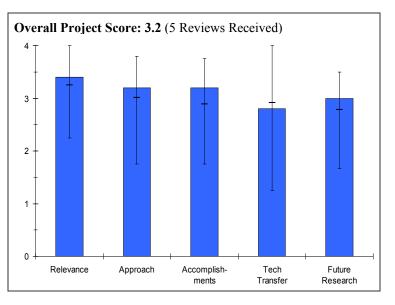
- The centrifugal compressors required for pipeline delivery, are projected to be the long-term low-cost option.
- Industrial compressors are one of the key barriers enabling cost effective hydrogen supply and distribution.
- This project is only relevant to central production and compression. This compression technology does not have a high enough compression ratio at 350 and 700 bar forecourt for production and compression.
- Various other compressor applications are outside of hydrogen and DOE program, and they should be explored.
- Improved compression vital to reducing delivery costs. Centrifugal compression for hydrogen represents major advance over existing compressors.
- This project is critical to selecting appropriate technologies for hydrogen delivery.

Project # PD-34: Oil-Free Centrifugal Hydrogen Compression Technology Demonstration

Hooshang Heshmat, Ph.D.; Mohawk Innovative Technology, Inc.

Brief Summary of Project

The objective of this project is to demonstrate key technologies needed to develop reliable and cost effective centrifugal compressors for hydrogen delivery. This project proposes to demonstrate that advanced and very highspeed, oil-free centrifugal compressors can meet hydrogen delivery needs. A key compressor stage will be designed, fabricated and tested to validate the concept and demonstrate overall system feasibility based upon advanced three dimensional aerodynamic designs combined with oil-free compliant foil bearings and close clearance compliant foil seals. Under this effort, compressor blade tip speeds and bearing and seal surface velocities exceeding state-of-art will be designed, built and evaluated.



Question 1: Relevance to overall DOE objectives

This project earned a score of 3.4 for its relevance to DOE objectives.

- The project's focus on centrifugal compressors required for pipeline delivery is relevant and projected to be the long-term low-cost option.
- Industrial compressors are one of the key barriers enabling cost effective hydrogen supply and distribution.
- This project is only relevant to central production and compression as this compression technology does not have a high enough compression ratio to 350 and 700 bar forecourt production and compression. However, it has various other compressor applications outside of hydrogen and DOE program and they should be explored.
- Improved compression is vital to reducing delivery costs. Centrifugal compression for hydrogen represents major advances over existing compressors.
- This project is critical to selecting appropriate technologies for hydrogen delivery.

Question 2: Approach to performing the research and development

This project was rated **3.2** on its approach.

- Contaminant-free hydrogen is required for low-cost fuel cell operation.
- The project team has an innovative high-speed super critical speed design.
- The team has a good approach to pick an established compressor design (NASA) and address the remaining issues with that design for prescribed application.
- Discharge pressures that the compressor technologies are aimed at (piston, guided rotor, centrifugal) is a bit confusing. The PI needs to make this clear as it is important for the intended application.
- The project team's use of computational fluid dynamics (CFD) modeling is a good approach.
- The project team needs to focus more on addressing potential H₂ leakage and durability issues.
- The team has a good use of simulation to address loads on shaft/bearings. The experiment correlates well with results.
- This project is sharply focused on demonstrating the feasibility and attributes of the centrifugal compressor technology as an input to a down-select.

Ouestion 3: Technical accomplishments and progress toward project and DOE goals

This project was rated **3.2** based on accomplishments.

- The project's initial frame design is a technical accomplishment.
- The project's analytical, multi-stage, and very high speed.
- The project's down-selected centrifugal vs. piston and guided rotor is a technical accomplishment.
- The project has had good progress on model-based design work.
- The project team needs to report progress on a more structured format including projections on life, cost and efficiency.
- The PI needs to set up a ranking system to evaluate the decision criteria shown (i.e., what are the most critical factors to address?). This needs to be developed in conjunction with DOE inputs.
- The PI needs to also address codes and standards issues and electrical area of classification requirements for H₂ applications.
- The project's 5% completion with \sim 50% of funding expended seems low.
- Objectives in this project are being achieved.

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated **2.8** for technology transfer and collaboration.

- Limited Collaboration is seen in this project.
- Good collaborations between Mitsubishi Heavy Industries (MHI) and Mohawk Innovative Technology, Inc. (MiTi), both being industrial players, is good.
- Perhaps the project team should consider having discussions with industrial gas compressor companies.
- Mitsubishi Heavy Industries is good partner for ultimate commercialization of this project.
- MHI is seamlessly incorporated into this project.

Question 5: Approach to and relevance of proposed future research

This project was rated **3.0** for proposed future work.

- Design fabrication and testing of concept is in the future plans of this project.
- There is a fair list of proposed work to accomplish this project's goals.
- The project team should consider addressing how the test will be set up to run the compressor on hydrogen.
- The project team should consider addressing safety codes and standards issues as well as durability.
- A timeline for the project's path forward should be shown. If funding is available, when would a compressor be seen?
- The project's future work is focused on supporting a down-select decision.

Strengths and weaknesses

Strengths

- The project's applications of lessons learned from the 70's by NASA are a strength.
- The project has good technical competency and industrial players.

Weaknesses

- The project's 500 tonnes per day (TPD) hydrogen compressors for hydrogen transport is a long-term application. The team should focus more on compressors at the forecourt.
- The project's low funding is a weakness.

Specific recommendations and additions or deletions to the work scope

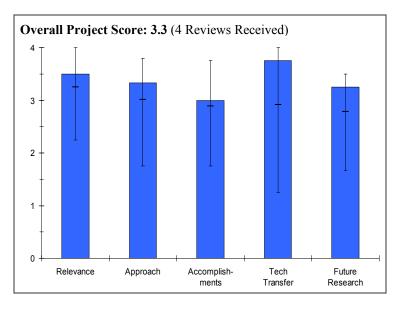
No specific recommendations were provided for this project.

Project # PD-35: Development of a Centrifugal Hydrogen Pipeline Gas Compressor

Colin Osborne and Francis A. Di Bella; Concepts NREC

Brief Summary of Project

The objectives of this project are to 1) design and demonstrate an advanced centrifugal compressor for high-pressure hydrogen pipeline transport; 2) investigate alternative system sizes, design options, operating conditions and costs; 3) select a baseline design able to meet near-term applications; 4) identify critical areas of development and operational limitations; 5) design and test critical components under design conditions; 6) build and demonstrate full-scale components in an integrated compressor system; and 7) prepare a development plan for industrial pipeline applications.



<u>**Ouestion 1: Relevance to overall DOE**</u> <u>objectives</u>

This project earned a score of **3.5** for its relevance to DOE objectives.

- The project's high-purity delivery of gas by pipeline is relevant.
- This project is relevant to DOE delivery program goals in compression cost reduction. Centrifugal compression would reduce down-time and O&M costs, which are typically significant for hydrogen compression and a significant barrier to hydrogen deployment.
- The development of lower cost compressors for hydrogen transportation via pipeline and other compression needs are essential for cost-effective delivery of hydrogen.
- This project is good at looking at current resources for developing compression solutions.

Question 2: Approach to performing the research and development

This project was rated **3.3** on its approach.

- The project team is "keeping their feet on the ground" with input from industry on requirements.
- The project's use of the shelf is state-of-the art.
- This project seems well designed to address DOE's technical barriers. Compression technology in the central plant must become more reliable and cheaper to enable central hydrogen production and pipeline hydrogen distribution. The project team is taking a very methodical approach to system design and is involving industry partners.
- The team's approach is good for objectives of the project. There is, however, a need to address the issue of hydrogen purity in more depth as design of preferred compressor advances.
- The PI moved too quickly through the technically detailed slides for comprehension.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated **3.0** based on accomplishments.

• An accomplishment of this project is the "go/no-go" decision point on alternative systems design from phase one.

- The project team should provide a Gantt chart showing tasks and funding in order to better judge progress. It is unclear if the project is on track to meet the July 2009 "go/no-go" decision milestone. It is very good to see the project has developed cost modeling components that are compatible with the H2A models.
- The project's design of a system and end rotor seems novel and well thought out.

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated **3.8** for technology transfer and collaboration.

- The project has an excellent mix of industry, university, and national lab with interactions on design.
- The project team's inclusion of industrial gas partner is valuable.
- The team has good collaboration with both industry and materials researchers in universities and the national labs. Industrial collaboration is particularly important considering the potential commercial viability of the compressor technology in the short term.
- Collaboration with Praxair, Texas A&M University and HyGen Industries seems to yield good results int his project.

<u>Question 5: Approach to and relevance of proposed future research</u>

This project was rated **3.3** for proposed future work.

- Phase 2 includes detailed design.
- The project is following good practices to update economics as it moves to phase two.
- The project's materials issues are key to success.
- The project's future work seems to be well planned. Several "go/no-go" decisions are part of the plan, which is good, but the team does not appear to be linked to any particular technology performance targets.
- Much work needs to be done on this project. Materials testing, compressor design, and gearbox all require attention. Funding should continue for these tasks to be accomplished.

Strengths and weaknesses

Strengths

- The project's mix of partners, input from industry and selection of near term available materials are all strengths.
- The project has a good collaborative team.
- Take current compressor designs and components to determine if adequate hydrogen compression can be done.

Weaknesses

• This project has had too little progress especially if funding will end.

Specific recommendations and additions or deletions to the work scope

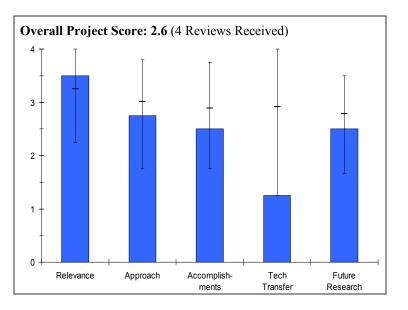
• The teams should consider availability of 70°F water at southern states compressor sites during the summer.

Project # PD-36: Advanced Hydrogen Liquefaction Process

Joe Schwartz and Jerry Jankowiak; Praxair

Brief Summary of Project

The overall objective of this project is to develop a low-cost hydrogen liquefaction system for 30 and 300 tons/day that meets or exceeds DOE targets for 2012. The objectives of this project are to 1) improve liquefaction energy efficiency; 2) reduce liquefier capital cost; 3) integrate improved process equipment invented since the last liquefier was designed; 4) continue orthopara conversion process development; 5) integrate improved ortho-para conversion process; and 6) develop an optimized new liquefaction process based on new equipment and new ortho-para conversion process.



<u>**Ouestion 1: Relevance to overall DOE**</u> <u>objectives</u>

This project earned a score of **3.5** for its relevance to DOE objectives.

- This project is very good and recognizes/uses liquefaction is a key process for efficient distribution and storage.
- The project's reduced energy process required to make liquid hydrogen economically viable as a transportation fuel is relevant.
- The project's reducing cost and increasing efficiency of hydrogen liquefaction is critical to meeting Hydrogen Program objectives.

Question 2: Approach to performing the research and development

This project was rated **2.8** on its approach.

- The project adapted a new equation of state. Can the team just use the NIST software directly?
- The project's proprietary approach was not presented at meeting for review.
- The team's work is at too early a stage to evaluate effectiveness of approach. Also, presenter was not able to describe proprietary process.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated 2.5 based on accomplishments.

- The project team has relatively little accomplished. This project is in the planning stages only.
- The project's phase 1 feasibility is underway.
- The project team is building on previous work by EMTECH, Inc.
- The team is creating a new software package when an acceptable tool already exists. This seems to be a waste of effort.
- Evaluation of the ortho-para conversion process (25% of the program) is not possible because no useful information was provided in the review.
- Project is at an early stage; I'm giving it the benefit of doubt.

<u>Ouestion 4: Technology transfer/collaborations with industry, universities and other laboratories</u>

This project was rated **1.3** for technology transfer and collaboration.

- No collaborations were listed in the project. This is partly justified by Praxair's dominant position.
- No collaboration or partners listed.
- No collaboration is evident.

Question 5: Approach to and relevance of proposed future research

This project was rated 2.5 for proposed future work.

- It is unclear what improvements will be incorporated into the system. The presentation seems vague, partly due to proprietary issues.
- The lack of information on plan for ortho-para conversion is a problem.
- This aspect of the project cannot be evaluated as no details were provided.
- This aspect of the project is hard to judge from information presented. The team's plan seems well laid out.

Strengths and weaknesses

Strengths

• This project has an important company leader in the field. The project has potential to greatly improve system efficiency and reduce cost.

Weaknesses

- Relatively little work is accomplished in this project. It is still in the earlier stages. Budget permitting, they have more to show in the future.
- Lack of collaborators and unwillingness of contractor to reveal critical details makes effective monitoring of the program impossible.

Specific recommendations and additions or deletions to the work scope

• If Praxair wants federal research money, they should be willing to be more open about their current performance figures. It is hard to evaluate progress and potential no details are provided.

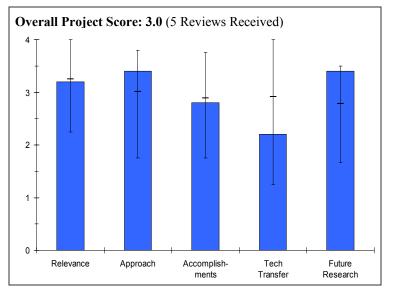
Project # PD-37: Active Magnetic Regenerative Liquefier

John A. Barclay; Prometheus Energy Company

Brief Summary of Project

The objective of this project is to provide a validated engineering basis for an advanced hydrogen liquefier technology that meets or exceeds DOE's targets for both capital and energy efficiency. Prometheus Energy intends to apply their technical knowledge of and experience with active magnetic regenerative liquefaction to sequentially analyze, design, fabricate, test and validate three experimental hydrogen liquefier prototypes.

<u>Question 1: Relevance to overall DOE</u> <u>objectives</u>



This project earned a score of **3.2** for its relevance to DOE objectives.

- This project has excellent potential relevance, but it is unclear if this system can really compete against conventional chilling and expansion systems.
- This project was well presented and the materials are technically feasible. Good presentation.
- This project addresses high capital cost and low efficiency of current liquefaction technology.
- The team is addressing the key cost challenge of H_2 liquefaction to cost effectively supply H_2 at 700 bar.
- Using a non-compression technique is novel and worth investigating.
- The likely intended application(s) of this technology (central, forecourt or both) is unclear.

Question 2: Approach to performing the research and development

This project was rated **3.4** on its approach.

- The project team has a good, detailed plan. The advantage of a magnetic refrigeration system for cooling between ambient temperature and 20 K is questionable.
- The project has had good accomplishments in spite of its late start.
- Increasing figure of merit efficiency from 0.35 to 0.5 would be a major breakthrough in this project.
- Continuous adiabatic conversion vs. step wise processing is a good approach.
- The project's execution plan seems logical.
- The project team should develop interim targets (efficiency & cost reduction) for each stage (290 K to 120 K & 290 K to 20 K).

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated 2.8 based on accomplishments.

- The project is behind schedule. The team has produced a design and calculated results.
- This project team has done very good work, technically on the right track.
- The project team has prototype parts on order but the cryocooler is in place.
- Significant progress in terms of actual testing due to company's ownership change is not seen and project is still in its early stages.

<u>Ouestion 4: Technology transfer/collaborations with industry, universities and other laboratories</u>

This project was rated 2.2 for technology transfer and collaboration.

- No collaborations have been made other than with suppliers.
- The project team has good interest in licensing technology.
- Little collaboration is listed in this project.
- No significant collaboration with other institutions has been seen.

Question 5: Approach to and relevance of proposed future research

This project was rated **3.4** for proposed future work.

- The project team has interesting plans, but this may be an academic exercise. Is this process going to be efficient and competitive at large (station or production facility) scale?
- The project team will complete assembly tests by September 2009.
- This project's first of its kind liquefier is an excellent project for DOE to support.
- The project team should consider concentration on efforts to address any scale up issues and limitations (magnet).

Strengths and weaknesses

Strengths

• This project has an interesting concept and is good idea.

Weaknesses

- The project's progress seems slow, possibly due to contractual reasons.
- The presentation was hard to follow. It would have been helpful to see a schematic of the system with all relevant components. The figure that was presented does not illustrate the thermodynamics of the whole process.

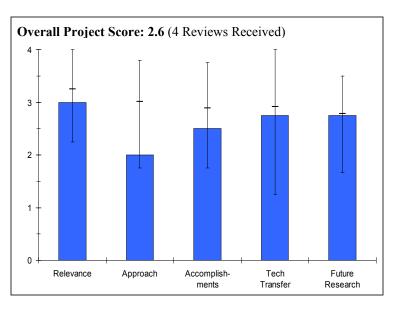
Specific recommendations and additions or deletions to the work scope

• A detailed system analysis to calculate expected performance and evaluate advantages/disadvantages with respect to conventional liquefaction process is recommended.

Project # PD-38: Reversible Liquid Carriers for an Integrated Production, Storage and Delivery of Hydrogen *Bernie Toseland and Alan Cooper; Air Products and Chemicals, Inc.*

Brief Summary of Project

The objective of this project is to enable a liquid carrier concept. This includes an economic study to determine the concept's viability. This project supports the liquid carrier by developing a dehydrogenation reactor system for hydrogen delivery. The packed bed reactor works well, but design limitations limit the reactor efficiency. Thinfilm catalysts (useful for monoliths and microchannel reactor) can be made with high catalyst efficiency. Monolith reactors are useable, but flow instabilities will cause design limitations. Micochannel reactors still look like the most viable alternative.



Question 1: Relevance to overall DOE objectives

This project earned a score of 3.0 for its relevance to DOE objectives.

- In this project, how close is the liquid carrier fuel to actual conditions? It seems that the team has its own safety and hazard analysis that needed to be done differently from the full-scale fuel. This is necessary to perform but deflects from the full scale project.
- The project's liquid carriers have potential for low-cost hydrogen delivery.
- Liquid organic hydrogen carriers in this project are one of the key options to reduce Hydrogen supply, distribution, as well as retail and storage costs.
- Liquid hydrogen carriers offer potential paths to hydrogen using conventional infrastructure.

Question 2: Approach to performing the research and development

This project was rated **2.0** on its approach.

- This project is half-way complete and has shown good results so far.
- The project team's time is better spent investigating alternative materials vs. moving ahead with toxic / corrosive liquid.
- The team's use and approach of the LOHC compound is not to my liking. Why not find and use the real commercial one? Everything about this research is to find that unique material and using a non-commercially viable model material doesn't do any good. The dehydrogenation process is not generic enough to be applied to all different compounds.
- It is unclear if the OEMs like the concept of micro-reactor onboard.
- The project team had a good choice of reactor designs. The microchannel is promising and the team has done good flow simulation work.
- Good work with kinetics modeling can be seen in this project.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated 2.5 based on accomplishments.

• This project appears to be on track.

- Utilizing H₂ fuel for an internal combustion engine (ICE) does not take advantage of the increased efficiency of a fuel cell and would be economically undesirable.
- The project has not had good progress on the microchannel reactor development front. The efficiency (10 15%) is very low seems like a dead end and a huge practical challenge. The computational fluid dynamics (CFD) modeling conclusions are useful to understand but the team needs to demonstrate it practically.
- Systems modeling work progress is fair in this project.
- It is somewhat disappointing that no reactor design has been identified that achieves high conversion, but problem of maintaining catalyst in "wet" state is daunting.
- Are issues expected with autothermal carrier to be the same, greater, or smaller?
- The quantification of projected reactor size is a good addition to this project.

<u>Ouestion 4: Technology transfer/collaborations with industry, universities and other laboratories</u>

This project was rated **2.8** for technology transfer and collaboration.

- Interaction between partners is not apparent in this project.
- The project has a good team of collaborators and right industry representatives in the project (OEM, IGC, Equipment Manufacturer).
- The project team's BMW collaboration is a good step. This collaboration adds the needed expertise from an automobile side. PNNL microreactor expertise has advanced this project.

Question 5: Approach to and relevance of proposed future research

This project was rated 2.8 for proposed future work.

- This project's microchannel reactor milestones are shown with "go/no-go" phase gate.
- This project has had a fair proposed list of future work.
- Reasonable extension based on current results can be seen in this project.

Strengths and weaknesses

Strengths

- The project team identified the toxic and corrosive property of N-Ethyl Carbazole.
- The team's liquid carrier approach is unique and worth considering.
- The project shows a good approach and has a capable team.

Weaknesses

- The project team did not discontinue work on toxic and corrosive carrier.
- The team is using the model compound approach. Why not develop/use the real compound?

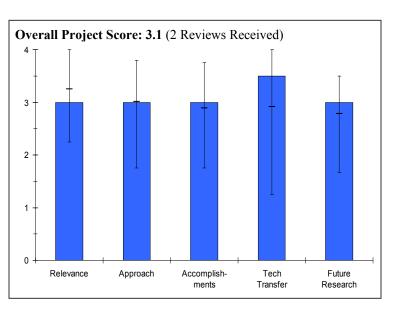
- The project team should compare the total weight and volume for liquid tanks and onboard dehydrogenation reactor vs. DOE targets for onboard storage.
- The team should consider the inclusion of autothermal material.

Project # PD-39: Inexpensive Delivery of Cold Hydrogen in High Performance Glass Fiber Composite Pressure Vessels

Andrew Weisberg, Salvador Aceves, Blake Myers, and Tim Ross; Lawrence Livermore National Laboratory

Brief Summary of Project

The overall objective of this project is to demonstrate inexpensive hydrogen delivery through synergy between low-temperature (200 K) hydrogen densification and glass fiber strengthening. Colder temperatures (~200 K) increase density ~35% with small increases in theoretical storage energy requirements. Low temperatures are synergistic with glass fiber composites. Glass composites (~\$1.50/kg) minimize material cost. Increased pressure (7,000 psi) minimized delivery costs. Dispensing of cold hydrogen reduces vehicle vessel cost about 25 percent.



<u>**Ouestion 1: Relevance to overall DOE**</u> <u>**objectives**</u>

This project earned a score of 3.0 for its relevance to DOE objectives.

- This project is a good match with the EERE program. It has had good technical progress in the one year time frame.
- This project reduced cost of storage and tube trailer delivery which is relevant to DOE's objectives.

Question 2: Approach to performing the research and development

This project was rated **3.0** on its approach.

- This project is well done.
- The team's selection of the operating regime to reduce delivery cost, while a good approach, should be reviewed in context of total cost.

Ouestion 3: Technical accomplishments and progress toward project and DOE goals

This project was rated 3.0 based on accomplishments.

- Project appears to have good progress.
- The project team's progress towards trailer delivery targets could provide lower cost hydrogen in the near term.

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated **3.5** for technology transfer and collaboration.

- The project team has had collaboration between national labs and industry.
- The project team's "teaming with an innovator" has allowed fast progress towards goal.

Question 5: Approach to and relevance of proposed future research

This project was rated **3.0** for proposed future work.

• The project team should include updated cost review as part of transitions between phases.

Strengths and weaknesses

<u>Strengths</u> No strengths were provided for this project.

<u>Weaknesses</u> No weaknesses were provided for this project.

Specific recommendations and additions or deletions to the work scope

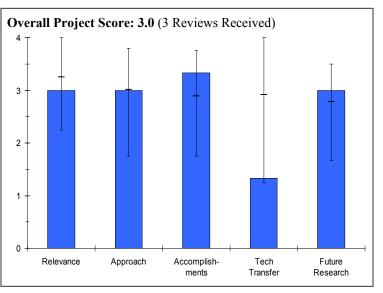
• The project team should consider the inspection of cylinders and potential build up of flammable gas mixture in closed container design.

Project # PD-40: Development of High Pressure Hydrogen Storage Tank for Storage and Gaseous Truck Delivery

Don Baldwin; Lincoln Composite Inc.

Brief Summary of Project

The objective of the project is to design and develop the most effective bulk hauling and storage solution for hydrogen in terms of cost, safety, weight, and volumetric efficiency. This will be done by developing and manufacturing a tank and corresponding ISO frame that can be used for the storage of hydrogen in a stationary or hauling application. The objective for the first year of this project (2009) is to design and qualify a 3,600 psi tank and ISO frame that will hold 510,000 in3 (~8,500L) water volume.



Question 1: Relevance to overall DOE <u>objectives</u>

This project earned a score of **3.0** for its relevance to DOE objectives.

- The project's high pressure storage and delivery of hydrogen, eliminating the need for additional compression at the stations is critical to the Hydrogen Program.
- The project aligns with DOE's Hydrogen Delivery element needs by design and development of cost-effective, high-pressure tanks for hydrogen bulk hauling and storage. Lincoln Composites is one of leading companies specializing in the high-pressure tanks development, and the company is well aware of DOE's targets and barriers.

Question 2: Approach to performing the research and development

This project was rated **3.0** on its approach.

- The project team should do more testing at 5000+ psig. There is not much value seen in 3600 psig tank activities. The team did not show a concrete plan to get to the 5000+ psig.
- The team's approach is sound and straightforward, starting from design and qualification of 3600 psi tanks to 5000 psi tanks. The cost reduction and risk mitigation are the driving forces.
- There is no innovation, and program risk is low.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated 3.3 based on accomplishments.

- The project team should consider more concentrated efforts on 5000+ psig tanks.
- The team needs to look into ambient temperature effects on tanks.
- Would like to see some work on addressing manufacturing of the tanks.
- It seems as if the program is delayed.
- The team has done a great job on development and qualification of the 3600 psi tank.

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated **1.3** for technology transfer and collaboration.

- Collaboration in the area of testing to ensure the damage tolerance of the design to realistic scenarios is needed.
- It is suggested that the team consider collaborating with vehicle storage tank projects to see if any synergies can be leveraged. Also collaborations with industrial gas companies might be worthwhile.
- There is no collaboration seen in this project. The team should collaborate with other companies who have similar experience on high-pressure tanks development.

Question 5: Approach to and relevance of proposed future research

This project was rated **3.0** for proposed future work.

- The project team should consider looking into addressing any potential codes, standards and regulatory issues.
- Future work to develop and qualify the 3600 psi tanks and 5000 psi tanks are very sound in this project.

Strengths and weaknesses

Strengths

• The company has great fabrication capabilities and facilities.

Weaknesses

- Risk assessment and hazard analysis of tank accessories and corresponding interfaces, (such as pressure relief valves), is lacking and should also be performed.
- The cost of delivery of hydrogen in this project is unclear.

Specific recommendations and additions or deletions to the work scope

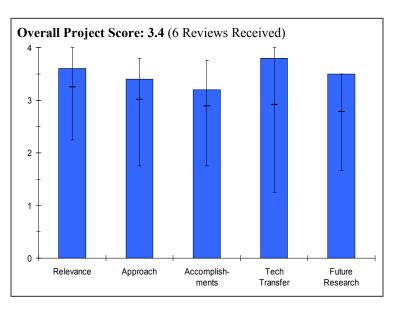
• Hydrogen's delivery infrastructure using high-pressure tanks is good for light use of hydrogen, but may not be applicable to daily/heavy use/transportation of hydrogen to H₂ refueling stations that particularly are located in metropolises. Under certain emergency situations (delivery truck involves an accident), a break or malfunction of the pressure relief valve or its interface to the tank may result in a release of 600 kg of H₂ at once. There is the potential that this could lead to a hazardous situation or possibly an explosion in population centers.

Project # PD-41: A Combined Materials Science/Mechanics Approach to the Study of Hydrogen Embrittlement of Pipeline Steels

P. Sofronis, I.M. Robertson, and D.D. Johnson; University of Illinois at Urbana-Champaign

Brief Summary of Project

The objectives of this project are to 1) come up with a mechanistic understanding of hydrogen embrittlement in pipeline steels in order to devise fracture criteria for safe and reliable pipeline operation under hydrogen pressures of at least 15 MPa and loading conditions both static and cyclic (due to inline compressors); 2) study existing natural gas network of pipeline steels or hydrogen pipelines; and 3) propose new steel microstructures. It is emphasized that such fracture criteria are lacking and there are no codes and standards for reliable and safe operation in the presence of hydrogen.



<u>**Ouestion 1: Relevance to overall DOE**</u> <u>**objectives**</u>

This project earned a score of **3.6** for its relevance to DOE objectives.

- This project has good relevance and much potential to characterize failure mechanisms in steel pipelines.
- The team's understanding of hydrogen embrittlement is critical to the design of hydrogen equipment.
- The project's study of pipeline steels is extremely important. Mechanistic understanding of the embrittlement processes is important for a hydrogen economy. Steel materials will likely be used throughout the hydrogen economy, whether in devices, in the existing pipeline network, or in pipelines repurposed for hydrogen.
- This project provides critical R&D to hydrogen pipeline delivery pathway and addresses potential hydrogen embitterment issue.
- I was unable to review due to a conflict.

Question 2: Approach to performing the research and development

This project was rated **3.4** on its approach.

- This project demonstrates a good combination of theory and experiments leading to better understanding.
- This project has a good blend of experimentation, characterization and modeling.
- Excellent fundamental work is shown in this project.
- The project is employing a sound mixture of modeling and experimental work. Models are validated with experimental data. This work increased the understanding of the fracture mechanics of pipeline steels in the presence of hydrogen. The methods developed in this project will have applications outside of pipeline steels.
- Significant amount of work was focused on simulation in this project. The project should have or build into some actual experiments to validate model.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated **3.2** based on accomplishments.

- This project's progress has been delayed due to funding issues.
- The project team is developing knowledge to set safety standards based on science.

- The project team has had great progress on gaining a better understanding of the fracture mechanics, as seen in slide 14. Strong results are seen in the understanding of the change of stress intensity factor in a hydrogen environment. Substantial progress with this team was made in 2009 in both experimental and theoretical work.
- Actual experimental results should be represented in this project. As with any modeling/simulation effort, one learns the most through doing the experiments.

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated **3.8** for technology transfer and collaboration.

- This project has multiple collaborations with appropriate institutions.
- This project contains an excellent mix of partners and "active partnership".
- Coordination and relationship between University of Illinois at Urbana-Champaign and SNL is excellent in this project. Collaboration with various industry members, such as Secat, Inc. and DGS Metallurgical Solutions, Inc. is strong and contributes to the project through their understanding of pipeline microstructures. Also, the participation of the project with the Hydrogen Pipeline Working Group is excellent. Collaboration resulting from the working group team is extensive and should be continued. International and standards-related collaborations are valued and add to the depth of this project and the Hydrogen Program as a whole.
- Excellent collaborations with various institutions are seen in this project. The industrial gas companies and energy companies have localized hydrogen steel pipelines in operations. It would be worthwhile to learn about their experiences regarding hydrogen embitterment in steel pipelines.

Question 5: Approach to and relevance of proposed future research

This project was rated 3.5 for proposed future work.

- The project team has proposed appropriate work.
- The team is working on both testing and modeling to increase understanding of mechanisms involved.
- The team's plans are well focused, both combining theoretical and practical approaches.
- The team's future plans are well laid out. Continued efforts to validate simulation tools, in collaboration with SNL, are an excellent next step. The work continues to increase the base knowledge of hydrogen effects on pipeline steels, with an eye for a better understanding of hydrogen embrittlement in metallic systems in general.
- The project team should do experiments to validate simulation.
- The project team should seek data from existing, real world hydrogen pipeline networks (places like greater Houston area where local hydrogen pipeline network near refineries is in place).

Strengths and weaknesses

Strengths

- The project team is not only good but also a prestigious researcher.
- This project has a strong team with active partnerships.
- Good collaborations are apparent in this project.
- The team's experimental and theoretical method is very strong. Collaborations with other DOE projects and external groups should serve as a model for other research projects.

Weaknesses

• The project team should elaborate on the current status of the technology, i.e., how is this project enhancing knowledge?

Specific recommendations and additions or deletions to the work scope

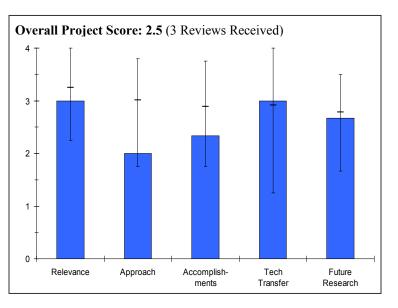
• This project should be continued.

Project # PD-42: Fiber Reinforced Composite Pipelines

Dr. Thad M. Adams and G. Rawls; Savannah River National Laboratory

Brief Summary of Project

The objectives of this project are to 1) investigate the influence of weld fabrication microstructure (especially weld heat affected zones [HAZ]) on hydrogen compatibility; 2) measure hydrogen transport (diffusivity) in HAZ materials; 3) determine HAZ material susceptibility to hydrogen embrittlement; 4) focus evaluation of fiber reinforced composite (FRP) piping for hydrogen service applications; and 5) assess the structural integrity of the FRP piping and leakage of existing commercial available FRP joint designs and joint components.



Question 1: Relevance to overall DOE objectives

This project earned a score of **3.0** for its relevance to DOE objectives.

- This project could be important for long term delivery if challenges are addressed.
- This project is important for the cost-effective distribution of H₂.
- It is absolutely critical to understand the requirements for installing FRP for hydrogen service. This project begins to address that need.

Question 2: Approach to performing the research and development

This project was rated **2.0** on its approach.

- This project should focus on technical details (permeability, leakage, strength) rather than in regulatory aspects. If the technology succeeds, then the industry will get it through the regulations.
- This project shows analytical work framing code and safety issues with limited technical investigation. It is possible that the properties of the piping are know, but were not reported or analyzed.
- What about finite element analyses (FEA) for understanding the maximum bend radii? Is this known from natural gas usage? The change in leak rate reported was not interpreted, even if upon reflection, it seems inconsequential.
- The team should pay attention to accelerated test protocols for e.g. H₂ permeation or other pipe aging mechanisms.
- The team's approach seems a bit distributed among several tasks. The team should consider increasing focus on understanding what close requirements are needed by authorities with jurisdiction for installing FRP for hydrogen service. The team should focus on the aforementioned goals first.

Ouestion 3: Technical accomplishments and progress toward project and DOE goals

This project was rated 2.3 based on accomplishments.

- This project has had reasonable accomplishments for the low budget allocation.
- The project's framing of the issues for adoption is well done.
- The team's technical depth and inspired analysis are both lacking.
- The project's accomplishments have been hampered due to the lack of funding. For the funding supplied, reasonable progress has been made.

<u>Ouestion 4: Technology transfer/collaborations with industry, universities and other laboratories</u>

This project was rated **3.0** for technology transfer and collaboration.

- This project has good collaborations with key institutions.
- The project's extent of interaction with ASME is not totally clear.
- The project team should consider trials of these materials in an industrial gas setting (APCI, Praxair, Linde, Air Liquide), with appropriate controls. A high interest in this is assumed.
- Reasonable cooperation with ORNL, Fiberspar, Polyflow and ASME can be seen in this project.
- The project team should consider stronger cooperation with the Department of Transportation and ASTM to address requirements.

Question 5: Approach to and relevance of proposed future research

This project was rated 2.7 for proposed future work.

- This project has good future plans. They seem to be better aligned with technical issues than with regulatory issues.
- Not much can be said about future plans due to the halt in this project's funding.
- The involvement of an industrial gas stakeholder is encouraged.
- This project plan set if funding appears.

Strengths and weaknesses

Strengths

- This project has potential for future advantage if successful.
- The project has the knowledge of practical requirements, especially safety and codes.
- The project's examination requirements for FRP installation for hydrogen service are a strength.

Weaknesses

- The project needs a better evaluation of system cost and performance to better justify the work.
- The PI needs to be better informed about basic facts (safety factor for pipeline?).
- The project team's technical depth focused on outstanding issues which is a weakness.
- The project team needs a more focused approach for limiting requirements by authorities with jurisdiction.

- The project team should evaluate potential reduction in hydrogen delivery cost. How does this compare to other hydrogen delivery technologies?
- The project team should consider collaborating with key stakeholders and conducting field trials.

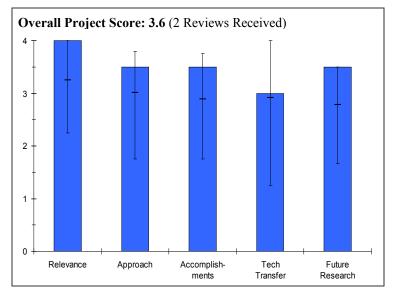
Project # PD-43: H₂ Permeability and Integrity of Steel Welds

Z. Feng, L. Anovitz, W. Zhang, and J. Wang; Oak Ridge National Laboratory

Brief Summary of Project

The objective of this project are to 1) quantify the effects of high-pressure hydrogen on property degradation of weld in pipeline steels; 2) develop the technical basis and guidelines for managing hydrogen, stresses and microstructure in the weld region to ensure the structural integrity and safety of H_2 pipeline; and 3) develop welding/joining technology to safely and cost-effectively construct new pipelines and/or retrofit existing pipelines for hydrogen delivery.

<u>Question 1: Relevance to overall DOE</u> <u>objectives</u>



This project earned a score of **4.0** for its relevance to DOE objectives.

• This project is extremely useful to the objectives of the DOE Hydrogen Program. It aims at analyzing the fracture behavior of welds in the presence of hydrogen.

Question 2: Approach to performing the research and development

This project was rated **3.5** on its approach.

• All four elements of the project's approach stated on slide #5 are important.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated 3.5 based on accomplishments.

- The project measured the permeability of the weld but it did not establish the diffusion coefficient of hydrogen through the weld at room temperature. This information is important because this is precisely the room temperature at which hydrogen embrittlement takes place.
- The team's baseline fracture tests with notched cylindrical bars of 4340 steel microstructures are good, but it is not clear how these tests and results help toward understanding the fracture response of the welds.
- The team's usage of the spiral notch torsion test (SNTT) for K_{th} measurement is an old test with questioned validity in particular with regard to mild and medium steel microstructures (yield strength less than 700MPa). The stress state locally in front of the notch is three dimensional despite the fact that an un-notched specimen experiences opening tension under macroscopic twist. Therefore, the mechanisms of fracture respond to all modes (opening, shearing, and tearing) and hence it is not correct to claim that the test isolates the mode I fracture response.

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated **3.0** for technology transfer and collaboration.

• The contributions of any of the partners listed on the opening slide were unclear.

<u>Ouestion 5: Approach to and relevance of proposed future research</u>

This project was rated **3.5** for proposed future work.

• With the exception of the K_{th} test with SNTT, the proposed work described on slide #19 is well thought out and important. In particular, the welding technology development and the management of the residual stresses in relation to the microstructure are both unique contributions. With regard to the K_{th} test with SNTT, it is an old technology and certainly does not isolate the opening mode of failure. The approach described in the ASTM standard E1681-03 is more precise and conclusive. In fact, there is doubt whether this SNTT test can yield any reliable information with regard to the proposed study of X52 welds (mentioned on slide #19). The X52 has a very mild microstructure and this makes it highly unlikely that conditions for pure mode I and small scale yielding are prevalent at the tip of the notch on the cylindrical bar subjected to macroscopic twist.

Strengths and weaknesses

Strengths

- The project's strength is in leadership and weldment expertise of Z. Feng.
- ORNL's capabilities in welding technology are project strength.

Weaknesses

• The project team's approach of analysis for fracture toughness of welds in the presence of hydrogen is a weakness.

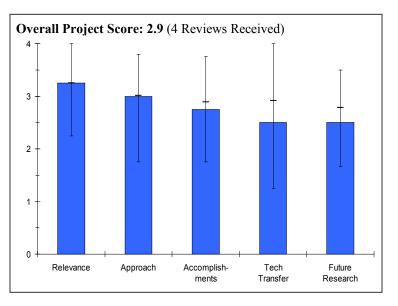
- More emphasis should be put on conventional welding processes, as opposed to friction stir welding.
- The project team should focus on the project strengths that are the weld microstructure, namely identify the type of the microstructure that is most compatible with hydrogen. The K_{th} analysis is inferior when compared with the one recommended by the ASTM Standard E1681-03. It is suggested that the ASTM standard be adopted.

Project # PD-44: Composite Pd and Alloy Porous Stainless Steel Membranes for Hydrogen Production and Process Intensification

Yi Hua Ma; Worcester Polytechnic Institute

Brief Summary of Project

The objectives of the project include; 1) synthesis of composite palladium (Pd) and Pd alloy porous Inconel membranes for water-gas shift (WGS) reactors with longterm thermal, chemical and mechanical stability with special emphasis on the stability of hydrogen flux and selectivity; 2) demonstration of the effectiveness and longterm stability of the WGS membrane shift reactor for the production of fuel cell quality hydrogen; 3) research and development of advanced gas clean-up technologies for sulfur removal to reduce the sulfur compounds to less than 2 ppm; and 4) development of a systematic framework towards process intensification to achieve higher efficiencies and enhanced performance at a lower cost.



Question 1: Relevance to overall DOE objectives

This project earned a score of **3.3** for its relevance to DOE objectives.

- Barriers related to the Hydrogen Program are addressed in this project. This project also focuses on research on developing advanced gas clean up system.
- This is an important and comprehensive project on development and testing of composite Pd-based alloys and Inconel membranes, highly relevant to DOE's hydrogen and fuel cell technologies. The researchers have excellent and methodic approaches for membrane development and testing. The presented results for FY08-09 indicate substantial progress in determining the effects of a number of contaminants and H₂-flux. The H₂-flux rates obtained from the developed membranes are significantly higher than DOE's targets for 2010 and 2015.
- A membrane of this type has the potential to enable several important applications.
- Addressing the membrane R&D needs for purification from coal-to-hydrogen process is relevant to DOE objectives.
- Typically when pressure swing adsorption (PSA) is used, no preferential oxidation and sometimes no low-temperature shift (LTS) is used (just a note on slide 4).

Question 2: Approach to performing the research and development

This project was rated **3.0** on its approach.

- The project team's approach is to fabricate Pd and Pd-alloy (Pd-Au) membranes on porous stainless steel tubes and test the membrane performance. It is unclear what was done to develop advanced sulfur clean up. Slide #4 showed the schematic approach of this project that included the advance sulfur cleaning unit but there was nothing about it in the rest of the presentation. Also, the adsorption work is unclear. Is this project trying to develop improved PSA system?
- Approaches used in this program are sound and carefully implemented. Nearly all aspects of the membrane productions and testing have been considered and evaluated. Modeling simulations of Methane Steam Reforming (MSR) have provided useful information. Effects of pressure, temperature and compositions have been predicted.

- Sequential characterization and testing activities are appropriate in this project.
- Regarding the tubular membrane: while it is useful to test the membrane with synthetic mixed gas stream, the project team needs to test with actual syngas from a gasifier.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated 2.8 based on accomplishments.

- It is claimed the membrane system had very high selectivity (nearly infinite selectivity for hydrogen). The detection limit of the gas analysis unit for CO, CO₂, and other species should be presented. No data was presented on the structural stability of the membranes under cycling conditions. Was there any interaction between the Pd membrane and the interface oxide layer?
- The project has shown very good progress regarding synthesis, fabrication and testing of Pd and Pd alloy composites membranes for applications in WGS reactors. Results of the tests are satisfactory and promising. Reported test results of the membranes, using simplified gas mixtures, indicate very good long-term H₂ selectivity and stability. However these tests should be extended to gas mixtures that are more realistic and similar in compositions with syngas.
- The data reported shows good progress toward the project's flux goals.
- Given the length of the project to date, there needs to be testing with real syngas from a gasifier.
- Regarding long term testing (slide 8), what are the concentrations of the gases entering the membrane (62%H₂, 37%CO₂, 1.2%CO).
- The project team needs to address the impurities and their levels in the product hydrogen stream and compare them to California Fuel Cell Partnership Hydrogen purity specifications.
- Presentation overall lacks cohesiveness and difficult to follow by the team.

<u>Ouestion 4: Technology transfer/collaborations with industry, universities and other laboratories</u>

This project was rated 2.5 for technology transfer and collaboration.

- Collaboration is seen with Adsorption Research, Inc., in the area of adsorption study but the objective of this collaborative work is not clear. Is it to develop an advanced PSA system or to develop advanced sulfur removal technology?
- It appears there is some collaboration with Adsorption Research, Inc. for production and testing of sulfur removal sorbents and for building and testing of the Pressure Swing Adsorption systems.
- Outside testing with Shell's reformer is useful for program validation.
- The project does not have significant collaborations with other institutions. The project team should work with other DOE sponsored projects to leverage any synergies.

Question 5: Approach to and relevance of proposed future research

This project was rated 2.5 for proposed future work.

- The project team has decided to continue the Pd-Au alloy membrane to improve the flux. Both Pd and Au are very expensive. Is there a plan to look into less expensive alternate membrane materials? How is the mass transfer resistance overcome in a very thin membrane?
- The project team's future work will include additional alloying studies for improving H₂ flux. Modeling studies will extend to a broader range of conditions and alloy types, including Pd-Au alloys. In addition to planned tolerance tests for CO and sulfur, poisoning effects of other major syngas contaminants should also be tested and evaluated. Major contaminants in a "typical" syngas, including halogens and nitrogen oxides, should be added to test mixtures and their poisoning effects should be evaluated and quantified.
- The project team should provide the connectivity to the baseline information that informed this project.
- The project team should also describe why this project is innovative in more detail then the general information provided. The concern about IP is understood but a credible examination of the claims of performance relies on some understanding of the mechanization.
- The project should compare the product against current hydrogen purity specs.

Strengths and weaknesses

Strengths

- The project team has significant experience with Pd membrane. The availability of graduate students and postdoctorate students to carry out the experiments and test new theories/hypothesis is beneficial. Professor Ed Ma is well respected in this field.
- The project applies sound and well-planned procedures for selection, fabrication and testing of the Pdcomposite membranes. The experimental testing methods are adequate and carefully performed. The modeling simulations are very useful for predicting the performance of the membrane in a broad range of conditions.
- The testing regime is thorough in this project.

Weaknesses

- The lack of knowing the detection limits for CO, CO₂ is a weakness. The selectivity numbers reported in this project are questionable (due to lack of detection limits for other gases). Nothing about an advanced sulfur cleaning unit was presented.
- No major weaknesses were identified.
- It is curious that no embrittlement has been reported by the project team. The representation that this simply does not occur is not credible without support.

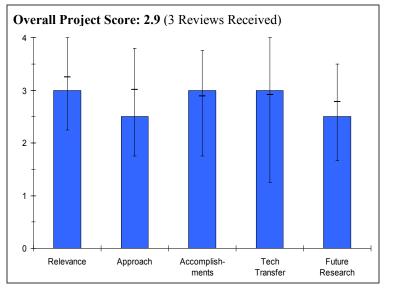
- The project team should perform an economic analysis for the Pd-Au alloy membrane. Will it meet the DOE cost target? How about sulfur poisoning of Pd membranes?
- The potential poisoning of all major syngas contaminants, particularly nitrogen and halogen compounds, should be tested and evaluated by the team.
- The analytical detection limits for H₂, CO and other relevant species should be carefully established and considered in error assessments of the data.
- No changes are recommended.

Project # PD-45: Development of Robust Metal Membranes for Hydrogen Separation

Brian D. Morreale; National Energy Technology Laboratory

Brief Summary of Project

Studies suggest that incorporating separation membranes into coal conversion processes can reduce costs. The overall goal of this project is the development of robust dense metal, hydrogen separation membranes for integration into coal conversion processes. A test protocol has been developed that allows technological progression and comparisons for application to coal conversion processes. Several alloy compositions have been fabricated and screened for performance, and some alloys have shown potential for S-tolerance.



<u>Question 1: Relevance to overall DOE</u> <u>objectives</u>

This project earned a score of 3.0 for its relevance to DOE objectives.

- This project is pertinent to industrial applications.
- This project addresses the membrane R&D need for purification from coal-to-hydrogen process.

Question 2: Approach to performing the research and development

This project was rated **2.5** on its approach.

- The project team's idea of intentionally degrading the system is interesting.
- It is unclear if using Pd alloy membranes is the best approach for separating hydrogen from coal-derived syngas The syngas contains more contaminants (to the membrane) as compared to a cleaner reformate stream from a steam methane reformer. Research on Pd and Pd alloy membranes integrated with a reformer has been done for many years and the technology has not been applied commercially. This project's application potentially can be more challenging for the membrane.

Ouestion 3: Technical accomplishments and progress toward project and DOE goals

This project was rated **3.0** based on accomplishments.

- More analysis is necessary in this project to contrast the performance of a degraded system vs. a non-degraded system.
- The project team has had good progress towards addressing the three main tasks of the project and addressing the barriers.

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated 3.0 for technology transfer and collaboration.

• This project has good collaborations with various institutions.

<u>Ouestion 5: Approach to and relevance of proposed future research</u>

This project was rated 2.5 for proposed future work.

- The project's Pd/Cu alloys have been used extensively in hydrogen work and it would be useful to have some connectivity to the baseline information that informed this project.
- It would be useful to describe why this is innovative in more detail then the general information provided. The concern about IP is understandable but a credible examination of the claims of performance relies on some understanding of the mechanization.
- The project team should consider developing a list of selection criteria in trying to optimize a membrane development.
- The project team should consider testing water-gas shift membrane reactor (WGSMR) with real syngas from gasifier.
- The project team needs to determine impurities and their levels in product hydrogen stream.

Strengths and weaknesses

Strengths

• The project's focus on durability is important to adaptation.

Weaknesses

• A degraded system has limitations that were not fully presented.

Specific recommendations and additions or deletions to the work scope

• None recommended.

Project # PD-46: Scale-up of Hydrogen Transport Membranes for IGCC and FutureGen Plants *Doug S. Jack; Eltron Research & Development Inc.*

Brief Summary of Project

The overall project objective is to develop a H_2/CO_2 separation system that; 1) retains CO_2 at coal gasifier pressures; 2) operates near water-gas shift conditions; 3) tolerates reasonable achievable levels of coal-derived impurities; 4) delivers pure H_2 for use in fuel cells, gas turbines and hydrocarbon processing; and 5) is cost effective compared to alternative technologies for carbon capture.

<u>Question 1: Relevance to overall DOE</u> <u>objectives</u>

Overall Project Score: 2.4 (4 Reviews Received)

This project earned a score of **3.3** for its relevance to DOE objectives.

- The objective of this project is to develop an H₂/CO₂ separation system that retains CO₂ at coal gasifier pressures, operates near water-gas shift conditions, tolerates reasonably achievable levels of coal derived impurities, delivers pure H₂ for use in fuel cells, gas turbines, and hydrocarbon processing, is cost effective compared to alternative technologies for carbon capture. Therefore this project supports DOE's Hydrogen from Coal Program.
- The development of practical and inexpensive membranes for hydrogen separation/purification for use in fuel cells is highly relevant to DOE's Hydrogen Program. However, most relevant and critical information necessary for evaluations of this project was not provided to reviewers. In the absence of such critical information it is difficult to evaluate the project, informatively and fairly, on its progress and soundness of future work.
- If this project is successful, this work would be highly relevant to DOE objectives.

Question 2: Approach to performing the research and development

This project was rated **2.5** on its approach.

- The project team's approach involves materials development, performance screening, mechanical design, process design and economics, and scale-up steps. The membrane and catalyst compositions are not disclosed; therefore it is difficult to determine whether the approach taken is right or wrong.
- The team's approaches utilized in this project are good and are now standard for development and testing of the separation membranes.
- The integrity of the welded seals mentioned might be sensitive to differences in hydrogen expansion. Welding has only been tested on disks so far.
- There seems to be an issue with the catalyst layer being affected by intermetallic diffusion in this project. Even at lower temperatures, this might become an issue over longer time periods.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated 2.0 based on accomplishments.

• The project's flux numbers are very impressive but they are measured under ideal conditions. The flux numbers should be reported using truly mixed-gas streams similar to a gasifier gas stream. What is the hydrogen recovery in experiments where fluxes over 350 SCFH/f² are obtained? Important information like gas flow rates, hydrogen recovery, and selectivity were not presented. It is difficult to evaluate the technical

accomplishments without knowing more about the membrane material and the catalyst used. This presentation appeared as if it was made by a representative from the Chamber of Commerce (to promote a business) rather than a scientific presentation for a peer review.

- No information was provided on the nature of the membranes used for testing. It is unclear if the project team has or will overcome the barriers for large scale and/or long term usage of the tested membranes. For example, if copper is a major component, based on several independent studies, exposure to sulfur will most likely rapidly destroy the membrane.
- The presented data indicates that the membrane material performance in this project will meet DOE's goals.
- The project's progress is hard to judge in this case. There was insufficient information provided to make a credible determination.
- Given that scaling up of the technology is the goal, the presented quantitative data on the basic problems (see above) do not address this goal. Maybe they are and the results are not made available to the reviewers?

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated **2.7** for technology transfer and collaboration.

- None of the project team's collaborators were disclosed. Partners include four membrane manufacturers and two industrial chemical producers.
- Information on collaborators in this project was not provided by the presenter.
- More information on collaborators would help address issues/uncertainties that the project can stand firmly on its merits.

<u>Ouestion 5: Approach to and relevance of proposed future research</u>

This project was rated **2.3** for proposed future work.

- It is stated (slide 6) that one alloy composition was down-selected for future testing and test results show the performance is meeting the targets. If this is the case, why will the team perform life testing on new materials? What is wrong with the already down-selected material?
- It is not possible to rate this project's proposed future work, when required information is not presented. For example, if the alloys to be tested contain Cu, a number of other recent studies have already reported various difficulties and performance problems with such alloys. Therefore, if this project intends to test copper containing alloys, it should present a convincing reasoning for repeating such studies.
- It would be useful to have some connectivity to the baseline information that informed this project.
- Also, it would be useful to describe in more detail why this is more innovative than the general information provided. The concern about IP is understood, but a credible examination of the claims of performance relies on some understanding of the mechanization.
- It might be too early for this project to scale up.

Strengths and weaknesses

Strengths

- The flux numbers in this project are impressive. Many years of experience on membranes is seen. The project team's ability to get new partners whenever needed is good (unfortunately no long-term partners).
- Developing and testing inexpensive, effective and durable H₂-separation membranes are of high priority for H₂ technology. Contributions of this project can be valuable to DOE's mission in advancing H₂ technology.
- This project has high potential if successful.

Weaknesses

- The PI was not able to disclose the material.
- Due to the lack of adequate quantitative data and information on composition of membranes developed and testing in this project, it is difficult to fairly assess the weaknesses or strength of this project.
- There is little attempt by the project team to actually describe the membrane or the methodology of testing the membrane.

- There was little effort to present any information other than unsupported claims in this project.
- No proof was provided that fundamental problems are sufficiently addressed in this project. It is too early for the team to focus on scaling up. Critical technology seems to be outsourced to subcontractors.

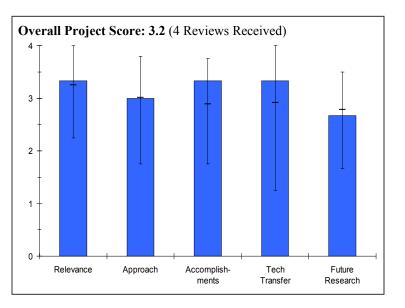
- The project team should address commercial scalability of the Eltron membrane and catalyst. They should study the stability of the membrane and catalyst under cycling of temperature and gas composition.
- Additional testing by the team for the membranes is needed before moving to the production stage. Particularly, in addition to sulfur and CO poisoning, effects of chlorine and nitrogen oxides should be tested and quantified.

Project # PD-47: High Permeability Ternary Palladium Alloy Membranes with Improved Sulfur and Halide Tolerance

Kent Coulter, Ph.D.; Southwest Research Institute

Brief Summary of Project

The overall project objective is to develop technologies that effectively and economically separate hydrogen from mixed gas streams that would be produced by coal gasification. The objectives of this project are to; 1) develop a process methodology for the cost-effective manufacturing of thin, dense, self-supporting palladium alloy membranes for hydrogen separation from the mixed gas streams of coal gasification processes; and 2) reduce Pd membrane thickness >50% over current state-of-art and show potential to meet the DOE 2010 technical targets.



<u>Ouestion 1: Relevance to overall DOE</u> <u>objectives</u>

This project earned a score of 3.3 for its relevance to DOE objectives.

• The objectives of this project are to develop and test Pd-based membrane that has improved tolerance to corrosive contaminants in syngas. The objectives of this project are in support of DOE's hydrogen and syngas technologies and results will help to achieving DOE goals

Question 2: Approach to performing the research and development

This project was rated **3.0** on its approach.

- The experimental and computational modeling approaches employed in this project are generally well planned and effective. However, the density functional theory (DFT) computational modeling efforts need improvement. Modeling procedures can be calibrated and verified by comparing modeling predictions for properties of certain alloys with experimental results for the alloy with same composition.
- The sealing can be improved in this project as well as the bottleneck on method.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated 3.3 based on accomplishments.

- The project team has reported significant progress towards objectives of the project.
- Eventual large scale applications of very thin membranes foils and disks for syngas-H₂ purifications is not likely due to a large number of technical difficulties in fabrication and using such foils and films. However, test results derived from this and similar projects are very useful in understanding chemical and physical properties of various alloys relevant to hydrogen purification and fuel cells.
- Results of this study on hydrogen permeability for various alloys and different temperatures are very valuable in assessing the preferred alloys for hydrogen purification.
- Data presented by the team was lucid, clear, and thorough.

<u>Ouestion 4: Technology transfer/collaborations with industry, universities and other laboratories</u>

This project was rated **3.3** for technology transfer and collaboration.

- The project team is working with a number of very capable groups, with complementary expertise, and is collaborating to achieve the objectives of this project.
- The project team performed all aspects of the studies, including design, modeling, fabrication, and testing of membrane.
- The project team can add work done by Lovvik et al, to incorporate in the theoretical model.

Question 5: Approach to and relevance of proposed future research

This project was rated 2.7 for proposed future work.

- The planned future work is generally sound and will help to achieve the stated goals of the project.
- It is recommended that more emphasis be given to improving and validating the modeling procedures for predicting hydrogen permeability of various alloys under different temperature and pressure conditions. If successful, modeling predictions should help in screening of a very large number of alloy compositions considered for testing. In the long run, using the modeling predictions for better selecting alloy compositions will lower the cost and shorten the time needed to achieve the objectives of the project.
- The goal of ultra thin membranes is constructive to integration and retrofit scenarios for several applications.
- Again, this project will encounter sealing barriers.

Strengths and weaknesses

Strengths

- This is a multi-approach and well-planned project. Collaborations among a number of expert groups with complementary capabilities have had past success and will help in achieving the future objectives of the project.
- The project represents a valid effort with 70 units fabricated.
- This project provides a powerful tool to make any alloy composition with high precision. This is highly valuable for the industry.

Weaknesses

- The computational modeling efforts are not well coordinated with laboratory studies. Hydrogen permeability for a large number of alloys has been determined experimentally and through modeling. However, alloy compositions used in modeling do not compare with those used in experimental studies. Consequently, direct comparison of the modeling and experimental results are not possible and experimental results cannot be used to calibrate the computational procedures.
- As test results from this work show, very thin membrane films are not likely to be durable for long-term applications. Alternative approaches, such as supporting of membrane on a durable base, should be considered.
- It would be useful to have some connectivity to the baseline information that informed this project.
- Sealing issues in this project are a weakness.

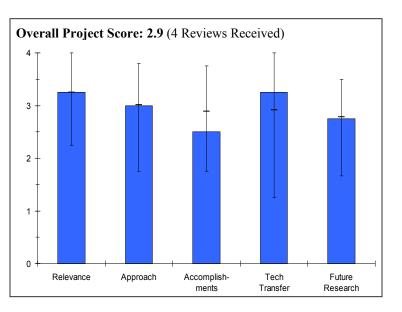
- It is recommended that more emphasis be given for improving the modeling procedures for predicting hydrogen permeability of various alloys under different temperature and pressure conditions. If successful, DFT modeling predictions should help in screening a very large number of alloy compositions considered for testing. And in the long run using the modeling predictions will lower the cost and shorten the time needed to achieve the objectives of the project.
- Continuing the testing of very thin membrane films should be replaced with other method(s) that provide more membrane durability.
- The Cu content of alloys may be responsible for rapid degradation and rupture of the membrane films.
- No changes are recommended.

Project # PD-48: Experimental Demonstration of Advanced Palladium Membrane Separators for Central High-Purity Hydrogen Production

S.C. Emerson, J.T. Costello, Z. Dardas, T. Hale, R.R. Hebert, G.C. Marigliani, S.M. Opalka, Y. She, R. Willigan, and T.H. Vanderspurt; United Technologies Research Center

Brief Summary of Project

The objectives of this project are to; 1) confirm the high stability and resistance of a PdCu trimetallic alloy to carbon and carbide formation and, in addition, resistance to sulfur, halides and ammonia; 2) develop a sulfur, halide and ammonia resistant alloy membrane with a projected hydrogen permeance of 25 m³m⁻²atm^{-0.5}h⁻¹ at 400°C and capable of operating at pressures of 12.1 MPa; and 3) construct and experimentally validate the performance of 0.1 kg/day H₂ PdCu trimetallic alloy membrane separators at feed pressures of 2 MPa in the presence of H₂S, NH₃ and HCl.



Question 1: Relevance to overall DOE objectives

This project earned a score of **3.3** for its relevance to DOE objectives.

- The objective of this project is to develop a sulfur, halide, and ammonia resistant alloy membrane for hydrogen separation and construct and experimentally validate the performance of 0.1 kg/day H₂PdCu trimetallic alloy membrane separators at feed pressures of 2 MPa (290 psia) in the presence of H₂S, NH₃, and HCl. This project supports the hydrogen from coal program (centralized hydrogen production).
- Objectives of this project include fabrications and testing of palladium-copper and tri-metallic membranes for hydrogen purification that are resistant to poisoning by syngas contaminants. Overall project objectives and technical plan may result in development of low-cost membranes for hydrogen production. This project is in line with DOE's cost goals.
- Currently, a H₂-flux of about 60 scfh/ft² with a 100 psi back pressure has been achieved. This flux is considerably less than the DOE 2010 target flux of 200 scfh/ft². Significant advancements by this team in membrane durability and H₂-permeation need to be made to achieve the DOE target. Also, tested membranes show inadequate lifetime and durability. Tests at higher backpressures have caused rapid membrane failures. Fundamental reasons for such failures need to be understood.
- It is very likely that significant amounts of copper content in Pd-Cu alloy react with sulfur and initiate failure of this class of membranes. Such failures have been reported in a number of independent studies.
- If this project is successful, this will be a very high-flux membrane.

<u>Ouestion 2: Approach to performing the research and development</u>

This project was rated **3.0** on its approach.

- The team's approach is to use advanced membrane property simulations by atomistic and thermodynamic modeling and experimentally verify the performance of hydrogen separator membranes made using the results of the modeling work. Unfortunately, all the membranes leaked and therefore the results are inconclusive.
- This project employs multiple testing procedures for designing and examining durability of Pd-Cu-based membranes. The approaches are sound. The durability tests indicate failure of the membranes after relatively short operating times. In addition to examining the physical reasons for failures, chemical effects of contaminant on the membrane, such as sulfur reactions with copper, should also be studied.

- In this study, a larger number of contaminants in the tests gases have been used, making the test results more realistic in comparison to several studies that have over-simplified the test gas mixtures.
- The project team has a good approach with proper tools.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated 2.5 based on accomplishments.

- The project team has evaluated the performance of fcc PdCu separators; quantified the effect of H₂S, CO, CO₂, N₂, and H₂O on H₂ permeability; demonstrated sulfur resistance of PdCu alloy; produced five (5) separators with United Technologies Research Center (UTRC) ternary composition; and has formed a secondary phase barrier on outer surface of membrane. There is a wide variation in flux for some membrane systems tested at nearly similar conditions but the reasons are unknown. Almost all the membranes leaked and there are defects in membrane tubes.
- Significant progress is being made in testing four separate Pd-Cu alloy membranes. Three of these membranes have failed. The Milestone Schedule indicated the project is near completion. However, several unresolved issues regarding the performance and durability of these groups of membranes still remain. The H₂ permeation needs to be substantially improved and reason(s) for relatively fast rupture of membranes should be established.
- The publication of information is important for this project.

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated **3.3** for technology transfer and collaboration.

- The project team collaborated with Power+Energy to manufacture the hydrogen separators and fabricate the UTRC alloys. Fundamental experiments on hydrogen solubility and experimental measurements of alloy systems for thermodynamic phase modeling were done in collaboration with Metal Hydride Technologies.
- This project is a collaborative team effort, involving four experienced groups.
- The University of Vermont and the Colorado School of Mines are valid collaborators in this project.

Question 5: Approach to and relevance of proposed future research

This project was rated 2.8 for proposed future work.

- The performance of a few more ternary alloys will be tested in 2009. The durability of membrane separators will also be studied. This project is scheduled to end in June 2009 and therefore no plans for future were given. Will there be a follow-up to this project?
- It is projected that two additional ternary Pd-Cu-based membranes will be manufactured and tested. In order to resolve the remaining issues with Pd-Cu ternary membranes a larger number of alloy types and performance tests need to be performed.
- Reason(s) for failure should be established and remedied in this project.
- The effort to connect with the 50kw fuel cell using logistics fuel for the Navy was interesting. A more thorough explanation of this effort would have been helpful.

Strengths and weaknesses

Strengths

- Collaboration with Power+Energy and Metal Hydride Technologies are a strength to this team.
- The project attempts to develop relatively inexpensive and durable membranes for hydrogen separations. A number of well-planned approaches have been utilized. Particularly the poisoning tests in this study are more realistic than those in a number of similar projects.
- Despite some shortcomings, results obtained from this project are valuable in better understanding of the factors affecting the performance of hydrogen separation membranes.
- The PI gave a frank presentation on this project.
- A high-flux membrane, from this project, would be enabling for many applications.

FY 2009 Merit Review and Peer Evaluation Report

• Encountered hurdles by the project team are well addressed.

Weaknesses

- In this project, all the membranes leaked and there is no apparent plan to address this issue. There is wide variation in flux for soae membrane system tested at nearly identical conditions, i.e., there is no reproducibility. There are no plans to control the defects in membrane tubes.
- The membrane manufactured and tested in this project has not performed as desired. Significant improvements are needed in the hydrogen permeation rate and durability of the Pd-Cu-based alloys.
- It would be useful to have some connectivity to the baseline information that informed this project.

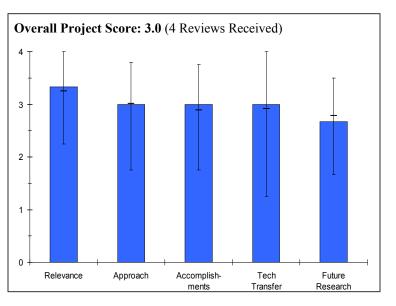
- Due to its weaknesses, this project should not be considered for continuation/renewal when the current term expires in June 2009.
- A larger number of alloy Pd-Cu-based alloy compositions, fabrication methods, permeation, poisoning and durability tests should be performed.
- Systematic variations in the composition may help identify the reason(s) for failures of Pd-Cu membranes in this project.

Project # PD-49: Integration of a Structural Water Gas Shift Catalyst with a Vanadium Alloy Hydrogen Transport Device

Tom Barton; Western Research Institute Morris Argyle; University of Wyoming

Brief Summary of Project

The 2007 objective of this project was to integrate the water-gas shift (WGS) catalyst and metallic membranes into a device and test under gasifier conditions. The 2008 objective of this project was to build a modular WGS/membrane integrated device capable of producing 10,000 l/day hydrogen from coal-derived syngas. The ceramic catalysts developed are superior to commercially available WGS materials with respect to survival in a pressurized device. Two different viable integrated device designs using vanadium membranes are under fabrication that should meet scalability issues and performance criteria.



Question 1: Relevance to overall DOE objectives

This project earned a score of 3.3 for its relevance to DOE objectives.

- The objective of this project for the current year is to build a modular WGS/membrane integrated device capable of producing 10,000 liters/day of hydrogen from coal-derived syngas. WGS catalyst and hydrogen separation membrane module development are key parts of this project.
- Objectives of this project include development and testing of WGS catalysts capable of operating at high pressures and manufacturing an integrated WGS membrane system to produce 10,000 liters/day of hydrogen from coal derived syngas. This is an excellent project with clear relevance to DOE's mission in coal and/or biomass conversion into syngas and subsequently hydrogen. The WGS catalysts-membrane process design and integration used in this project should allow for better efficiency and greater flexibility.
- The project's approach has very good potential to be scaled up for commercial applications.
- This project has practical goals.

Question 2: Approach to performing the research and development

This project was rated **3.0** on its approach.

- There are four tasks in this project; 1) to develop WGS catalyst; 2) scale up the integrated devices catalyst plus membrane; 3) test the integrated module in a fluidized bed coal gasifier; and 4) perform economic analysis. The project's approach to develop a catalyst is good. The catalyst development was the objective for FY2006 and this objective was met in 2008. However, there is nothing in the approach that addresses how to overcome the membrane's oxidation problem.
- This is an excellent project relevant to DOE's objectives. A number of WGS catalysts have been developed and tested. Catalysts with Al and Ce show higher activity than other tested catalysts (vanadium-based).
- The process design and approaches used by the team can be utilized for large-scale operations. Two integrated WGS devices have been built and tested. The target rate of 10,000 liters/day at 600 psi for hydrogen production has been reported.
- The project's integrated system allows for using different membrane materials with the WGS catalyst.

<u>Ouestion 3: Technical accomplishments and progress toward project and DOE goals</u></u>

This project was rated 3.0 based on accomplishments.

- The structural WGS catalyst developed with Al and Ce shows higher activity and is more appropriate for the integrated WGS -membrane device than the commercial catalyst. The two scale-up designs for the membrane modules are carried out (one with Chart Engineering and the other with REB Research, Inc.). Two integrated devices were constructed that met the 10,000 liters/day hydrogen goal at 600 psig and 400°C in coal derived syngas. One device was constructed to incorporate anyone's best membrane material. The vanadium alloy membranes are challenging to manufacture.
- The project is near completion. Fabrication and testing of the integrated WGS units have been completed and testing is 90% complete. Overall, the technical accomplishments for this project have been very good.

<u>Ouestion 4: Technology transfer/collaborations with industry, universities and other laboratories</u>

This project was rated **3.0** for technology transfer and collaboration.

- This project involves collaboration with University of Wyoming, Chart Energy and Chemicals, REB Research and Consulting, U.S. DOE Ames Laboratory. The roles played by the collaborators are clearly described in the presentation.
- The project team has good collaboration between the team members from academics, industry, national lab and small business consulting. Team members' responsibilities and their work and part in the team clearly described.

Question 5: Approach to and relevance of proposed future research

This project was rated 2.7 for proposed future work.

- The commercialization of the WGS catalyst monolith will be pursued with the assistance of a catalyst manufacturer. Completion of the testing of the two-scaled integrated devices will be followed by the design and fabrication of the 10x assembly based on the economic and performance data for testing under coal gasification conditions. The flux for the vanadium alloy membrane is low. Are there any plans to improve its flux and are there any plans to look into other membranes?
- Upon completion of testing of two more WGS integrated devices, the project has plans of commercializing the WGS units. Collaborations with large scale catalyst manufacturers will be required. The team's plans build on progress and address the barriers for commercialization of the WGS devices.
- The PI gave a frank presentation of the project.

Strengths and weaknesses

Strengths

- The project's strength is shown in developing a new catalyst and methods to incorporate the catalyst on membrane structural units. The researcher at REB Research, Inc. has strong background in membranes area. Chart is well known in developing engineering components for energy applications.
- Practical, efficient and durable catalysts-membrane combinations have been developed, tested and utilized in this project. The return for investment on this project is very good.

Weaknesses

- The project team should focus on vanadium alloy membrane especially if it cannot meet the 2010 flux target. It is very difficult to make vanadium alloy. There is no focus to avoid the problems with vanadium system. And there is no attempt to look into other candidate materials.
- The poisoning and durability tests have not used more realistic syngas compositions. The project's potential contaminants such as trace heavy metals or halogens may affect the performance and durability of the catalysts and membrane.
- The team should have some connectivity to the baseline information that informed this project.
- Also, the focus on vanadium should have been contrasted with other candidate materials more clearly.

- The project team should drop the vanadium alloy work and try to incorporate the catalyst onto a more practical membrane system.
- The performance tests for the WGS catalysts and membranes should be extended to conditions that better mimic more realistic syngas compositions.

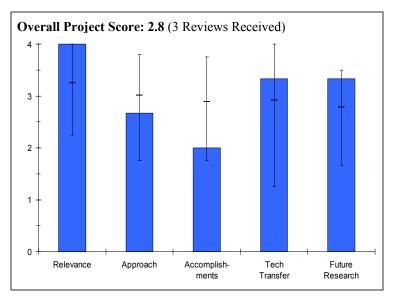
Project # PD-50: Hydrogen Delivery in Steel Pipelines

Doug Stalheim; Secat, Inc.

Brief Summary of Project

The objective of this project is to develop materials technologies to minimize embrittlement of steels used for highpressure transport of hydrogen. The deliverables are to 1) identify steel compositions/microstructures suitable for construction of new pipeline infrastructure; 2) develop barrier coating for minimizing hydrogen permeation in pipeline and associated processes (on hold per DOE); and 3) understand the economics of implementing new technologies.

<u>Question 1: Relevance to overall DOE</u> <u>objectives</u>



This project earned a score of **4.0** for its relevance to DOE objectives.

- This project is dealing with material microstructures that are hydrogen compatible. The main investigator, D. Stalheim, is an authority in the field of steel microstructure as it relates to mechanical properties. The proposed four steel-microstructures, namely A, B, C, and D are promising micro-alloyed steels we can manufacture today for hydrogen compatibility.
- Success in identifying/developing embrittlement-free and corrosion-free alloys and welds would have significant effects on building hydrogen pipelines. This would also be the most cost-effective means for delivering hydrogen from central production areas to hydrogen refueling stations. This project aligns with DOE's goals.

Question 2: Approach to performing the research and development

This project was rated 2.7 on its approach.

- The project's focus on the effects of steel structures on hydrogen sulfide stress cracking is well known and may be applied directly to loss of ductility due to high-pressure gaseous hydrogen charging.
- The project has analyzed the microstructure of four promising steels (A, B, C, and D) and established their grain morphology. The project has also studied the hydrogen effect on the uni-axial tension response of these steels. In particular, the project established the hydrogen effect on the yield and ultimate strength and the reduction in area as a function of hydrogen pressure.
- The microstructural analysis results of this project are very important since they will help in the analysis of the hydrogen-induced fractures. Therefore the project's approach to ascertain the steel microstructures in relation to the mechanisms of fracture is extremely important. The uni-axial tension results though are not important as they do not correlate with material fracture toughness.
- The evaluation matrix is well established for the project. This project relies on the existing pipeline materials and lacks novelty.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated 2.0 based on accomplishments.

- The effect of strain rate on tensile testing steels in high-pressure hydrogen needs to be evaluated, in order to fully interpret the project results to date.
- The proposed steel microstructures and their microstructural characterization is an important development. In fact, the project should focus on further developing and analyzing potential microstructures that are hydrogen compatible. To do this, the project should proceed with the fracture toughness assessment of the steel microstructures termed as A, B, C, and D, and establish what new advances in the material microstructures are needed to improve fracture resistance. As explained below, the project has already planned for these fracture assessment experiments. Therefore, the project is on the right trajectory.
- The project has very limited accomplishments and progress has been made, but these are proportional to the project schedule and DOE's funding.

<u>Ouestion 4: Technology transfer/collaborations with industry, universities and other laboratories</u>

This project was rated **3.3** for technology transfer and collaboration.

- The team's collaboration between SECAT, DGS Metallurgical Solutions, and Sandia National Laboratories is outstanding. It sets the project on the proper trajectory toward achieving its goals.
- There is a good team structure involving a national laboratory and other companies. The majority of accomplishments presented were made by ORNL, and contributions from other team members are unclear.

<u>Question 5: Approach to and relevance of proposed future research</u>

This project was rated **3.3** for proposed future work.

- It is unclear what new insights the proposed validation of select reduction in area values of alloys B, C, and D in hydrogen will bring about in this project. As was mentioned above, uni-axial tension tests offer negligible information on the relationship between microstructure response and hydrogen embrittlement.
- Future work for this project is listed in detail. Economic analysis will be very helpful to determine the viable approach.

Strengths and weaknesses

Strengths

- The identification, development and analysis of promising modern low-carbon steel microstructures are a strength of this project.
- The participation of Mr. D. Stalheim is a strength of this project.
- This project has low risk of utilizing existing commercial products.

Weaknesses

- This project has no fracture assessment of the microstructures as of yet. However, the proposed collaboration with Sandia National Laboratories aims to do exactly that.
- This project is scheduled to be completed by 2011. It is unclear if this project meets the time frame of DOE's "go/no-go" decision milestones.

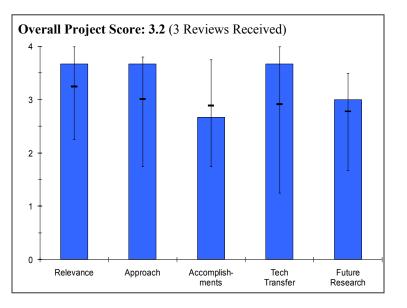
- Study of the uni-axial tension characteristics offers negligible information on the material resistance to hydrogen-induced fracture. This is a well-documented fact in the hydrogen literature. The project team should focus on fracture toughness assessment. They should redirect and work toward microstructural development, alloy modification and improvement, perhaps through thermo-mechanical or chemical treatment, after input is received from Sandia on the fracture behavior. In other words, capitalize on the project's personnel strengths that lie on alloy development.
- The project team needs to evaluate impurity effects on steel, especially for impure gases like moisture and trace of H₂S.

Project # PDP-01: Development and Optimization of Cost Effective Material Systems for Photoelectrochemical Hydrogen Production

Eric McFarland; University of California, Santa Barbara

Brief Summary of Project

The overall project objective is to discover and optimize an efficient, practical and economically sustainable material system for photoelectrochemical (PEC) production of bulk hydrogen using solar light energy as the primary energy input making use of novel syntheses and high throughput experimentation methods. The task objectives of this project are to 1) identify improved materials for solar photon absorption using high throughout methods and exploratory design and synthesis of new mixed metal-oxides; and 2) optimize the morphology of the PEC material system for maximum efficiency.



Question 1: Relevance to overall DOE objectives

This project earned a score of 3.7 for its relevance to DOE objectives.

- The project's development of a viable form of iron oxide for PEC water splitting is extremely relevant to Hydrogen Program goals.
- The team's long-term renewable hydrogen production supports Hydrogen Program objectives.
- Yes, this project is relevant to DOE's overall objectives.
- This project uses a greater than 2.2 eV band edge criteria for "go/no-go" decision screening.
- This project uses a 10% conversion "go/no go" decision screening.
- This project uses >8% solar H₂ production efficiency as "go/no-go" decision screening.
- This project uses <\$5/kg of H₂ criteria for the "go/no-go" decision screening.
- The materials development piece of this project is impressive and important to the goal of efficient PEC-based water splitting. The new modifications to Fe₂O₃ appear encouraging in lowering band gap of the metal oxide photo-electrodes.

Question 2: Approach to performing the research and development

This project was rated **3.7** on its approach.

- The project has done a good job of integrating state-of-the-art theory, synthesis and characterization approaches to tackle the difficult job of refining oxide materials and interfaces for PEC water splitting. Further emphasis on this integrated approach is strongly encouraged; both in continued research into hematite-based systems, and in the discovery of new material systems, such as the delafossites.
- The project team's approach is directly addressing key efficiency, durability, and cost.
- Focusing on cheap & abundant material is a logical approach by the project team.
- The PI has shown steady progress toward understanding of the chemical mechanisms that limit materials synthesis. This is not an easy problem to tackle.
- McFarland has a good grasp of materials issues and his approach to combine combinational synthesis with theory has a good chance of achieve many of the project's objectives.
- It is important for the PI to remain focused on the big picture. And as such, via tasks #6 to #9, must begin evaluating the conceptual reactor designs and ultimately, an estimation of the hydrogen production costs both with and without sacrificial reagents (e.g. municipal waste water, etc.).

Ouestion 3: Technical accomplishments and progress toward project and DOE goals

This project was rated 2.7 based on accomplishments.

- The project team's integrated approach has yielded impressive results, particularly in the demonstration of record levels of unbiased PEC water splitting in modified hematite materials. Though these levels are below DOE targets, the results are encouraging and represent a significant step forward. Integrated multi-junction configurations might be of interest using the current forms of this material. Preliminary results from the delafossites are less auspicious, but the successful implementation of integrated theory/synthesis/characterization approach in the research of this "new" material class represents a good accomplishment.
- The projects use of iron oxide is not promising. More focus on other more promising materials is needed by this team. Significant improvement in incident photon conversion efficiency (IPCE) is still needed.
- No progress has been made on an actual reactor design and H2A cost analysis in this project.
- The high-temperature electrolysis (HTE) of Al doped hematite was identified 0.3-0.5% as optimal, and IPCE increased it 4-5 times over control samples.
- The PI's group has synthesized new CuMO₂ delafossites, M=Cr, Fe, Ga, La, as well as new oxides (CuCr₂O₄), sulfides (SnS, CuGaS₂), & selenides (WSe₂, CuInSe₂, CuGaSe₂). This project has had very good progress.
- The project team's fluorine surface modification was able to shift conduction band-edge of Ti-doped hematite producing zero bias (two electrode) efficiency for hematite ~ 1% at 450 nm.
- The project has had four times improvement on the performance of NiFe electro-catalysts.
- The PI's have shown that biomass analogues can be photo decomposed with increased performance (15 times or higher than NaOH). This is not surprising. It has merit for near-term applications of the technology but may not help with the ultimate objective of water splitting. It is unclear even if biomass assisted PEC hydrogen production will be economical and/or meet DOE's near- and long-term hydrogen production cost goals. The H2A analysis of this approach is in order.
- At this point in the team's research (5th year and 90% completion), the long-term catalyst stability data is still lacking in order to draw solid conclusions.
- McFarland and his group have made good progress in identifying potential materials for splitting water.

<u>Ouestion 4: Technology transfer/collaborations with industry, universities and other laboratories</u>

This project was rated **3.7** for technology transfer and collaboration.

- The team's collaborations with the DOE PEC Working group, including efforts in theory, synthesis, characterization and techno-economics analysis have been exemplary.
- The project team has had good collaborations with NREL and various universities.
- A moderate number of publications and presentations have been done by the project team all in good archival journals. The PI's interactions with PEC community and others are noteworthy.

Question 5: Approach to and relevance of proposed future research

This project was rated **3.0** for proposed future work.

- The team's future work is well laid out and is consistent with meeting the fundamental needs of PEC materials discovery and development.
- More focus on other more promising materials is needed by the project team. Significant improvement in ICPE is needed.
- The project needs multiple miracles to happen to overcome the barriers.
- The PI has made good progress in addressing issues related to catalyst stability and conversion efficiency.
- Future plans for the project are reasonable if additional DOE funding can be made available. This should be predicated upon a system-level cost analysis using H2A platform to better define the cost-efficiency goals for the prospective catalysts and photo-reactors.

Strengths and weaknesses

Strengths

- This project has had good Progress, excellent collaborations and has a clear vision of research needs for future successful implementation of PEC hydrogen production.
- The project team's combinatorial materials synthesis is a strength.
- This project has a highly skilled group in material synthesis and characterization.

Weaknesses

- The team's scope of work is somewhat over-ambitious within the limits of current funding levels. There are still some fundamental 'mysteries' regarding performance of different hematite materials that should be pursued more aggressively. Perhaps using collaborative partners in characterization would be a benefit.
- No progress has been made on an actual photo-reactor design and H2A cost analysis in this project.
- No material with good long-term stability and photon to hydrogen conversion efficiency has been found yet.
- The use of biomass or other organic analogous present distraction to this DOE-EERE funded project.

Specific recommendations and additions or deletions to the work scope

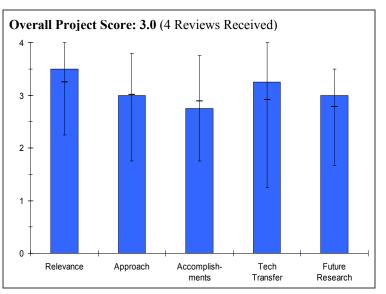
- This project should have a continued expansion of collaborative efforts, especially in future work related to advanced material characterization and screening, but also in theoretically guided materials modification experiments.
- The project team should perform H2A analysis as they go along.

Project # PDP-02: Semiconductor Materials for Photoelectrolysis

John A. Turner, Todd G. Deutsch, and Huyen Dinh; National Renewable Energy Laboratory

Brief Summary of Project

The objective of this project is to discover and characterize a semiconductor material set or device configuration that 1) splits water into hydrogen and oxygen spontaneously upon illumination; 2) has a solar-to-hydrogen efficiency of at least 5% with a clear pathway to a 10% water splitting system; 3) exhibits the possibility of 1,000 hours stability under solar conditions; and 4) can be adapted to volume-manufacturing techniques. The main objective for the past year has been to develop and optimize state-of-the-art materials that we have identified as promising for meeting the DOE's near-term efficiency and durability targets.



Question 1: Relevance to overall DOE objectives

This project earned a score of 3.5 for its relevance to DOE objectives.

- The PEC fits the long-term renewable hydrogen production goal.
- This project has a very broad and long-term approach to address PEC production.
- The project's development of a viable form of high-performance III-V material for PEC water splitting is extremely relevant to Hydrogen Program goals, and investigating other important material classes is of high relevance.
- The project's discovery and characterization of materials that have the potential water splitting application to produce "green" hydrogen, if successful, is very relevant to the Hydrogen Program goal.

Question 2: Approach to performing the research and development

This project was rated **3.0** on its approach.

- This project uses cheap, durable and efficient materials for photoelectrode and is the key enabler for PEC success.
- The project team's approach is sharply focused on the "big three" challenges. By breaking down the very large set of possible materials into two general categories, it makes the progress more tangible to non-experts.
- The project has done a good job focusing on important material classes meeting some (though not all) of the critical requirements for practical PEC hydrogen production. Stabilization of the III-V materials class appears to be of central focus, but other important classes remain under investigation. Further emphasis on collaborative approaches integrating theory, synthesis and characterization are strongly encouraged; both in continued research into stable, lower-cost III-V semiconductor systems, and in the discovery and development of new material systems.
- This project has been on going for a long time. The team's approach appears too much trail-and-error. They need a more systematic approach to selecting and/or eliminating materials.
- The project team needs to include cost as one of main criteria (material and synthesis/manufacturing method).

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated 2.8 based on accomplishments.

- The project's milestones were met on time.
- More durability data is needed from the team. What is the pathway to 10 % efficiency?
- There was clear progress in the synthesis and characterization of InGaN-based materials, though the presentation could have better pulled-together the key results on performance and stability, especially in relation to future directions for the research. There was also progress in the evaluation of CGS, a-SiN_X and copper spinel materials developed at NREL. Again, the presentation could have done a better job in tying together the results with synergetic activities within the DOE PEC working group, and the implications for future work. The work in this project is an important part of the validation process of new approaches integrating materials theory, synthesis and characterization, and this validation process should be strongly emphasized, especially at NREL (which is ideally suited for a leadership role in this area).
- The project team still has had no significant step change in improving combination of efficiency and durability.

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated **3.3** for technology transfer and collaboration.

- The project team has had good collaboration with members of the PEC working group.
- The project team should have more industry collaborations.
- There was an impressive list of collaborators, particularly within NREL and with international participants in the research. Collaborations with the DOE PEC Working Group were also implicit, though better integration of synergistic activities and results could have been demonstrated in the presentation.
- The team had strong collaborations with institutions doing similar researches.

Question 5: Approach to and relevance of proposed future research

This project was rated **3.0** for proposed future work.

- The project's durability testing is not explicitly mentioned in the future work.
- Future work on this project is somewhat open-ended, though well laid out in the presentation. Future work needs to focus strongly both on improving the stability and reducing the cost of the III-V focus materials, and this project needs to implement all available tools in materials theory, synthesis and characterization toward this end.
- The team needs to clearly show how to achieve incremental improvement in efficiency, instead of just continuing on with trail-and-error approach.

Strengths and weaknesses

Strengths

- Technical capabilities of the people involved in this project are a strength.
- Progress was made on several fronts in the development of PEC materials for solar hydrogen production in this project. Good synthesis and characterization results have been achieved.

Weaknesses

- This project has taken a long time to mature.
- The presentation could have better represented collaborations, synergies, and motivations for future work critical to the success of renewable PEC hydrogen production.

Specific recommendations and additions or deletions to the work scope

• Continued expansion of collaborative efforts, especially in future work related to advanced material characterization and screening is needed, but also in theoretically guided materials modification experiments. Pathways toward low-cost synthesis of III-V materials should be a stronger focus for the project team.

Project # PDP-03: PEC Materials: Theory and Modeling

Yanfa Yan, Muhammad Huda, Aron Walsh, Su-Huai Wei, Mowafak Al-Jassim, and John Turner; National Renewable Energy Laboratory

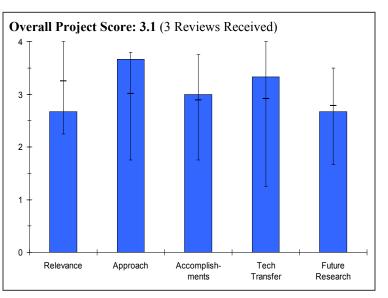
Brief Summary of Project

The main focus of the project is to 1) understand the performance of current photoelectrochemical (PEC) materials; 2) provide guidance and solution for performance improvement; 3) design and discover new materials; and 4) provide theoretical basis for "go/no-go" decisions to DOE PEC H₂ programs.

<u>Ouestion 1: Relevance to overall DOE</u> <u>objectives</u>

This project earned a score of **2.7** for its relevance to DOE objectives.

 The PEC is relevant to long-term renewable hydrogen production. The project's modeling shall be a key enable;



- project's modeling shall be a key enabler to PEC materials search.
- It is uncertain why this project needs to be independent. This should be part of any PEC project. How this project adds value in addition to other on-going PEC projects is not apparent. Why does DOE need a separate project to study why certain materials work and do not work? Should this be the task of the PI's of the PEC projects?

Question 2: Approach to performing the research and development

This project was rated **3.7** on its approach.

- The density functional theory (DFT) is the right approach to perform material discoveries in this project.
- The team has had good coordination between theory and experiments.
- The team has a good effective use of modeling to understand materials performance

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated 3.0 based on accomplishments.

- Project milestones have been met in time. Continuous search for new materials is still a part of this project but there is some delay due to fabrication of materials.
- Good progress is shown in working with other PEC projects to understand materials performance and issues.

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated **3.3** for technology transfer and collaboration.

- The PEC team has outstanding coordination within their group.
- More industry collaborations would be good for this project.
- This project has good collaborations and is in support of other PEC projects.

<u>Ouestion 5: Approach to and relevance of proposed future research</u>

This project was rated 2.7 for proposed future work.

- The project team has a good approach to iterate between models and experiments.
- The project team should consider merging the work with other PEC projects (if funding is available).

Strengths and weaknesses

Strengths

• The team has the right approach for problem solving. Their combination of theory and experimental work is a strength.

Weaknesses

• This project has taken a long time to mature.

Specific recommendations and additions or deletions to the work scope

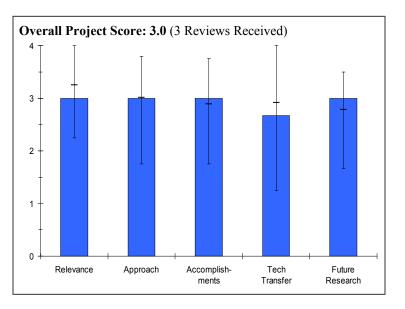
• The project team should consider not doing this project on its own. The task of understanding materials performance should be done by all of the PIs of the PEC projects.

Project # PDP-04: Progress in the Study of Amorphous Silicon Carbide (a-SiC) as a Photoelectrode in Photoelectrochemical (PEC) Cells

Arun Madan; MVSystems, Inc.

Brief Summary of Project

The objective of the project is by September 2009, to fabricate the hybrid a-Si tandem solar cell/a-SiC photoelectrode (PV/a-SiC) device, which exhibits a photocurrent greater than or equal to 4 mA/cm², and durability in the electrolyte of greater than or equal to 200 hrs. In the past year, this project has 1) fabricated an integrated hybrid PEC device containing a-Si tandem solar cell and a-SiC photoelectrode; 2) investigated the effect of surface oxide (SiOx) on the photocurrent; and 3) improved the PV performance of a-Si tandem solar cell used in the hybrid PEC device.



Question 1: Relevance to overall DOE objectives

This project earned a score of 3.0 for its relevance to DOE objectives.

- This project addresses the program objectives related to PEC Hydrogen efficiency and durability.
- This project is in line with hydrogen project objective to produce low-cost, renewable hydrogen.
- This project has efforts to utilize full solar spectrum to raise efficiency, which is relevant to DOE's objectives.

Question 2: Approach to performing the research and development

This project was rated **3.0** on its approach.

- This project would benefit from a cost assessment to ensure their technology is on the path to achieving overall hydrogen production cost targets.
- The project team's approach to improving efficiency and durability seems logical.
- Tailoring the bandgap with deposition control and multilayer films is a good strategy for capturing solar spectrum.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated 3.0 based on accomplishments.

- The project team's corrosion resistance data looks good and at least some hydrogen was evolved during testing last year. More work is needed to generate hydrogen at the required rate.
- Major technical barriers still exist in this project to demonstrate the necessary current, but there appears to be a path to achieving the desired results.
- There were a very large number of publications listed for this project, but many of them were written before this project started. Listed publications should be those that derived directly from this research project.
- This project has had good progress in materials development and testing.
- The project's efficiency improvement is still minimal.
- Test data on corrosion after 150 hours is promising in this project.

- The project's multi-layer films appear to have good efficiency and corrosion resistance. The STH efficiency lagging is well below target.
- The project's HF etch study gave good results

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated 2.7 for technology transfer and collaboration.

- It was unclear how well coordinated this project is with the listed partners. More collaboration may be beneficial.
- The project had good collaborations with various institutions.
- The project had collaborations with NREL.

Question 5: Approach to and relevance of proposed future research

This project was rated **3.0** for proposed future work.

- The project's list of future work looks appropriate, but there may not be enough time and funding to achieve the project goals.
- The team needs to focus on longer term testing (>150 hrs) to investigation corrosion issue, while addressing efficiency improvement.
- It is not totally clear on how >10% STH efficiency can be achieved.
- The project has a good listing of potential improvement mechanisms.
- Are the project's criteria for "go/no go" decision set? If so, what are they?

Strengths and weaknesses

Strengths

- The project's corrosion resistance looks good and at least some hydrogen was evolved during testing last year.
- There appears to be a path to overcoming the major technical barriers and achieving the desired results in this project.
- Good expertise in film production/characterization/testing can be seen in this project.

Weaknesses

- This project would benefit from a cost assessment to ensure the technology that is on the path to achieving overall hydrogen production cost targets.
- More work is needed to generate hydrogen at the required rate in this project.
- Listed publications should be those that derived directly from this research project.
- It was unclear how well coordinated this project is with the listed partners. More collaboration may be beneficial.

Specific recommendations and additions or deletions to the work scope

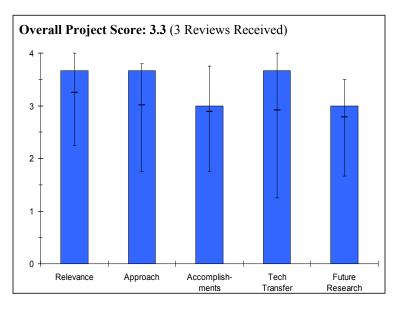
• The list of future work looks appropriate, but there may not be enough time and funding to achieve the project goals.

Project # PDP-05: Progress in the Study of Tungsten Oxide Compounds as Photoelectrodes in Photoelectrochemical Cells

Nicolas Gaillard; University of Hawaii

Brief Summary of Project

In the past year, this project has 1) continued WO₃ bulk modification using ion incorporation with synthesis of new alloys and theoretical analysis on band-gap reduction; 2) investigated the WO₃-based bilayer concept with fabrication of new devices, surface electronic properties analysis and crystallographic and structural analysis; and 3) evaluated RuO₂ nanoparticle deposition for catalytic treatment with deposition of thick (1 micron) films, characterization of RuO₂ film's oxygen evolution rate vs. that of Pt foil and the first evaluation of RuO₂ nano-particle onto WO₃ film.



Question 1: Relevance to overall DOE objectives

This project earned a score of **3.7** for its relevance to DOE objectives.

- The project team's work is relevant in establishing the next steps for photoelectrochemical hydrogen production (PEC) electrode structures.
- The project's photoelectrochemical hydrogen production is within the DOE Hydrogen Program plan.
- The project's use of WO₃ is shown to be a promising material.

<u>Ouestion 2: Approach to performing the research and development</u>

This project was rated 3.7 on its approach.

- The team had a very methodical approach that evaluates the individual layers of the PEC electrode. Overall improvement in performance is obtained by the improvement in one or more PEC electrode layers in this project.
- The team's work on tailoring band gap/band-edge is good.
- The team has a good use of theory.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated 3.0 based on accomplishments.

- A continuous improvement in WO₃-based PEC electrode performance has been demonstrated via new materials/fabrication techniques in this project.
- The team has demonstrated an increase in photocurrent using new bilayer structures.
- The project's further improvement in SiC & WO₃ PEC electrodes are required to meet the STH efficiency target of ~5%.
- The project team has made reasonable progress towards goals. The 3D growth of catalyst particles is promising.

<u>Ouestion 4: Technology transfer/collaborations with industry, universities and other laboratories</u>

This project was rated 3.7 for technology transfer and collaboration.

- The project is a well rounded team effort between institutions covering the theory, synthesis, and characterization R&D effort. The knowledge gained appears useful to all partners involved.
- Collaborations in this project were okay.

Question 5: Approach to and relevance of proposed future research

This project was rated **3.0** for proposed future work.

- New materials and fabrication techniques have been identified to further improve PEC performance in this project.
- Are the criteria for "go/no-go" decision in this project set? If so, what are they?

Strengths and weaknesses

Strengths

• There has been good collaboration between partners and DOE PEC working group.

Weaknesses

• The low current densities will result in relatively large systems for hydrogen production, which is a weakness of this project.

Specific recommendations and additions or deletions to the work scope

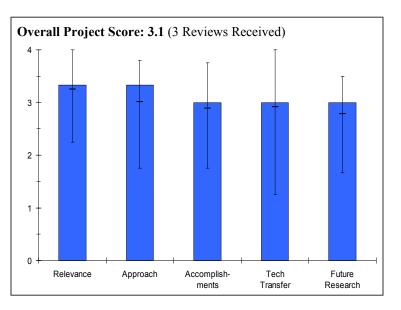
• This may be too early to say but the project team should complete an economic analysis of a PEC system to demonstrate feasibility of this technology for hydrogen-production.

Project # PDP-06: Photoelectremical Hydrogen Production

Jess Kaneshiro; University of Hawaii at Manoa

Brief Summary of Project

The objective of this project is to develop copper chalcopyrite materials for incorporation into a hybrid photoelectrode (HPE) device capable of splitting water for hydrogen production when immersed in a suitable electrolyte and illuminated by sunlight. Material development objectives are to 1) identify methods of increasing the bandgap of copper chalcopyrite films; 2) make thinner copper chalcopyrite films; and 3) make surface modifications. Device development objectives are to 1) use material development to synergize different components of HPE; 2) identify suitable underlying photovoltaic (PV) cells, possibly also copper chalcopyrite-based; and 3) identify suitable photoelectrochemical-PV interfaces.



Question 1: Relevance to overall DOE objectives

This project earned a score of 3.3 for its relevance to DOE objectives.

- The PEC is relevant to DOE's goal of renewable hydrogen production.
- The project's link to pdp_02_turner is unclear? It is assumed that it is shown in the collaboration with NREL.

<u>Ouestion 2: Approach to performing the research and development</u>

This project was rated 3.3 on its approach.

- The project's investigation of copper chalcopyrite is a good as these materials are cheaper and durable.
- The project team's focus towards reducing voltage bias is the right approach.
- The project team has good use of theory to guide experimental work.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated 3.0 based on accomplishments.

- The team has demonstrated some progress in reducing the voltage bias via sulfur incorporation in the materials.
- The project team needs to have a crisp milestone plan.
- High currents are achieved in this project.
- The team has made not much progress on stability, but issues are being addressed.
- The team's look into the device's efficiency has not yet started.

<u>Ouestion 4: Technology transfer/collaborations with industry, universities and other laboratories</u>

This project was rated **3.0** for technology transfer and collaboration.

- The PEC team has outstanding coordination.
- Are there other possibilities for industry collaborations in this project?
- The team has had good work with theorists and co-investigators.

FY 2009 Merit Review and Peer Evaluation Report

Question 5: Approach to and relevance of proposed future research

This project was rated **3.0** for proposed future work.

- The project team has continued to focus on the reduction of voltage bias through looking at new and/or different materials.
- Are the criteria for "go/no-go" decision set? If so, what are they?

Strengths and weaknesses

Strengths

• This team has had good technical background and coordination.

Weaknesses

• This project has taken a long time to mature.

Specific recommendations and additions or deletions to the work scope

No specific recommendations were provided for this project.

Project # PDP-07: Critical Research for Cost-Effective Photoelectrochemical Production of Hydrogen

Liwei Xu; Midwest Optoelectronics, LLC Anke Abken; Xunlight Corporation William B. Ingler, Jr.; University of Toledo

Brief Summary of Project

The objectives of this project are to 1) develop critical technologies required for cost-effective production of hydrogen from sunlight and water using thin film (tf)-Sibased photoelectrodes; and 2) develop and demonstrate at the end of the three-year project, tf-Si-based photoelectrochemical photoelectrodes and device designs with the potential to achieve systems with 10% solarto-hydrogen efficiency with a durability of 5,000 hours by 2018.

Question 1: Relevance to overall DOE objectives

This project earned a score of **2.7** for its relevance to DOE objectives.

- Overall Project Score: 2.5 (3 Reviews Received)
- The project is well aligned with the program goals, in particular finding low-cost PEC technology and materials.
- The work in this project has general relevance to the broad Hydrogen Program, although only a small fraction of the tasks are directly relevant to the goals of PEC hydrogen production, as outlined in the DOE MYPP.

Question 2: Approach to performing the research and development

This project was rated 2.3 on its approach.

- The team's approach appears to be reasonable given the early stage of R&D.
- Of the tasks presented, Task 1 is completely outside the scope of hydrogen production; Task 2 is more suited to research funding under PV and/or electrolysis systems; Task 3 has relevance to renewable hydrogen production using PEC solar water-splitting; and Task 4, based on waste-water treatment, is interesting, but outside the scope of renewable PEC hydrogen production from sunlight and water..

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated 2.7 based on accomplishments.

- The project shows some good potential, but significant technical barriers still exist.
- Progress was made in the different tasks presented, though much was unrelated to progress in the development of PEC water-splitting materials and devices. The critical issue in PEC is the development of new efficient and cost-effective materials and interfaces to better utilize the solar spectrum in photoelectrochemical processes for splitting water, and only Task 3 attempts to address these issues. Unfortunately, the scope of work within Task 3 is limited, and does not incorporate research approaches and progress from within the DOE PEC Working Group.

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated 2.7 for technology transfer and collaboration.

- The project's collaboration appears to be sufficient.
- The role of collaboration in this project was not made clear within the presentation, though there appears to be some collaborative results.

Question 5: Approach to and relevance of proposed future research

This project was rated **2.0** for proposed future work.

- There may not be enough time and funding to achieve the project goals.
- The future work outlined for Task 3 is somewhat limited in its scope and definition. Better integration of the materials R&D efforts with the broader efforts in the DOE PEC Working Group is strongly encouraged.

Strengths and weaknesses

Strengths

- The project is well aligned with the program goals, in particular finding low-cost PEC technology and/or materials.
- The team's approach appears to be reasonable given the early stage of R&D.
- The project team's collaboration appears to be sufficient.
- Progress was made in several different directions in this project, though few of these were directly tied to the advancement of PEC water splitting for solar hydrogen production.

Weaknesses

- Significant technical barriers still exist in this project.
- Too much work unrelated to PEC hydrogen production was presented by the team. Other funding sources would have been better suited to this project. Collaborative efforts need to be strengthened. The incorrect poster ID was listed on the first panel (pdp 24), indicating perhaps that some of the information may be from an outdated source.

Specific recommendations and additions or deletions to the work scope

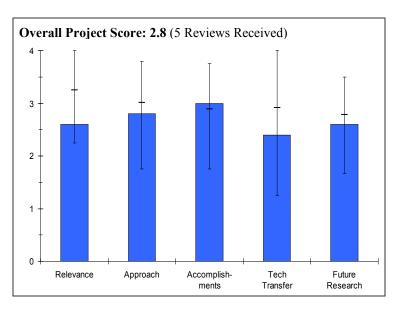
- There may not be enough time and funding to achieve the project goals.
- The project team should find alternative funding venues for Tasks 1, 2 and 4. They also need to strengthen the materials R&D directions within Task 3.

Project # PDP-10: Composite Bulk Amorphous Hydrogen Purification Membranes

T. Adams, K. Brinkman, S. Garrison, and P. Korinko; Savannah River National Laboratory

Brief Summary of Project

Metallic glass materials offer the potential for excellent membrane function at a fraction of the cost of Pd-based alloys. The objectives of this project are to 1) examine novel Pd free membranes for hydrogen separation; 2) address the potential challenge of crystallization during operation at elevated temperature; 3) quantify hydrogen permeation properties of commercially available metallic glass membranes; 4) evaluate and understand crystallization and hydrogen flux behavior in metallic glass membranes; and 5) integrate permeation, crystallization behavior and modeling effort on materials chemistry to guide synthesis and characterization of novel metallic glass materials for hydrogen separation.



Question 1: Relevance to overall DOE objectives

This project earned a score of 2.6 for its relevance to DOE objectives.

- The project fits in to DOE's hydrogen separation R&D objectives. However, the work provides little support to DOE's hydrogen separation technology R&D intended results. This is because the DOE 2010 membrane flux performance target is 200 SCFH/ft² at 340-400°C and 100 psig trans-membrane ΔP.
- The project's concept is not novel; glass membranes have been studied before, generally with not much potential. The separation conditions are not synergistic with upstream process operating conditions and the separation flux is order of magnitude lower than would be required to process the throughputs of WGS reactors. It is doubtful the material can achieve DOE 2010 flux and other performance targets.
- The research is attempting to develop novel membranes to produce high-purity hydrogen. The researchers are aware of the need to develop effective hydrogen separation membranes and are aware of the DOE goals and targets (slide #3). This is a high-risk approach that would likely be much longer term than the DOE target timeframe. It is unlikely that any of the DOE targets will be met, but the work may provide some fundamental information on alternative membranes.
- This project meets some aspects of DOE goals.
- The project's hydrogen purification is a necessary step after onsite reforming or within the station to satisfy fuel cell purity requirements. Work in using low-cost metallic glass instead of high-cost palladium is absolutely in line with DOE programmatic goals.
- A cost effective membrane hydrogen separation system has the potential to lower the cost of several hydrogen production methods. Although some success has been obtained with palladium-based membrane systems, there are still some issues with this project's approach. Metallic glass membranes are an interesting alternative approach to explore.

Question 2: Approach to performing the research and development

This project was rated **2.8** on its approach.

- The work conducted thus far in this project is of academic value. The hydrogen separation mechanism is not clear. The work is in its fundamental stages and the success potential of the glass membrane, if any, is difficult to predict.
- The team's approach is reasonably novel and gets away from the use of high-cost precious metal membranes. The work is attempting to build on hydrogen separation using micro-porous glass membranes, which has shown some success for hydrogen separation. This is a high-risk approach, which is appropriate for a basic research laboratory like SRNL. The project is beginning to look at supported thin films, which would be the next logical step in the development of this type of membrane system. The work involves a high level of fundamental characterization and modeling which is acceptable for a project of this type operating on a minimal budget.
- The concept of using isomorphous alloys is intriguing and potentially a method to make cheaper membranes. Avoiding crystallization of the alloy is a key to the success of this method.
- Work towards understanding metallic glass hydrogen permeation is important in this project. The use of alloying to control glass transition temperature looks promising, as does use of thin film systems. The project team should continue to work on both increased flux but also hydrogen recovery.
- The approach being taken is to first look at the key issue of potential re-crystallization at elevated temperatures needed for use as well as to measure the hydrogen flux rate. This is a good first step for the project team.
- Computational molecular modeling is also being used to try to determine which glass metal alloys should have the best hydrogen permeability.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated **3.0** based on accomplishments.

- The project's flux data is much lower than the immediate DOE 2010 target. Membrane separation performance varies with temperature exponentially and the separation mechanism is unclear. High-temperature membrane operating conditions may not be compatible with upstream gas clean up or water gas shift reactor conditions. The separation flux is an order of magnitude lower than DOE targets. Some knowledge applicable to advanced materials development may evolve.
- Unfortunately, the project has little technical success. Flux rates are very low and the project lacks a clear path to improve on these is proposed. The differential scanning calorimetry (DSC), X-ray diffraction (XRD), X-ray photoelectron spectra (XPS) and permeations studies are scientifically interesting but do not appear to be providing any valuable information for future material development. However, the researchers are to be commended for attempting a new and innovative approach. For a fundamental and novel approach, the results are considered reasonable, appropriate and acceptable.
- The project team's experimental work appears to be solid and well focused. Primarily screening different alloys for susceptibility to crystallization.
- Adding a computational modeling effort is a good idea to lead to possible other combinations of alloy components in this project.
- Experiments involving realistic feed gases are lacking in this project. All that is seen are experiments on just H₂ or Ar/H₂. What might be the effect of other compounds (H₂O, CO₂, etc.) on membrane stability?
- Especially considering a lack of funding in 2009, the project made substantial progress. Work towards understanding crystallization mechanisms looks good and promising in the future. The project team's work looks very promising to develop an excellent replacement for Pd membrane materials.
- The project team successfully used calorimetry to determine crystallization temperatures of metallic glasses. The team found that some crystallization can occur in the temperature range of interest depending on the metallic glass used.
- The project team measured hydrogen flux rates and compared them with palladium. Crystallization did decrease the hydrogen flux rate as expected and the rates were generally an order of magnitude below those of palladium. The team's work is now in progress to generate thing films of the metallic glass to improve hydrogen flux rates.
- The project team's computational modeling is in progress to help define the alloy compositions that should have enhanced properties for hydrogen separations.
- A lot of progress has been made in a short time with very modest funding for this project.
- The project team should include work to ensure a high selectivity separation of hydrogen from a mixture of gasses can be obtained with these metallic glasses.

<u>Ouestion 4: Technology transfer/collaborations with industry, universities and other laboratories</u>

This project was rated **2.4** for technology transfer and collaboration.

- Some industry partnership has been reported in this project.
- Outside collaboration (based on slide #2) appears reasonable in this project. However, with the exception of MetGlas who provided samples) it is not clear what the involvement of the other partners actually entails. It is valuable that the investigators are actively seeking outside industrial participation. In addition, with the limited budget (\$200K), it is likely difficult to interest outside industrial involvement.
- It is unclear how effective the list of consulting partners were or if they were even used. Partners could have perhaps provided some of the metals?
- Partnership with manufacturers is good, but not discussed in the presentation. Do partners provide anything other than samples?
- There appears to be good collaboration with private sector companies working on metallic glasses.

Question 5: Approach to and relevance of proposed future research

This project was rated **2.6** for proposed future work.

- The project has not been funded in FY09 and future funding is not known. The project PI has listed some future work, at the fundamental level, which does not include selectivity and flux measurements, or integration potential with WGS reactors of Integrated Gasification Combined Cycle (IGCC)-Carbon Capture and Sequestration (CCS) plants.
- Scoping projects such as these, especially at low budget levels, are valuable to the Hydrogen Program. Without new, innovative ideas being developed, significant advancements are not possible. Although only minimal results have been obtained, it would be useful to consider funding this work for an additional year to allow the researchers to examine other materials of this class for hydrogen separation/purification. The planned future work is generally just a continuation of the ongoing effort, but should be considered a reasonable extension of the original fundamental effort. Additional funding, at the same level, would be appropriate.
- This work deserves consideration for future funding. The combination of experimental and computational modeling is good.
- Future work on integrating modeling with experimental work is an excellent next step. Initial work looks promising there, and a continuation of that work is important for additional materials development. This project has had excellent progress considering its funding.
- The project's future plan is well thought through. It includes work to generate and measure flux rates in thin films, additional modeling work, and testing of alloys suggested by the modeling work.
- This project needs clear milestones and a "go/no-go" decision built into the future work.

Strengths and weaknesses

Strengths

- The project is a good alternative and has a novel approach for development of hydrogen separation/purification membranes without the use of high-cost precious metals. Considering preparation of supported thin films this early in the work is a plus and could provide early cost information on producing larger scale units and also identify technical problems in scale-up/production of larger size membranes.
- The Savannah River group appears to be competent.
- The project team's combination of theoretical and experimental work is good. Their use of multiple analytical techniques to better understand metallic glass diffusivity with hydrogen. This project directly addresses DOE programmatic goals of reduced cost and hydrogen purity.
- A cost effective membrane hydrogen separation system has the potential to lower the cost of several hydrogen production methods. Although some success has been obtained with palladium-based membrane systems, there are still some issues with this approach. Metallic glass membranes are an interesting alternative approach for the project team to explore.
- Computational molecular modeling is being used to try to determine which glass metal alloys should have the best hydrogen permeability by the project team.

- This project has made a lot of progress in a short amount of time with very modest funding.
- The future plan for this project is well thought through. It includes work to generate and measure flux rates in thin films, additional modeling work, and testing of alloys suggested by the modeling work.

Weaknesses

- This project had no clear weaknesses for a fundamental membrane materials scoping project.
- This project has a fairly academically focused at this point.
- The collaboration in this project is a weakness.
- The project team should include work to ensure a high selectivity separation of hydrogen from a mixture of gasses can be obtained with these metallic glasses.
- The project needs to have clear milestones and a "go/no-go" decision built into the future work.

Specific recommendations and additions or deletions to the work scope

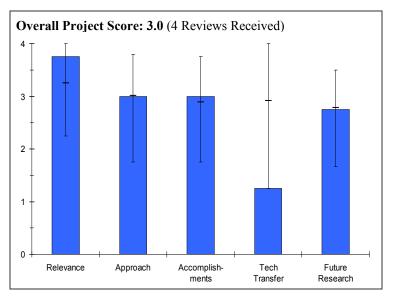
- This project is worth considering continuation with the current/future work scope at the same funding level.
- This project includes realistic gas feeds to test membrane stability.

Project # PDP-12: Catalytic Solubilization and Conversion of Lignocellulosic Feedstocks

T.A. Semelsberger, Kevin C. Ott, Rod L. Borup, and Roshan Shrestha; Los Alamos National Laboratory

Brief Summary of Project

The objective of this project is to develop novel low-temperature chemical routes and catalysts to produce hydrogen/syngas from lignocellulosic feedstocks. The most abundant constituent of biomass is lignocellulosic (~80%). Discovering new chemistries and catalysts that can convert lignocellulosic into hydrogen/syngas will be critical if biomass is to be used as a feedstock for hydrogen or other alternative fuels. The target for this project is to, by 2012, reduce the cost of hydrogen produced from biomass gasification to \$1.60/gget at the plant gate (<\$3.30/gge delivered). The target for 2017 is to reduce the cost of hydrogen produced from biomass gasification to \$1.10/ggeat the plant gate (\$2.10/gge delivered).



Question 1: Relevance to overall DOE objectives

This project earned a score of **3.8** for its relevance to DOE objectives.

- This project is a really good idea where it explores catalytic approaches to directly treat cellulose and lignin.
- The project's focus on biomass sourced from non-food/feed crops is an excellent feedstock for the production of hydrogen. It is plentiful and can be developed to be even more plentiful. The production cycle of plant growth through hydrogen production is near zero in GHG emissions and can reduce GHG air concentrations if the GHG generated in the production process is sequestered. Aqueous Phase Reforming (APR) of sugars and other compounds derived from biomass is a low-temperature and low-cost process to produce hydrogen. If the cost of the feedstock (sugars, etc.) could be reduced, it could be a very low-cost green approach to hydrogen production that could exceed the DOE hydrogen cost targets. This project is targeted at finding lower cost processing and digestion of biomass to produce sugars or other compounds that can be used in APR.
- This project's process uses a very abundant feedstock for H₂ production. This route can have a very favorable central and semi-distributed production economics.
- Based on the project team's presentation materials, their appeared to be good relevance toward the development of biofuels pathways toward the DOE's hydrogen goals.

Question 2: Approach to performing the research and development

This project was rated **3.0** on its approach.

- A crisp rationalization for the approach or the investigation that could lead to a preferred approach is not apparent.
- The team's approach that has been taken is to perform screening experiments with an array of potential catalysts using solid biomass and potential biomass digestion products to look for evidence of biomass breakdown to APR processable intermediates. APR catalysts were used in conjunction with other catalysts in some experiments to seek evidence of combined biomass digestion and APR in one pot. Several different analytical techniques were used to identify the products produced. The screening approach allowed examination of a wide array of catalyst options.

- It appears the team's entire effort went into screening experiments. It would have been better to identify some of the more encouraging catalysts earlier and done more extensive experiments to try to improve on the results achieved with them.
- LANL is applying the right tools for developing understanding of this difficult chemistry environment. The process can also have offshoot technology applications and side products that improve the economics of the process.
- The team's approach was laid out clearly in the presentation.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated **3.0** based on accomplishments.

- Objectives for current fiscal year are not well detailed in this project. Funding is practically close to nothing. It is not clear what has been done recently by this team.
- The screening experiments in this project resulted in some encouraging results including: the demonstration of catalyzed hydrolysis of cellobiose to glucose, conversion of cellobiose to syngas but only to 5%, demonstrated catalytically enhanced decarboxylation of lignin and low-temperature catalyzed gasification of lignin.
- It appears that the entire team's effort went into screening experiments. It would have been better to identify some of the more encouraging catalysts earlier and done more extensive experiments to try to improve on the results achieved.
- In many cases, the analysis of the products, particularly the gas phase products was incomplete.

<u>Ouestion 4: Technology transfer/collaborations with industry, universities and other laboratories</u>

This project was rated 1.3 for technology transfer and collaboration.

- There were no apparent collaborations in this project.
- LANL has had no collaborators on this project. There has been a great deal of research over the past 20 years on the digestion of biomass to sugars and other compounds. Much of this work was based on enzymes and thus the reason for this project. However, some work has been done on thermochemical breakdown of biomass and those in the field of enzymatic biomass digestion could have brought some valuable insights to this project. NREL and PNNL have been working on biomass digestion for decades. Many universities have also been in this field for a long time. In addition, Virent has pioneered APR and PNNL has recently been studying it as well. Thus there is a long list of potential collaborators that could help in this effort.
- This project can be leveraged a lot more. For example similar consortium can be applied as the one for PEC.
- Not applicable. It would have been helpful to involve a commercialization partner in some aspect of the project.

Question 5: Approach to and relevance of proposed future research

This project was rated 2.8 for proposed future work.

- Project plans are not written in way that can give confidence, The PI has any specific ideas to explore.
- The future project plan includes both additional screening experiments and some focused work on lignin, which has proven to be the most difficult part of the biomass to digest. This project has shown some degree of success in converting cellulose to APR processable sugars and oligomers. If low-cost catalytic digestion of biomass to lignin and APR processable products could be developed, this could be a major success. The lignin could be used to generate power and the rest of the biomass could be a low-cost feedstock for APR generation of hydrogen. Research on this approach should also be a part of the future work plan.
- The project's work scope needs to be in line with other work happening outside LANL, in order to improve the general technology development.
- The "future work" pathway looks like an expanded investigation work similar to what has already been done. No pathway to commercialization clearly identified in this project.

Strengths and weaknesses

Strengths

- The biomass sourced from non-food/feed crops is an excellent feedstock for the production of hydrogen is a strength. It is plentiful and can be developed to be even more plentiful. The production cycle of plant growth through hydrogen production is near-zero in GHG emissions and can reduce GHG air concentrations if the GHG generated in the production process is sequestered. Aqueous Phase Reforming (APR) of sugars and other compounds derived from biomass is a low-temperature and low-cost process to produce hydrogen. If the cost of the feedstock (sugars, etc.) could be reduced, it could be a very low-cost green approach to hydrogen production that could exceed the DOE hydrogen cost targets. This project is targeted at finding lower cost processing and digestion of biomass to produce sugars or other compounds that can be used in APR.
- The project team has taken an approach to perform screening experiments with an array of potential catalysts using solid biomass and potential biomass digestion products to look for evidence of biomass breakdown to APR processable intermediates. APR catalysts were used in conjunction with other catalysts in some experiments to seek evidence of combined biomass digestion and APR in one pot. Several different analytical techniques were used to identify the products produced. The screening approach allowed examination of a wide array of catalyst options.
- The project's screening experiments resulted in some encouraging results including: the demonstration of catalyzed hydrolysis of cellobiose to glucose, conversion of cellobiose to syngas but only to 5%, demonstrated catalytically enhanced decarboxylation of lignin and low-temperature catalyzed gasification of lignin.
- The project team has provided strong technical detail.

Weaknesses

- It appears the entire effort went into screening experiments in this project. It would have been better to identify some of the more encouraging catalysts earlier and done more extensive experiments to try to improve on the results achieved.
- LANL had no collaborators on this project. There is a long list of potential collaborators that could help in this effort.
- Partnering and commercialization efforts in this project are weak.

Specific recommendations and additions or deletions to the work scope

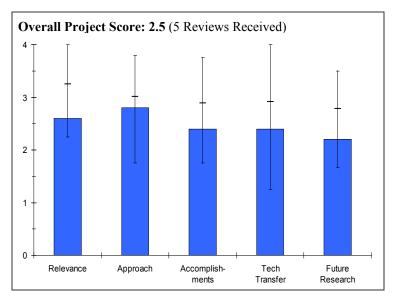
No specific recommendations were provided for this project.

Project # PDP-13: Novel Low-Temperature Proton Transport Membranes

Andrew Payzant; Oak Ridge National Laboratory

Brief Summary of Project

The objective of this project is to develop a novel ceramic proton conductor based on $La_2Mo_2O_9$ for use as a hydrogen separation membrane. The objective will be achieved through 1) compositional development; 2) characterization of the electrical properties, chemical stability, hydrogen flux and thermo-mechanical properties; 3) neutron diffraction analysis of selected materials to better understand the hydrogen transport properties; and 4) evaluation of surface exchange catalysts. The goal will be to synthesize this asymmetric membrane from candidate materials with and without exchange catalysts for additional flux testing to determine the range of fluxed possible in these materials.



Question 1: Relevance to overall DOE objectives

This project earned a score of **2.6** for its relevance to DOE objectives.

- The team's work provides little support to DOE's hydrogen separation technology R&D efforts. This is because the DOE 2010 membrane flux performance target is 200 SCFH/ft² at 340°-400°C and 100 psig trans-membrane ΔP.
- The project's proposed proton transport membrane flux performance, although above the above leak level, is orders of magnitude lower than the immediate-term target.
- The membrane looked interesting, perhaps as a hydrogen purification membrane, perhaps only as a solid oxide fuel cell material, perhaps neither. Either objective would be worthwhile; however, it would be nice to know which it is at this stage. The project has been defunded, so cannot expect too much from the researchers.
- This is a novel and high-risk approach to develop materials and membranes for hydrogen separation. The investigators are well aware of the DOE targets and goals and are striving to meet these goals and targets while still conducting a fundamental development project (at minimum cost). Although not successful, their efforts are to be commended.
- A reliable, cost effective, stable hydrogen separation membrane that could operate below 500°C could be a key enabler for the Hydrogen Program. It could reduce the cost of thermochemical hydrogen production in general and for reforming of natural gas and biofuels in particular. The Pd membranes are beginning to be commercialized but an alternative that might have some advantages could be very useful.

Question 2: Approach to performing the research and development

This project was rated **2.8** on its approach.

- The proton transport membrane (PTM) R&D work has been going on and off for several years with no significant progress and the findings presented are not new. All of the DOE 2010 membrane performance parameters need to be studied and satisfied; this is not expected to happen. The team's work is at a very fundamental level and may be of some academic value.
- The researchers made a membrane and presented data on transport at low pressures, but did not examine the effect of pressure. The project team examined the effects of temperature, but the results were quite aberrant,

suggesting high-flux solid-state transfer with almost no activation energy and 100% selectivity. No analysis was done as to why transport properties were this way.

- This is a good approach for basic development of new separation ceramic materials that may operate at reduced temperatures. The compositions are based on materials that have shown some promise and further examination is warranted for this project.
- The project team understands and has defined all the key properties needed for a hydrogen membrane to be useful. It is testing the novel LAMOX-based material for these properties, as well as developing improved LAMOX-based materials where the properties are deficient.
- This project includes a fundamental approach by obtaining crystal structures and other fundamental properties and using atomistic computer modeling to identify potential improved ceramic materials.
- The first LAMOX material to be identified as promising has a H₂ flux rate 5-6 orders of magnitude, which is too low. The researchers have identified plausible approaches to solve this fundamental problem including: generating a thin membrane, use of higher pressure across the membrane, increase the proton conductivity by using dopants to alter the crystal chemistry, and increase the H₂ proton dissociation rate with a surface catalyst.
- The project's diffusion of impurities should be evaluated in this system. The project's 100% hydrogen is an optimistic assumption. The project's CO₂, CO, and H₂O need to be accounted for in purity measurements at the least.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated **2.4** based on accomplishments.

- As of now, the membrane separation performance is not of any significance to this project. The flux improvement strategies, based on known theories, are speculative and may not apply to this membrane. It is not even guaranteed the material is truly transporting protons. Besides, even the desired low operating temperature is not compatible with upstream process conditions.
- This project was defunded a year ago, so not much progress can be expected with only carry-over funds. The project team's graduate student has left. The data that was taken looks very interesting except for the holes that suggest something odd is going on behind the scenes.
- Unfortunately the project's technical progress is limited. The overall flux is still very low and it is unclear how this can be improved. The development of low temperature ceramic materials for hydrogen/proton is a difficult problem and the investigators have made a good attempt to improve on past materials.
- The project has successfully synthesized 10 micron films on Y-stabilized zirconia.
- The project has demonstrated that LAMOX is stable in H_2 at 500°C and CO₂ at 800°C.
- The project's crystal structure of the LAMOX material has been determined with XRD.
- This project has had very good progress for the funding level. The diffusion rate appears to be very low, or the diffusion gradient is not there. If dilute hydrogen is used, the concentration on the purified side at ambient pressure would predict no diffusion. The project team should show pressure differential effects. The team should also describe the bulk proton transport mechanism that they are hypothesizing.

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated 2.4 for technology transfer and collaboration.

- Collaborations in this project include ORNL, the University of Cincinnati (hydrogen permeation tests), and the Imperial College.
- Project work is being done at different groups, but there was no effort to combine the results from the different groups.
- External collaborations are limited to academics and national laboratories in this project; however; this is appropriate for this type or research.
- The project is collaborating with the University of Cincinnati for permeation measurements, Imperial College, London for impedance spectroscopy, and other scientists at ORNL for NMR to identify H₂ bonding.
- There is a lot of excellent work being done at several universities and national labs on ion and proton conducting membranes. It seems that collaboration with some these efforts would be very helpful in this project.

<u>Ouestion 5: Approach to and relevance of proposed future research</u>

This project was rated 2.2 for proposed future work.

- The project has not been funded in FY09 and future funding is unknown.
- The team researcher hopes to keep carrying on with this project. This is heroic given that the project was defunded a year ago.
- The additional slides for reviewers only indicate that this project is being terminated. However, this reviewer would strongly suggest that DOE continue to allow this project to continue at a moderate level. The Hydrogen Program needs some need ideas and direction and this work is providing this approach. The work may not be successful, but it may provide data and information for future research direction.
- There is no future work-plan presented by this team. The researchers appear to be assuming that this project will not receive additional funding.

Strengths and weaknesses

Strengths

- At first glance, the project has a miracle material, and a durable, solid-state transport membrane that has 100% selectivity, and very low activation energy for transport. This could be used as a low-temperature separation membrane, or as a low-temperature solid oxide fuel cell.
- A reliable, cost effective, stable hydrogen separation membrane that could operate below 500°C could be a key enabler for the Hydrogen Program. It could reduce the cost of thermochemical hydrogen production in general and for reforming of natural gas and biofuels in particular. The Pd membranes are beginning to be commercialized but an alternative that might have some advantages could be very useful.
- The project understands and has defined all the key properties needed for a hydrogen membrane to be useful. It is testing the novel LAMOX-based material for these properties and developing improved LAMOX-based materials where the properties are deficient.
- The project includes a fundamental approach by obtaining crystal structures and other fundamental properties and using atomistic computer modeling to identify potential improved ceramic materials.
- The first LAMOX material to be identified as promising has an H₂ flux rate 5-6 orders of magnitude which is too low. The researchers have identified plausible approaches to solve this fundamental problem including: generating a thin membrane, use of higher pressure across the membrane, increase the proton conductivity by using dopants to alter the crystal chemistry, and increase the H₂ proton dissociation rate with a surface catalyst.
- The project has successfully synthesized 10 micron films on Y-stabilized zirconia.

Weaknesses

- What was transferred in this project, O, H, or both, is not apparent. We do not know how it was transported nor why there activation energy with 100% selectivity is lacking.
- The hydrogen flux rate needs to be improved by 5-6 orders of magnitude in this project.
- There is a lot of excellent work being done at other several universities and national labs on ion and proton conducting membranes. It seems that collaboration with some these efforts would be very helpful.
- There is no future work-plan presented by the project team.

Specific recommendations and additions or deletions to the work scope

- This project should be re-funded. The team researcher should measure H₂ transport using a simple, Sievert transport apparatus at different pressures and different gases so we know if O, O₂, H, H₂, or some combination is being transported. The team should also conduct either nuclear magnetic resonance (NMR) or infrared (IR) work to understand how atoms are moving.
- The project team should continue at a moderate level. Fundamental material development is a necessary part of an overall program and could have a longer-term payoff.

Project # PDP-14: Ultra-thin Proton Conduction Membranes for H₂ **Stream Purification with Protective Getter Coatings**

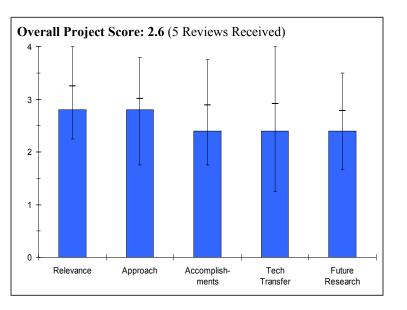
Dr. Margaret E. Welk, Dr. Robert Grubbs, and Dr. Andrea Ambrosini; Sandia National Laboratories

Brief Summary of Project

The objectives of this project are to 1) provide a functional support that will protect membranes from corrosive species in reformate gas stream; and 2) synthesize an "ultra-thin" dense ceramic proton conducting membrane to increase hydrogen flux over existing membranes. Dense membranes, whether metallic or ceramic, are especially vulnerable to sulfur attack. Sandia was successful in the deposition of Titania and recently SrO. The deposition of ZnO was also successful.

Question 1: Relevance to overall DOE objectives

This project earned a score of **2.8** for its relevance to DOE objectives.



- This project will develop a hydrogen purification membrane technology that incorporates sulfur getter-ing to address DOE hydrogen production targets for impurities, flux, durability, and hydrogen selectivity.
- This project aims to extend the life of oxide membranes by coating them with ZnO to protect against H₂S poisoning. The project team has achieved the desired protection, however, they do not have selectivity. This project was defunded. Ideally, the team should try to work with some other project where they produce membrane with selectivity, but short life in H₂S.
- The PCM is relevant to renewable hydrogen production goals. It is not clear if this is the right time to look at H₂ separation membranes
- The project team's approach is interesting, but is unlikely to be able to compete with cheap guard bed based on solid ZnO-based sorbents.

Question 2: Approach to performing the research and development

This project was rated **2.8** on its approach.

- The project's approach integrates sulfur getter and H₂ separation into a multifunctional membrane. Their use of ALD for materials deposition for both getter and proton conducting material should allow thin film deposition on surfaces of support and fine control of film properties.
- The work done by the team is nothing spectacular, but it worked to the extent that work was done. The team coated with ZnO, got H₂S protection. They, however, still do not have the flux and selectivity problem solved.
- A high-cost membrane is not a good solution for H₂ separation. The PCM themselves have a cost barrier to overcome and this makes the task all the more challenging.
- The project team has performed good work on deposition and stabilization on ZnO thin film.
- The project team should show how this would be scaled up in a manufacturable scale. Large areas of this material would appear to be fragile and challenging for handling. Is tube arrangement the geometry of choice?

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated 2.4 based on accomplishments.

- Initial attempts to deposit SrTiO₃ using ALD were not successful, but had never been previously demonstrated. The project team's effort has transitioned to a new Sr precursor identified in a recent literature report. There has been good success in demonstrating uniform deposition of ZnO getter in Al₂O₃ substrate, and initial results indicate this material can be cycled and fully utilized to purify a gas stream containing H₂S. The estimated performance of an S-getter was based on this technology and assumed full utilization, but did not compare to existing S-getter technologies to baseline pros/cons of this approach.
- The project team has had good progress in the area worked on. The project was defunded; therefore only carryover funds were used. The team should have a better membrane underneath in terms of flux and selectivity.
- Not much progress has been made since the last time, possibly due to lack of funding for this project.
- The project team has done good work to solve problems in depositing uniform films.
- The project's 70 days operation is very short for a complex and expensive film like this.

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated **2.4** for technology transfer and collaboration.

- The project team identified other partners, but did not pursue further after a decision made to end this project.
- The team should collaborate with someone that has a better membrane, and try coating it with their ZnO. The lack of funding is hindering, but still would expect that there are other people who would like to piggyback on the work.
- The PECM team has good coordination within themselves.
- This project team has done okay considering funding was cut.
- This project could leverage a lot of participants. BASF, for example, has extensive interest and experience in similar filtration systems.

Question 5: Approach to and relevance of proposed future research

This project was rated 2.4 for proposed future work.

- The project team will determine whether appropriate $SrTiO_3$ stoichiometry can be achieved, and if so, then they will measure H_2 flux of films. The project team will also determine the rate of sulfur uptake.
- No particular future work is planned for this project.
- The project's lack of funding from DOE would be a major obstacle.
- The project team needs a realistic estimate of reactor cost and comparison with sacrificial ZnO guard bed.

Strengths and weaknesses

Strengths

- The project team's integrated/monolithic approach to S gettering/H₂ purification should provide a simplified system design and good robustness.
- This is a nice part of a membrane durability project.
- None.

Weaknesses

- The project team needs to baseline component (getter and H₂ membrane) performance by comparing with existing technologies/approaches.
- The team needs to work better with others so that this part does not stand alone, but becomes part of a viable membrane.
- This project is an outside focus area for PCM research. Firstly, the right PEC materials should be obtained and then the team should focus on H₂ separation/purification.
- This project has questionable economics.

Specific recommendations and additions or deletions to the work scope

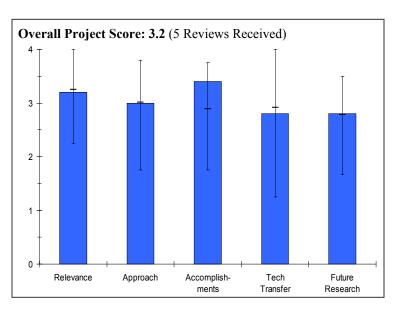
• The project team should get a good oxide membrane substrate, coat it, and repeat tests comparing it to the uncoated oxide membrane in terms of flux, selectivity, and life.

Project # PDP-15: Distributed Bio-Oil Reforming

S. Czernik, R. French, and M.M. Penev; National Renewable Energy Laboratory J. Marda and A.M. Dean; Colorado School of Mines

Brief Summary of Project

The overall objective of this project is to develop the necessary understanding of the process chemistry, compositional effects, catalyst chemistry, deactivation and regeneration strategy as a basis for process definition for automated distributed reforming. The fiscal year 2009 objectives are to 1) improve bio-oil atomization with less MeOH addition; 2) demonstrate noncatalytic partial oxidation of bio-oil at the bench scale; 3) demonstrate catalytic conversion of bio-oil to syngas at the bench scale; and 4) provide mass balance data for H2A.



<u>**Ouestion 1: Relevance to overall DOE**</u> <u>objectives</u>

This project earned a score of 3.2 for its relevance to DOE objectives.

- This project is going to develop distributed bio-reforming capabilities that directly address H₂ production targets for fuel feedstock issues, operation and maintenance, and control and safety.
- Bio-oil is a low-cost, renewable fuel, far cheaper than hydrogen. In this project, it is being reformed to H₂ and other gases that can be used in a fuel cell or for other power applications. This is a good and simple project. The work is straightforward and relevant to the hydrogen goals. The team's results are also good results; however, more work is needed.
- While this project meets the scope of direction and supports DOE objectives, converting biomass to hydrogen may not be the smartest thing to do.
- This project broadly supports objective of producing hydrogen from renewable sources. The project's cost potential is low; however, this low-cost potential comes at a price.
- This project has a fatal flaw in that it requires distribution of very dirty pyrolysis oil to forecourt locations. The distribution chain can't be made tolerant of dirty, unstable liquids; these bio-oils will need to be substantially upgraded before they can be distributed and stored for forecourt use; and these steps will add exactly the cost that this project seeks to avoid.
- This project presents a good analysis of a hydrogen production pathway that is not getting a lot of attention.

Question 2: Approach to performing the research and development

This project was rated **3.0** on its approach.

- The project team's approach addresses key individual processes, as well as overall system considerations. The team has a good understanding of how its research must feed into the overall system to achieve DOE's targets. It also has a good balance of fundamental experiments and practical system considerations.
- This project's experimental apparatus appears straightforward. The team has good experiments as well as analysis and has done good work. It would be better if the team looked at a lower-cost catalyst.
- This project has had a sound process path during period of performance that is consistently seen year to year. The team is well focused on the challenges and it is challenging to find how they can improve on their processes. This project team has done outstanding work in all aspects.

- This project's barriers are mischaracterized. The team's use of a dirty feed (pyrolysis oil) addresses the barrier of feed cost, by substituting a lower cost feed (than ethanol for example). Framed this way, a key issue is whether these cost advantages are outweighed by logistical (distribution) disadvantages.
- The boundary limits in this project need to be widened to include pyrolysis oil manufacture, distribution, and storage. In this project, it appears that oil handling distribution and storage are the most important barriers.
- This project has a good approach and the misting reactor is non-standard. The investigator needs to carry out studies using traditional reactors under a variety of conditions and compare results to ultrasonic nozzle reactor to establish its advantages and justify its use. The reactor has made interpretation of results difficult because temperatures are not well defined.
- The project team needs to look at steel reactors to explore higher pressures.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated **3.4** based on accomplishments.

- This project team has had significant progress in testing a range of feedstocks and conditions using the benchtop reactor both developed and built previously. The quantitative results for providing good insight for optimizing the overall reaction process from bio-oil to syngas. The initial results indicate that either a system that operates on a range of feedstocks could be developed or that the individual components could be developed to enable optimized systems in distributed locations for the primary feedstock in that location.
- This group is developing a technology that could be used in current or near-future fuel cells. The catalyst is still expensive and it would be better if Pt-Ni were used in the project instead. Also, the data should be presented in terms of turn-over numbers, and other, more normal, terms. Still, this project shows good solid work.
- While one may question the value of the objectives, the project clearly achieves steady technical accomplishments during the period of performance. The team's ultra-sonic nozzle development might prove to be very interesting, and beneficial. This is an outstanding performance by the project team.
- The project's objectives are well detailed for 2009, and are mostly accomplished despite minimal support.
- The team's reactor appears to generate consistent results. The team has also achieved good conversions of biomass and shown the effect of oxygen partial pressure.
- The project team has not made it clear that material balances are closed.

<u>Ouestion 4: Technology transfer/collaborations with industry, universities and other laboratories</u>

This project was rated **2.8** for technology transfer and collaboration.

- This project has strong collaboration with key partners that provide complimentary expertise and capabilities.
- This project has a good collection of distributed work, plus various students and collaborators. More input from catalyst researchers and a commercial catalyst supplier is recommended.
- The project team has met the requirements of collaboration with other institutions.
- This project has a little more than a catalyst supplier relationship with Lanny Schmidt and a funding relationship with Chevron.
- This project has collaborators listed, but no elaboration of how they contributed to program.

Question 5: Approach to and relevance of proposed future research

This project was rated 2.8 for proposed future work.

- The team's proposed future work builds on prior results and is focused on an ultimate system design concept and demonstration.
- This project seemed to be winding down. The team also seems open to looking at other catalysts, but had no particular plans to test them. They have no plan to feed into FCs, or to reorganize the data either.
- The project team has clear plans to address "what's next." It is also clear that future plans capitalize on progressto-date and that past progress supports future.

- This project needs to consider the whole "life cycle" of oil creation, storage, transportation, storage, and conversion.
- The project team needs to collaborate more. More industrial collaborations are suggested to better understand data needs for scale-up and consider improving reactor design.

Strengths and weaknesses

Strengths

- This project is a good idea. Making hydrogen from renewable cellulosic materials has allowed for good results.
- This is a very well thought out project and has a nice progress of getting from point A to point B.

Weaknesses

- This project should be continued, however it should look at less-expensive catalysts. Would like to see different data presentation, and more next-generation planning.
- The hydrogen cost chart seems to raise as many questions as it answers. The project team might want to make this chart clearer.
- The project team needs a better reactor design so that the temperature is controlled and measured.

Specific recommendations and additions or deletions to the work scope

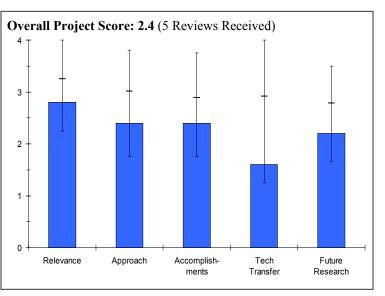
- The project team should feed gas to current or near-future fuel cells. It would be nice to see results in terms of residence time vs. extent of reaction. Also, the catalyst is still expensive and it would be better if Pt-Ni were tested instead of Rh.
- The project team needs to consider the whole "life cycle" of oil creation, storage, transportation, storage, and conversion.
- The project team should improve the reactor design. The team should look at pyoil from a variety of pyrolosis conditions and determine optimum conditions for process.

Project # PDP-16: Pressurized Steam Reforming of Bio-Derived Liquids for Distributed Hydrogen Production

Sheldon H.D. Lee, Dennis Papadias, and Shabbir Ahmed; Argonne National Laboratory

Brief Summary of Project

The objective for this project is to develop a distributed hydrogen production process 1) from hydrated ethanol and other bio-derived liquids; 2) using a pressurized steam reforming reactor; 3) to develop an efficient hydrogen production/purification process by reducing the hydrogen compression penalty. The rationale for this project is that steam reforming of liquid fuels at high pressure can reduce hydrogen compression costs. In addition, high-pressure reforming is advantages for subsequent separations and hydrogen purification.



<u>Question 1: Relevance to overall DOE</u> <u>objectives</u>

This project earned a score of 2.8 for its relevance to DOE objectives.

- This project supports the DOE Hydrogen Program objectives.
- Based on slide 3, the researchers are aware of the DOE goals and targets. The work is attempting to address the target of efficiency. However, there appears to be little consideration about the cost. In particular, increasing reactor pressures in a membrane reactor will likely require more robust materials and seals (which will increase the cost). Coupled with the need for a turbo-compressor, reaching the cost target may not be realistic. The work, overall, does not address any cost issues.
- This program provides a key understanding of relative merits of the key reforming and separation routes (membrane vs. PSA) for H₂ manufacture. This is a small but very important point, as projects will emerge that purport advantages via one route or the other.
- The distributed reforming of bio-based liquids such as ethanol is a promising near-zero GHG emissions route for the production of hydrogen if the capital costs can be reduced and selectivity improved. The DOE Hydrogen Program is funding several projects in this area. This project is trying to achieve cost reduction by operating at higher pressures and employing an *in situ* palladium hydrogen membrane. This can reduce capital costs to a degree but does not have the potential of more significant cost reductions of other options being researched.
- This technology has a potential of reducing the already low-cost steam methane reforming (SMR) hydrogen production. The process has relevance in both long-term biogas applications, as well as today's refinery SMR applications.

Question 2: Approach to performing the research and development

This project was rated **2.4** on its approach.

- The rationale behind the technical approach in this project is unclear.
- The team's energy and cost analysis data should substantiate the claim why it is cheaper to pressurize an incompressible fluid (fuel and water) compared to hydrogen, a compressible fluid. It is well known that compressing hydrogen is energy intensive. A Google search shows that to compress hydrogen from 100 psi to 700 psi, the energy need is 2.6-3.6 kWhe/kg. Energy needs to compress liquid fuel and water is necessary for comparison.
- The project team has idealized assumptions on membrane performance without identifying a membrane operating at 650°C and achieving DOE 2015 performance targets.

- The recovery of a non-permeate streams' temperature and pressure energy into shaft work is not a new idea. The availability of appropriate capacity turbo-machinery for distributed production scenario is not discussed in this project.
- If a reactor operates at 800°C and 80 atm, it is unclear which membrane is available to separate the hydrogen at DOE's 2015 flux target. It is also not explained why it is so cost-effective and operationally simple to operate a SMR/membrane integrated reactor at 800°C and 80 atm.
- The project's engineering design and plant operation of the proposed approach may not be practical.
- The overall approach to evaluate/model a high-pressure reaction on the reaction side of the membrane does not appear to make sense. Increased pressure may increase flux (due to a higher partial pressure differential) but the product pressure will not be affected.
- This may have benefit for a conventional SMR reaction but increased pressure for SMR has already been examined in detail in many studies in the past. In addition, this appears to be a pure modeling effort with little experimental results to back up the modeling results. There needs to be a better balance in the approach of this project. Slide 9 simply uses the DOE target. This is not a reasonable approach. The actual flux rates (with mixed gas) need to be incorporated for realistic model results. This work also needs some independent verification.
- The project's model approach is perfect for this program.
- The team's approach to this effort over the past year consisted solely of modeling several options for distributed ethanol reforming including the high-pressure *in situ* membrane approach being taken by this project and the more conventional approach using lower pressures and PSA technology. Although modeling can be very useful, this modeling work only included performance (energy efficiency) without any analysis of costs which is the issue for ethanol reforming.
- There was no experimentation done to verify the modeling effort or to further the development of the approach being researched by the team.
- There was no collaboration mentioned with the other DOE Hydrogen Program funded projects working on ethanol reforming. Collaboration with these efforts would be very beneficial to this effort as well as the other projects.
- This team has demonstrated outstanding systems engineering and optimization of its technology. This process can be used to evaluate the performance of other similar applications of hydrogen separation. It would be worthwhile to benchmark the various technologies of this flavor in this fashion.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated **2.4** based on accomplishments.

- The team's studies and reports have areas where analysis is based on ideal assumptions. The project team has not analyzed if the technical strategy is practical, nor has analyzed or substantiated some of the technical claims.
- The team's summary statement of higher efficiency at 10,000 psi delivery pressure is made with ideal assumptions. The DOE target is 100 psi trans-membrane ΔP. The project team needs to say what feed pressure they recommend to achieve the delivery pressure to exceed the efficiency of a conventional, proven, SMR-PSA system.
- The project's results are minimal for the funding provided. There has been very little advancement since last year. The work has changed to look at ethanol, which should be easier to reform; however, few results are actually provided. Efficiencies are still not reaching the targets and increasing efficiency by even a few points is a difficult problem with systems such as these. The only potential result appears to be that addition of a turbo-compressor may add some benefit to the efficiency. The cost of it may cause this benefit to be impractical.
- The team's objectives are poorly expressed in the poster for the specific piece of work that was executed and described. However, the project accomplishments are very good.
- The team's modeling work performed is quite good and does help to understand the potential performance (energy efficiency) leverage of the approach to ethanol reforming being researched. However, there is no cost analysis work being done to quantify the potential benefits of this approach. Cost is the key issue.
- The future plan from last year's merit review presentation included exploring O₂ and CO₂ membranes. There was no work done on this.
- The team has done good systems analysis work. More results from material performance and properties were expected and this technology may need to be demonstrated in scaled up reactor.

<u>Ouestion 4: Technology transfer/collaborations with industry, universities and other laboratories</u>

This project was rated **1.6** for technology transfer and collaboration.

- The project team is working with REB Research and Consulting, but the extent of their collaboration is not discussed.
- Outside collaboration appears minimal to none in this project. Some interaction appears to be with REB; however, the REB membrane is used for a small scale system and has minimal flux at moderate conditions. They are neither considering nor addressing conditions that would be used in a larger scale process. All other project work is being done within Argonne. In order for this work to be credible both industry input and collaboration is necessary. The models need some independent verification outside the lab to have any meaning of value.
- There are not a lot of collaborations in current phase nor do there need to be.
- The only collaboration mentioned by the team is within ANL and with REB who supplied the palladium membrane. There are several other excellent ethanol reforming projects being funded by the DOE Hydrogen Program. Collaboration with these efforts would be very beneficial to this effort as well as the other projects.
- The modeling work performed by the team is quite good and does help to understand the potential performance (energy efficiency) leverage of the approach to ethanol reforming being researched.
- This project can benefit itself and other projects by collaborating. This can especially benefit others with issues such as systems engineering capabilities and practices.

Question 5: Approach to and relevance of proposed future research

This project was rated 2.2 for proposed future work.

- This section is missing from the project.
- This is a project that should be considered for termination. Few results have been obtained and the results thus far do not suggest continuing the project. The future plans are standard and vague and still appear to focus on modeling with little experimental verification. There is considerable other work in the suggested areas that is being conducted by other researchers. The team's work is not providing any new or novel insight that could not be obtained elsewhere.
- The team should complete the economics due to being the highest priority of the several items identified.
- The project's future plan includes cost analysis, which is good. However, it should have been part of this project from the beginning.
- The team's future plan appears to include experimentation work with other biofuels based on the proposed approach which would be useful.
- The future work for this team includes evaluating systems based on CO₂ removal. It is unclear if this approach could significantly reduce the cost of biofuels reforming. A very simple analysis might determine this.

Strengths and weaknesses

Strengths

- No clear strengths are identified in this project.
- Distributed reforming of bio-based liquids such as ethanol is a promising near-zero GHG emissions route for the production of hydrogen if the capital costs can be reduced and selectivity improved which is a strength.

Weaknesses

- Minimal results have been shown for an estimated investment of \$750K. The work is not achieving the DOE efficiency target and cost has not been clearly considered at all. There are no clear targets or milestones for this work and seems to be simply continuing on a random path to provide some basic, minimal results.
- The DOE Hydrogen Program is funding several projects in this area. This project is trying to achieve cost reduction by operating at higher pressures and employing an in-situ palladium hydrogen membrane. This can reduce capital costs to a degree but does not have the potential of more significant cost reductions of other options being researched.

- The approach to this effort over the past year consisted solely of modeling several options for distributed ethanol reforming including the high-pressure *in situ* membrane approach being taken by this project and the more conventional approach using lower pressures and PSA technology. Although modeling can be very useful, this modeling work only included performance (energy efficiency) without any analysis of costs which is the issue for ethanol reforming.
- There was no experimentation done to verify the modeling effort or to further the development of the approach being researched by the team.
- There was no collaboration mentioned with the other DOE Hydrogen Program funded projects working on ethanol reforming. Collaboration with these efforts would be very beneficial to this effort as well as the other projects.

Specific recommendations and additions or deletions to the work scope

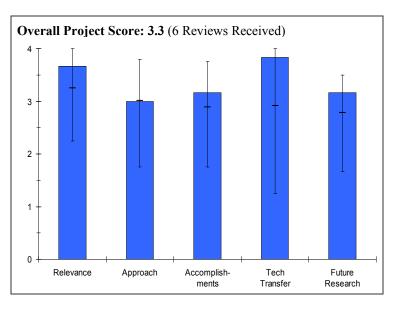
- Many assumptions realistic for engineering development.
- This project should be considered for termination. No additional funding should be obligated.

Project # PDP-17: Renewable Electrolysis Integrated System Development and Testing

Kevin W. Harrison, Greg Martin, Todd Ramsden, and Genevieve Saur; National Renewable Energy Laboratory

Brief Summary of Project

The objectives of this project are to 1) characterize electrolyzer performance with variable input power; 2) design, build and test shared power electronics; 3) identify opportunities for system cost reduction and optimization; and 4) test, evaluate and model the renewable electrolysis system. The National Renewable Energy Laboratory (NREL) has increased energy capture of the second generation wind to stack power electronics and verified stack voltage efficiency to help meet the DOE milestone. NREL has also integrated grid, wind and photovoltaic functionality into single power electronics module to reduce capital cost.



<u>Ouestion 1: Relevance to overall DOE</u> <u>objectives</u>

This project earned a score of 3.7 for its relevance to DOE objectives.

- This project addressed a highly relevant topic. There will be significant payoff if project is successful. This could be highly significant for industry, military, and individual consumers.
- The project team broadly supports renewable energy to fuel hydrogen.
- The project's wind to H₂ project fully supports the DOE Hydrogen Program.
- The project's focus on the need for "as close to direct coupling" of renewable sources to electrolyzers is important and relevant. This is because, in the end (when fossil sources get prohibitively expensive), renewable electricity would be the only logical power for electrolysis of water to produce hydrogen.
- The project's hydrogen-oxygen redox couple is not convincing especially regarding the claim that it is the best couple for renewable energy storage. This exercise is useful in developing the groundwork for understanding the rate-limiting challenges in this source especially load coupling.
- The project supports critical analyses of renewable hydrogen production systems.
- This is an important project that helps to assess the capability of hydrogen to serve as a storage medium and to maximize the use of intermittent renewable resources.

Question 2: Approach to performing the research and development

This project was rated **3.0** on its approach.

- Barriers appear to be accurately identified in this project.
- The team's approach clearly addresses barriers, but this is a very expensive, pre-commercial scale activity. It is possible that this work was done too soon before there was adequate commercial interest to take the findings into commercialization.
- With the push to get renewable energy onto the grid, the assumption of a dedicated solar or wind facility for hydrogen generation seems unlikely in near future. If the benefit of the advanced power electronics is in elimination of the turbine's power electronics (which is what the cost analysis shows), then this part of the project should be deferred until closer to when it is likely that a wind turbine that is dedicated to hydrogen production would occur. Doing this research does not seem effective since it is likely that turbines and electrolyzers of the future (when the power electronics are needed) will be substantially different requiring the power electronics to be re-developed. In addition, the power electronics seem to be turbine type specific,

therefore power electronics for each manufacturer and model of turbine would be required. It is hard to see how the power electronics will be used in the time frame the team envisions.

- The barriers addressed by the project team (capital cost, system efficiency, and renewables integration) do not include the design, construction and commissioning of a fuel cell vehicle filling station. This should not be part of this project, but it should be in Tech Validation. The Production and Delivery budget is too small to maintain a filling station. Resources from Production and Delivery should not have been spent on the filling station. This portion of the project should be given to Tech Validation.
- The team should have spent more effort on getting long-term on-wind or on-solar hydrogen production generation. Showing a limited number of hours on-sun or on-wind hydrogen generation is not impressive considering the very large budget of the project and the length the project has been in place.
- The team's approach is solid and reasonable but efficiencies developed here tend to be individual component efficiencies rather than a "quantum leap" in system-integrated efficiencies.
- Numerous barriers are being addressed in a well-integrated project.
- The team's approach for research and development seems generally good, but it would help to have a more specific approach to meeting technical barriers such as overall system efficiency, auxiliary power losses, etc.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated 3.2 based on accomplishments.

- The project team's stack size reductions are commendable. The whole process to make a more-durable, more size-economic system could be well received.
- Overall, the team's accomplishments are great, but presentation does not identify what was actually planned or executed in 2008 or 2009, and a lot of this material has been around for a while.
- This project started in FY06 and has been very well funded (\$4.625M), but has produced relatively little on-sun or on-wind data. One would expect long term (days at a minimum, preferably weeks or months) worth of data to show how the system operates over a wide variety of conditions. The hydrogen does not necessitate the need to be captured for this operation, it could be vented or consumed (they have a generator).
- DOE provided the 2008 AMR presentation. In that presentation, the PI said that they were validating their cost/performance models that NREL was developing. The results of the validation were not presented. It is unclear where these results have been presented.
- Seeing new wind to hydrogen data from the team was good.
- The power electronics improvements from generation 2 to generation 3 did not seem extremely significant; however, power electronics improvements are difficult to achieve.
- Since the power electronics are a major focus of this project, a more detailed explanation on why the 3rd generation did not achieve the anticipated improvements would be useful.
- The team's cost analysis assumes that the wind turbine would be used exclusively for hydrogen production. This is not a realistic assumption in the current rush to put renewables on the grid. The cost analysis should be done again, with the assumption that the wind turbine will be used primarily for electricity generation and then curtailed wind will be used for hydrogen generation. This is a more realistic scenario.
- The team's development of standardized testing protocols is an important accomplishment.
- The project team accomplished straight-forward experiments and well-presented results (e.g., the direct coupling for PV-PEM.)
- The team produced good, reasonable, conclusions related to criticality of power electronics (command and control), need for greater standardization of interconnects and components, and need to define redundancies.
- The findings and lessons learned document shows strong progress in the team overcoming barriers.
- Several significant improvements have been developed and implemented by the project team.

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated **3.8** for technology transfer and collaboration.

- A significant number of partner activities are involved in the program.
- There seems to be good collaboration with other institutions including international collaborations in this project.

- It is unclear how the team is sharing and offering feed back regarding its information and what information on the electrolyzer is being fed back to electrolyzer manufacturers. Are the electrolyzer companies interested in using the power electronics? Who will manufacture the power electronics? Since it is unlikely that the electrolyzer companies will manufacture power electronics, have they talked with power electronics companies?
- A large component of this project is integration with wind and solar. Collaborations with wind and solar companies are not apparent.
- The team's collaborations are solid because of the equipment supplied by the many players.
- There are several partners that are well integrated into this project.

Question 5: Approach to and relevance of proposed future research

This project was rated **3.2** for proposed future work.

- A compelling argument to do any of this is not apparent.
- The team has been working on the system upgrades for unattended operation for at least two years without being able to begin unattended operation.
- What is the purpose of the higher-pressure storage? Is an renewables to electrolyzer project? Should storage be part of a storage project or tech validation project?
- The team has well developed plans for future work should continue progress in addressing the specified barriers.
- The team could use more specific plan.

Strengths and weaknesses

Strengths

- The project addresses a technology that could be beneficial to a great number of users.
- The team has a good relationship with electrolyzer manufacturers and utilities.
- The team is providing a necessary and needed independent testing facility to the DOE to validate the electrolyzer projects results.
- The team has been very involved in the international community and given many presentations and published many reports.
- This project is somewhat unimaginative project but well-executed and presented.
- The team's conclusions are good (and expected) however no major revelations or show-stoppers are seen (other than system costs.)
- Strong technical integration is widely evident in this project.
- The team addresses a key area of hydrogen use with renewables.
- The team has a good combination of analysis and experimental results.

Weaknesses

- The team has been working on the system upgrades for unattended operation for at least two years. If it is that difficult to design a system for unattended operation, is this technology viable?
- The team needs to talk with wind and solar companies to get their "buy-in" on dedicated renewables for hydrogen.
- The project's progress seems slow, especially for the amount of resources they have received.
- It seems that the team has gotten side tracked. For example, the team worked on electrolyzer cost modeling for a few years and then stopped, but the outcome has not been presented. The team is putting in a fueling station and high-pressure storage, but it has not produced any long-term wind-to-hydrogen results. The compressor studies were interesting, but it is unclear why these studies were not done under Hydrogen Delivery element funding?
- There are no apparent weaknesses because this project's objective is to explore system interactions.
- The team should develop more specific technical targets.

Specific recommendations and additions or deletions to the work scope

- Because of the design differences between more-traditional fuel cell stack and tube-like systems, one could suspect that the team's system's ability to manage freeze conditions is a significant advantage over traditional stacks as water can more efficiently drain off.
- The project should focus on getting renewables-to-hydrogen data, especially long-term data.
- The power electronics development should be deferred until closer to when large central production facilities are necessary.
- The project should turn the fueling station to the Technology Validation Subprogram.
- The project should turn the compressor testing to the Hydrogen Delivery element.
- The project should work closer with electrolyzer companies on helping the companies understand the impact of renewables on the electrolyzers. However, this cannot be done until they have long term data is available.
- The team should continue the work but figure out an open portal for spiral integration of new technologies. They should explore more close-coupling (direct-coupling) projects.

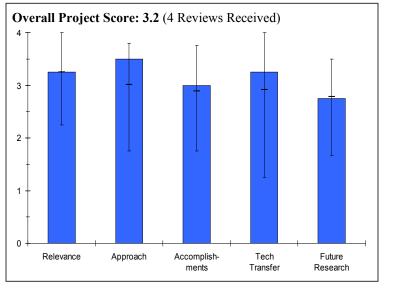
Project # PDP-18: Hydrogen from Water in a Novel Recombinant Oxygen-Tolerant Cyanobacterial System

Qing Xu; J. Craig Venter Institute Pin-Ching Maness; National Renewable Energy Laboratory

Brief Summary of Project

The objective of this project is to develop an oxygen tolerant cyanobacterial system for continuous light-driven hydrogen production from water. The approach is to transfer oxygen tolerant hydrogenases into cyanobacteria to overcome the hydrogenase oxygen sensitivity issue. Environmental deoxyribonucleic acid encoding hydrogenase was converted into a functional hydrogenase with both hydrogen evolution and uptake activities.

<u>**Ouestion 1: Relevance to overall DOE**</u> <u>**objectives**</u>



This project earned a score of **3.3** for its relevance to DOE objectives.

- Biological hydrogen supports the Hydrogen Program's RD&D objectives.
- This project aligns with the need for a renewable hydrogen production technology.
- Several approaches are being taken to add oxygen tolerant hydrogenases to cyanobacterial systems. This is key as the only real source of electrons is water and therefore oxygen will always be present.

Question 2: Approach to performing the research and development

This project was rated 3.5 on its approach.

- The approach is very systematic and well thought out.
- The project team has good focus on one key barrier: oxygen tolerance; however, it is unclear whether the final objective is to demonstrate an approach or an enzyme that can be manipulated into other more attractive organisms. It is unclear whether this organism would be stable. This is excellent science. There is not an obvious plan to incorporate other barriers for this type of technology.
- The project team is combining metagenomic searches for oxygen tolerant hydrogenases with expression in T. roseopersicina. The team is also taking a known oxygen tolerant hydrogenase gene from Rubrivivax gelatinosus CBS and expressing it in the cyanobacterium SynechocystisPCC6803. The metagenetic approach in particular has great promise.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated **3.0** based on accomplishments.

- The team is achieving difficult milestones.
- The PI clearly identifies accomplishments and contributions of partner.
- Although NREL has received similar funding, they seem to be lagging behind J. Craig Venter Institute (JCVI).
- The project team has made excellent accomplishments in transferring genes and expressing a better oxygen tolerant hydrogenase.
- The project team is observing some hydrogenase activity from hydrogenase genes found and expressed in T. roseopersicina. The team has been trying to transfer the system into Synechococcus and can do this with the native hydrogenase from T. roseopersicina. NREL is having problems with the expression in synechocystis of

an oxygen tolerant hydrogenase from Rubrivivax gelatinosus CBS in terms of activity of the enzyme, though some subunits are present. They have demonstrated protein expression of the catalytic subunit in E. coli.

<u>Ouestion 4: Technology transfer/collaborations with industry, universities and other laboratories</u>

This project was rated **3.3** for technology transfer and collaboration.

- The project team has good collaborations with other institutions and they clearly identify partner contributions.
- There is a good collaboration with NREL, but no mention of Vanderbilt University or University of Szeged, Hungary. It is unclear whether any of this work is linked to the Office of Science and if so what type of collaboration there may be.
- This appears to be a strong collaborative effort between JCVI and NREL.

Question 5: Approach to and relevance of proposed future research

This project was rated 2.8 for proposed future work.

- Continuing analysis does not seem very specific. More description in future work would be nice.
- More characterization and transfer is planned; however, nothing is mentioned about the stability of the hydrogenase through a number of generations. The work should at least validate the new gene sequences will remain active before additional bacteria systems are tested.
- In both JCVI and NREL, the proposed work is largely to continue optimizing the expression and activity of the hydrogenases in cyanobacteria.

Strengths and weaknesses

Strengths

- The team has a vast library to examine and the tools to examine it.
- The team is strong and they are communicating well.
- This is a good research team.
- The team has a well thought out plan for an oxygen tolerant hydrogenase.
- The strong capability in metagenomics of JCVI is the biggest strength. This, combined with the ability to identify and express the various components of the oxygen tolerant hydrogenases that they find, is potentially very powerful.

Weaknesses

- Contingency plans need to be developed.
- Understanding of the outcome is limited beyond the funding of good science. Does this work have any practical use in a real production system?
- The project is still at a point where it is very hard to extrapolate to commercial value or scale.

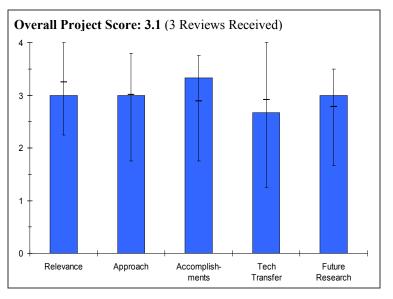
Specific recommendations and additions or deletions to the work scope

No specific recommendations were provided for this project.

Project # PDP-19: Use of Biological Materials and Biologically Inspired Materials for H₂ Catalysis John W. Peters, Trevor Douglas, and Mark Young; Montana State University

Brief Summary of Project

The objectives of this project are to 1) optimize the hydrogenase stability and electron transfer; 2) optimize the semiconductor nano-particle photocatalysis, oxygen scavenging and electron transfer properties of protein nano-cages; 3) perform gel/matrix immobilization and composite formulation of nano-materials and hydrogenase; and 4) perform device fabrication for hydrogen production. Montana State will incorporate hydrogenase and mimetics into stabilizing matrices as well as into electroactive poly (viologen matrices).



Question 1: Relevance to overall DOE objectives

This project earned a score of 3.0 for its relevance to DOE objectives.

- The project consists of two parts: hydrogenase studies and biomimetic devices. The former aligns very well with the Hydrogen Program's objectives, although the latter seems to be too basic to be funded by EERE.
- The project goals are well-aligned with DOE program targets for improving both stability of hydrogen production and rate of electron transfer
- The focus on the hydrogenase of the purple sulfur bacterium is relevant since it is one of the most stable one reported thus far.
- Encapsulation of the hydrogenase will eventually improve stability, coupling that with a photosensitizer will improve the efficiency of solar hydrogen production.
- The project aligns well with DOE's objectives for biological hydrogen production.

Question 2: Approach to performing the research and development

This project was rated **3.0** on its approach.

- The approaches are good, although it would probably be better for the PIs to focus in a fewer approaches in the future.
- Good approach and synergy between biochemistry and material science
- Hydrogenase from Thiocapsa is a good model to determine protein structure and the possibility of uncovering underlying mechanism conferring overall stability
- The use of carbon nanotube, sol gels, photosensitizer, and polyethylene glycol may improve overall protein stability and rate of electron transfer while harnessing solar energy for hydrogen production. The team is also developing various materials for light capturing properties to harness solar energy.
- Approaches are logical. Focus on encapsulation of active hydrogenases in gels is good.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated **3.3** based on accomplishments.

• The accomplishments are good and exciting, particularly in the area of hydrogenase studies. The accomplishments regarding the Thiocapsa roseopersicina hydrogenase's C-terminal and its possible relationship

to high O_2 tolerance are very promising in terms of future molecular engineering and biotechnology approaches to modify other hydrogenases.

- The progress toward goals was good.
- Protein alignment suggested the extra amino acids in the C terminus of the hydrogenase small subunit may confer stability, although no biochemical data supporting this hypothesis yet.
- The EM pictures revealing supermolecular structures of Thiocapsa hydrogenase is an important achievement
- Hydrogenase activity was demonstrated when it was entrapped in silica gel and was further enhanced when carbon nanotube is added.
- Low but obvious hydrogen production was observed in the nanotube in the absence of methyl viologen
- The finding of enhancement by polyethylene glycol (PEG) is novel, suggesting improvement in mass transfer is the contributing factor.
- The project team determined the photocurrent with hematite and methyl viologen (MV). Hydrogen production is to be expected with reduced MV, although the data was not shown.
- Good progress has been made. 100% recovery of hydrogenase activity encapsulated in Sol-Gel was achieved and gel encapsulation may be used to stabilize Fe-Fe hydrogenases. Identification of the C-termini end that contributes to the stability of Thiocapsa hydrogenases is interesting.

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated **2.7** for technology transfer and collaboration.

- Both PIs belong to the same institution and there are no outside collaborators. The two projects (hydrogenases and biomimetics) could be better coordinated.
- The collaboration is among the team members of this project: a multidisciplinary team comprising of biochemists and material scientists.
- This project is not yet ready for technology transfer.
- Good collaboration was demonstrated.

Question 5: Approach to and relevance of proposed future research

This project was rated **3.0** for proposed future work.

- Plans are good.
- A clear plan is laid out for device testing and evaluate hydrogen production efficiency
- Device optimization is underway
- Proposed future work is appropriate. The plan to establish benchmarks for hydrogen production efficiency is good.

Strengths and weaknesses

Strengths

- The PIs are knowledgeable in their respective areas of research and the institution is well-positioned to address the proposed research plans.
- This multidisciplinary team comprises expertise in hydrogenase biochemistry, crystallization, and material sciences.
- The investigators have demonstrated progress toward meeting well-defined goals.
- The biochemistry side of the research is strong, with the PI being a leader in the field of crystallography of difficult hydrogenase protein.
- This research may lead to identification of protein structure conferring its overall stability. This knowledge can serve as a model to study other hydrogenase and to improve their stability.
- The material sciences part of the team can generate materials with properties for improving electron transfer, mass transfer, and light capturing.
- The investigator is an expert in structures and structure-function relationship of NiFe-hydrogenases and Fe-Fehydrogenases.

Weaknesses

- The is a lack of coordination between the different projects.
- It is unclear as to a final choice between hydrogenase and platinum/palladium as the hydrogen-producing catalyst.
- Similarly, it is not clear as to whether ferritin or Ru(bpy)³ is preferred as the photosensitizer. There should be a more logical plan to include or eliminate and focus on the more promising materials.
- Ferritin needs ethanol as the sacrificial electron donor, but this may or may not be practical.
- The project's goal is not specific and there are no benchmarks for hydrogen production.

Specific recommendations and additions or deletions to the work scope

• The project team should focus more on down-selecting different configurations for the biomimetic device, at this point.

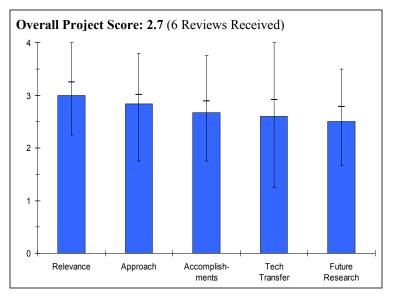
Project # PDP-20: Hydrogen Embrittlement of Structural Steels

Brian Somerday; Sandia National Laboratories

Brief Summary of Project

The objectives of this project are to 1) enable application of structural integrity models to steel hydrogen pipelines; and 2) enable development of micromechanics models of hydrogen embrittlement in pipeline steels. Models can demonstrate that hydrogen embrittlement can be accommodated and pipeline safety margins can be quantified. Micromechanics model are essential for understanding the fundamentals of hydrogen transport and embrittlement in steels.

<u>**Ouestion 1: Relevance to overall DOE**</u> <u>**objectives**</u>



This project earned a score of **3.0** for its relevance to DOE objectives.

- The project team should address how embrittlement rates compare to other forms of degradation.
- The acceptable performance target for these materials is unclear.
- This subject is important but in the overall list of items is probably ranked in lower quartile. The multiplier effect would have been to tie in this project with infrastructure validation programs fro end-of-life analysis.
- Knowledge of metal behavior in hydrogen service is important to delivery scenarios.
- Hydrogen pipelines may or may not be critical to the long-term success of fuel cells and the Hydrogen Program.
- It is unclear what the current hydrogen pipeline materials lack in properties.
- Knowledge of embrittlement required for use of steel in pipe and parts of hydrogen systems.

Question 2: Approach to performing the research and development

This project was rated **2.8** on its approach.

- The round robin approach will improve confidence in the data. It is unclear whether the different lab equipment/tests been calibrated.
- The sampling preparation and the hydrogen leakage were difficult issues and affected the program. The sampling issue could have been resolved by connecting this program with ongoing infrastructure validation projects to get field data and samples.
- It is not clear why the particular steels were chosen for evaluation.
- Evaluating the samples by ASME procedures is technically sound.
- This project measures material properties for use in hydrogen pipelines. Existing materials are evaluated for their use with hydrogen. It is unclear if the current material properties lack sufficient properties or not.
- Materials testing in support of ASME B31.12

Ouestion 3: Technical accomplishments and progress toward project and DOE goals

This project was rated 2.7 based on accomplishments.

- Some test apparatus issues still remain.
- Good progress has been made considering no funds were made available this year.
- This is not reflective of the PI's work but the organizational and budgeting issues.

FY 2009 Merit Review and Peer Evaluation Report

- Low funding for FY09 has hindered progress.
- Some data have been generated in round robin tests. Conclusions are weak. Metal behavior as a function of composition should be addressed to validate the original reasons for choosing the candidate metals.
- This project received no funding in FY09, thus accomplishments for FY09 were minimal. It is not fair to evaluate a project which was not funded in the current fiscal year.
- The project team should duplicate testing to demonstrate reproducibility.
- This project needs continued funding!

<u>Ouestion 4: Technology transfer/collaborations with industry, universities and other laboratories</u>

This project was rated **2.6** for technology transfer and collaboration.

- This is not a criticism of the PIs but rather an indication of lack of coordination between the ongoing and parallel programs within the entire hydrogen effort. While as is, this project provided good data, but it could have had a higher potential to be a very useful and practical project.
- The problem that beset this project could have been worked out if the program was coordinated with the ongoing infrastructure projects for sample recovery.
- Participation of DOE Pipeline Working Group is positive but there seems to be weak participation of steel and pipe supplier companies.
- Work with the Pipeline Working Group is good.
- It seems as though there should be emphasis on industry: energy and industrial gas companies, as they have working hydrogen pipelines.
- Work with the DOE Pipeline Working Group is an excellent example of collaboration.
- Round robin testing is being conducted.

Question 5: Approach to and relevance of proposed future research

This project was rated **2.5** for proposed future work.

- The reliability of the testing methods is still outstanding. This should be first on the agenda.
- As the program appears to be at an end, there is no significant work planned.
- DOE funding is in question.
- Future work at some point should include an analysis of metal properties and behavior as functions of composition.
- No additional work is planned in FY09 due to lack of funding

Strengths and weaknesses

Strengths

- Embrittlement is an important issue with hydrogen.
- Round robin testing is a good approach.
- Useful concept with wide industrial application.

Weaknesses

- Issues with testing methods should have been resolved earlier.
- There has been a lack of coordination.
- This project has had limited budget.
- The experimental set up and procedure were weaknesses.

- It is unclear what other materials are being proposed for these pipelines.
- It is unclear whether the round robin partners have calibrated their tests with a known/standard material.

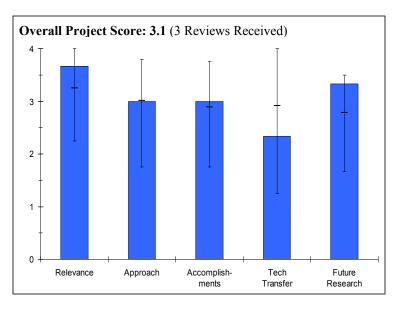
- The slide on critical assumptions discusses the issues, but there is no resolution for these. For example, it is unclear whether this program can work in conjunction with the infrastructure validation program to analyze the on-site steel storage tanks that have been through multiple cycles at pressures up to about 6000 psi.
- It appears a highly useful and practical program but it is handicapped by lack of adequate planning and interprogram connections and collaboration.
- The budgeting cycle could have been timed better to coincide with the end of the other programs for sample recovery.

Project # PDP-21: Oil-Free Rotor-Bearings for Hydrogen Transportation & Delivery

Hooshang Heshmat, Ph.D.; Mohawk Innovative Technology, Inc.

Brief Summary of Project

The objectives of this project are to 1) assess the feasibility of centrifugal compressors for hydrogen transmission and delivery; 2) demonstrate full-scale oil-free foil bearings in a compressor simulator rig; and 3) test candidate bearing/shaft materials and coatings. The hydrogen centrifugal compressor operated at very high speeds and required oil-free compliant foil bearings. Multi-stage, high-speed centrifugal compressors operating in series are necessary and feasible as demonstrated by low friction and long wear life of Korolonä.



Question 1: Relevance to overall DOE objectives

This project earned a score of 3.7 for its relevance to DOE objectives.

- Research in any new modes of efficient compression for bulk hydrogen handling is an important subject with wide reaching application.
- This project is a Phase II SBIR project aimed at the development of foil bearings (journal and thrust) for hydrogen pipeline compressors. This project directly addresses hydrogen compression targets and barriers.

Question 2: Approach to performing the research and development

This project was rated **3.0** on its approach.

- The project is segmented in different parts and funded separately. It was somewhat difficult to grasp the entire approach without knowing the entire scopes of the work. Apparently this project was just the preliminary modeling and scoping phase.
- The project team has a good approach based on foil bearing technology developed for air and gas turbine applications. Phases I and II of the project are focused on development and testing of bearings in non-conventional gases that simulate hydrogen e.g., use He to simulate lightweight properties of hydrogen. He tests appear to validate models, which can then be used to predict lift-off speeds and rotor dynamics in hydrogen.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated **3.0** based on accomplishments.

- Based on the materials and the objectives, the project has made steady progress and is on its way to the next proto-type setup and testing.
- One of the problems is reducing environment with hydrogen. This project could have benefited if it had a closer collaboration with the other project (ANL, PDP-25) on coating tests.
- Good progress on modeling rotor dynamics and lift-off conditions for He. In final stage, project started to address seals and appears to settle on dynamic compliant foil seals.

<u>Ouestion 4: Technology transfer/collaborations with industry, universities and other laboratories</u>

This project was rated **2.3** for technology transfer and collaboration.

- This is partly because of the PI issues and proprietary nature of the work. It would have been useful if the PIs would allow ANL to test their coating. It is understood the reducing hydrogen environment can rapidly affect the coating performance.
- There was limited collaboration with outside firms. Mitsubishi Heavy Industries (MHI) interaction was noted, but no details were given on the interaction. It would be nice to know details of MHI interaction and if MHI intends to be involved in testing/demonstration of prototype compressor, and if prototype will be designed for hydrogen or natural gas.

Question 5: Approach to and relevance of proposed future research

This project was rated **3.3** for proposed future work.

• Future activities on this specific project will focus on final report of overall project and dynamic seal tests at high pressures, speeds, and temperature.

Strengths and weaknesses

Strengths

- This is an innovative concept with wide ranging application.
- The design of foil bearing seal technology can enable significant design improvements in centrifugal compressors.

Weaknesses

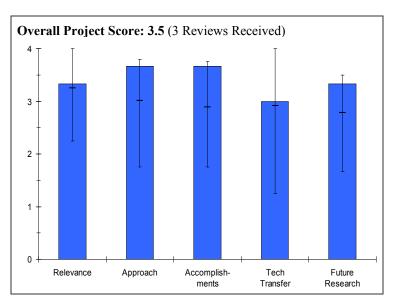
- There has been a lack of collaboration.
- Reliability and durability of bearing and seal materials in hydrogen environments does not appear to be considered in test plans. It is unclear whether the proposed materials and coatings survive in hydrogen environments.

- It would have been useful to have the entire roadmap for the project. Also, it would have been useful to have the PI at the poster session.
- Project is in final stage and is transitioning to larger design project with MHI. Would like to see a trade-off design comparing overall performance of a centrifugal compressor using current off-the-shelf bearings and seals against foil bearings and seals. Comparison should include parasitic losses, leakage, and anticipated durability/reliability. The project team should look at how predicted leakage of foil seal technology compares to an optimized labyrinth seal. The team should examine how much is gained by using foil bearing technology over a well-designed/optimized compressor using conventional bearings and seals.

Project # PDP-22: Development of Highly Efficient Solid State Electrochemical Hydrogen Compressor (EHC) *Ludwig Lipp; FuelCell Energy, Inc.*

Brief Summary of Project

The objectives of this project are to 1) demonstrate feasibility of a solid-state hydrogen compressor cell capable of compressing hydrogen to 2,000 psi; 2) increase the cell performance (power consumption, compression efficiency) while lowering the cost compared to previous designs; and 3) study thermal and water management to increase system reliability and life. FuelCell Energy increased compression mode operation capability from 500 psi to 4,000 psi in a single state EHC cell and completed >100 pressure cycles from 100 to 3,000 psi without performance loss.



<u>**Ouestion 1: Relevance to overall DOE**</u> <u>objectives</u>

This project earned a score of 3.3 for its relevance to DOE objectives.

- The project goals and development efforts aligned to delivery barriers on the development of high-pressure forecourt hydrogen compressors.
- The project supports a critical delivery objective within the Hydrogen Program.
- The project provides improved means of compressing hydrogen, which can facilitate refueling with highpressure hydrogen storage tanks on vehicles.

<u>Ouestion 2: Approach to performing the research and development</u>

This project was rated 3.7 on its approach.

- The approach is well thought out and described. Specific goals/milestones and metrics (2000 psi/FY08, and 6000 psi/FY09) were identified. Plans to scale up capacity to 2 #/day are presented.
- The project is clearly focused on technical goals and objectives to enable future delivery targets.
- Technical barriers were well addressed. The project team should perform cost analysis to help establish design and capital cost goals. The project team should compare these goals with goals for PEM fuel cells and electrolysis on a cost per active area basis.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated 3.7 based on accomplishments.

- Good progress is being made. The ability to provide a 300:1 compression ratio is impressive. Durability studies (1000 cycles to 3000 psi) demonstrate good durability.
- The project team has made excellent progress within scope of an SBIR project.
- The project team has made very good progress for Phase I. This project is promising.

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated **3.0** for technology transfer and collaboration.

- Collaborations and coordination with FuelCell Energy are in place and offer a route to integrate there process with a fuel cell developer.
- Collaboration was noted but not detailed in presentation.

Question 5: Approach to and relevance of proposed future research

This project was rated **3.3** for proposed future work.

- Proposed future effort to 6,000 psi and 2 lb H₂/day are in line with the process. The project team still needs to make significant advances in capacity (kg/day) to make this work attractive.
- Plans for future work appear positioned to continue success of first two years.
- The project team should establish cost goals in addition to performance in order to focus future work.

Strengths and weaknesses

Strengths

- High compression ratio (300:1) and capability to reach pressures up to 6,000 psi.
- The project team uses a solid technical approach with good initial progress.

Weaknesses

- Low capacity is a weakness.
- The project team needs to identify how much scale-up will be required to make this technology commercially viable, and give an indication of the magnitude of development needed.
- The project team needs to establish commercial viability by assessing capital cost issues.

Specific recommendations and additions or deletions to the work scope

• The project team should discuss the potential to go to 100 to 1000 kg/day, and what barriers exist in terms of size/footprint, and size/pressure differential over membrane. The project team should provide estimates of (capacity * delta-P) verses power requirements for this concept as compared to other compressor technologies.

Project # PDP-24: Composite Technology for Hydrogen Pipelines

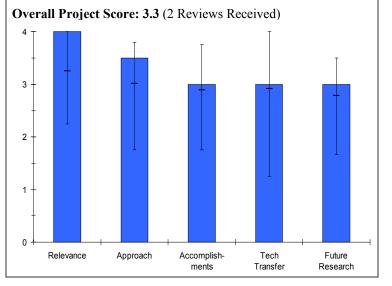
Barton Smith, Barbara Frame, and Lawrence Anovitz; Oak Ridge National Laboratory

Brief Summary of Project

Oak Ridge National Laboratory will investigate the applicability of composite pipelines in use in oil and gas gathering operations and develop a path forward for hydrogen delivery. The cost scenario shows composite pipeline will meet the DOE 2012 goals and are close to the 2017 goals. The hydrogen compatibility of pipeline materials is acceptable. The pipeline leakage rates are better than predicted.

<u>Question 1: Relevance to overall DOE</u> <u>objectives</u>

This project earned a score of **4.0** for its relevance to DOE objectives.



- Nonmetallic pipeline could meet DOE's target cost
- This project meets a critical need for high quality, cost effective pipeline distribution of hydrogen.

Question 2: Approach to performing the research and development

This project was rated **3.5** on its approach.

- The project team is investigating the application of commercially available fiber-reinforced polymer (FRP) piping for hydrogen application, which could result in identifying a low-cost alternative to steel.
- The approach shows solid engineering work built upon a strong scientific base. Go/no-go decisions have been built into the plan.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated **3.0** based on accomplishments.

- Joining technology is critical to the use of plastic piping.
- The researchers found unexpected success, (i.e., better results than they expected or could explain). Further investigations of possible explanations might lead to a short cut or a better cost model.

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated **3.0** for technology transfer and collaboration.

- There is a mix of industry and national labs, as well as a pipeline working group.
- The list of collaborators is impressive, but the presentation does not provide any information on the nature of the collaboration.

Question 5: Approach to and relevance of proposed future research

This project was rated **3.0** for proposed future work.

- Permeation and diffusion testing of liner materials would provide additional information of the suitability of FRP to hydrogen service.
- Future work should include consideration of codes and standards.

Strengths and weaknesses

<u>Strengths</u> No strengths were provided for this project.

<u>Weaknesses</u> No weaknesses were provided for this project.

Specific recommendations and additions or deletions to the work scope

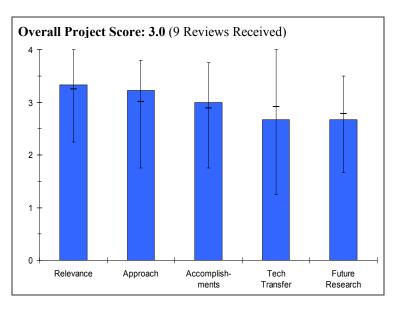
No specific recommendations were provided for this project.

Project # PDP-25: Coatings for Centrifugal Compression

George Fenske, Robert Erck, and Osman Eryilmaz; Argonne National Laboratory

Brief Summary of Project

The objective of this project is to identify and develop as required, advanced materials and coatings that can achieve the friction, wear and reliability requirements for dynamically loaded components (seal and bearing) in high-temperature, high-pressure hydrogen environments prototypical of pipeline and forecourt compressor systems. The reliability and efficiency of hydrogen compressors will depend on the tribological performance of critical bearings and seals. Knowledge of the tribological performance of materials and coatings in hydrogen environments is currently insufficient to design reliable, efficient hydrogen compressors. The rule of thumb/target is friction < 0.1.



Question 1: Relevance to overall DOE objectives

This project earned a score of **3.3** for its relevance to DOE objectives.

- The lubrication and coating issues in reducing environment such as pure hydrogen is very practical but critical work. This has wide implications and application industry-wide.
- Identification of suitable materials for use in compression in pipeline and forecourt service needed to utilize hydrogen as a motor fuel.
- Methane work is interesting, but not critical to the DOE program.
- This project is relevant only to central applications (compression <2000 psig for pipeline).
- Potentially, this research could benefit any compression applications (outside of hydrogen) to address reliability and operating costs.
- High-speed centrifugal compression critical component of delivery.
- This project supports delivery reliability goals.
- Understanding hydrogen effects on the tribological behavior of contacting surfaces is extremely important to the development of hydrogen compressors. Hydrogen effects on friction is an area totally unexplored and the current project aims at achieving exactly that: to shed light on the hydrogen effect on friction and assess the presence of surface coatings. In fact, to the best of my knowledge, this is the only project in the US exploring the interaction between hydrogen and friction. Another effort underway is in Japan, but it has not addressed coatings as of yet.
- This project seems somewhat general and needs more specific goals.
- As long as this work is transferable to higher pressure hydrogen systems, it could help reduce operating costs. The PI believes the work is transferable. If not transferable, then (in my opinion) this project only has a fair relevance to DOE objectives as large-scale centrifugal compressors seem unlikely to be deployed in hydrogen infrastructure for several years.

Question 2: Approach to performing the research and development

This project was rated **3.2** on its approach.

• The approach is sound. The testing is bench-scale simulating various parts in control environment. It would have been useful to broaden the scope to more than centrifugal compressor system.

- It also would have been useful to tie in this project with infrastructure technology validation for testing and consultation/collaboration.
- The project team is conducting tribological testing of materials used in critical compressor components.
- Approach to address reliability and H₂ embitterment related to critical components is logical.
- This project needs to have clear targets and decision criteria.
- It is not clear why there is a need to conduct tests on any gas other than hydrogen. Methane, air, and inerts WILL have different effects on compressor components.
- The project team has done good testing of materials and novel coatings.
- Scope appears to be fairly limited and focused. Materials and coatings characterization is being addressed. Future progress appears to be dependent on obtaining a new test device.
- The approach of the project is the right one. A great number of coatings are investigated at room temperature and coefficients of friction are determined. Magnitude comparisons between coefficients of friction in hydrogen and other gases are made. The effect of normal load and relative velocity (motor speed) between the contacting surfaces are addressed. The project is moving to address the effect of hydrogen on friction at high temperature. This will also be an important development, since compressor operation takes place at high temperature environments.
- The project team should focus on coatings, but needs to consider base materials as well. The team should look at whether hydrogen will diffuse through coating to base metal.
- The project team has a well thought out approach. For the amount of funding, the PI covers several topics and options.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated 3.0 based on accomplishments.

- Considering the budget issues, the program has been steadily progressing and yielding good data.
- The high-speed, hydrogen tribometer is now operational and the team is testing materials.
- The project team needs to have some real life test data on running on hydrogen.
- The project team's accomplishments have been good considering the lack of funding.
- Near-frictionless carbon (NFC) materials show great promise.
- Progress is being made in characterizing materials issues, but it is not clear that pathways to overcome barriers and meet goals are being developed.
- A great number of coatings have been investigated at room temperature and coefficients of friction have been determined. Magnitude comparisons between coefficients of friction in hydrogen and other gases have been made. The effect of normal load and relative velocity (motor speed) between the contacting surfaces has been addressed. The project has identified that in the absence of coatings hydrogen prevents oxide formation which serves as a friction reducing agent. In addition, hydrogen was found to increase wear between the contacting surfaces. An interesting result is that in some occasions (short duration tests) hydrogen was found to increase the coefficient of friction (e.g., MoS₂/Graphite) relative to air and decrease the coefficient of friction under long duration tests. Japanese researchers also reached a similar conclusion. These results are interesting and merit further study.
- Progress has been limited so far, which is understandable since the project is in early stages. Several coatings are identified for analysis.

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated 2.7 for technology transfer and collaboration.

- There are many material failures in compressor and higher pressure mechanical devices that could have benefited from this work. This is not reflective of PI's work, but rather the potential that this work could have had if it were connected to the infrastructure program.
- This project has involved a good mix of national lab and industry.
- Collaboration with Mohawk Innovative Technologies Incorporated (MITI) is a plus. The project team should also consider working industrial gas companies and compressor companies.

- Partners are bearing and coating suppliers. The extent of collaborator involvement in the development of technology solutions is not evident.
- Collaboration with MITI on oil-free centrifugal compressors is a good one. Pursuing it further will give the project industrial relevance.
- Collaboration with the University of Illinois on carrying out focus ion beam (FIB) lift-out of material to investigate cracking and embrittlement of surfaces in contact will be a high impact one. This approach is truly novel and never has been undertaken before in this area of hydrogen effects on tribology.
- Not a lot of detail was offered on collaboration and roles of the project partners.

Question 5: Approach to and relevance of proposed future research

This project was rated 2.7 for proposed future work.

- The team's future plans include coating and testing of materials.
- The team should consider looking into addressing issues related to startup/shutdown issues, extreme cold ambient temperatures, and impurities in hydrogen stream (e.g., moisture and trace H₂S).
- It is not clear that pathways to overcome barriers and meet goals are being developed. Plans focus on characterization of materials issues, but need to state how that understanding can be translated into solutions.
- The proposed FIB work is outstanding. The proposed electron microscopy of wear is indeed the next level where the project ought to be heading.
- The high-temperature hydrogen tribometer is needed to study the temperature dependence of the hydrogen effect as it relates to the tribology of the contacting surfaces.
- The team's future work should include positive displacement compression and higher pressure applications.

Strengths and weaknesses

Strengths

- The team has used a very practical and useful approach to material failure in reducing environment
- Several promising coatings have been tested side-by-side, so that valid comparisons can be made.
- The systematic study of hydrogen interaction with various coatings is a strength. Another strength is the experimentally observed relationship between the friction coefficient and the relative velocity (motor speed) of the surfaces in contact. These studies provide a valuable collection of experimental data that can be used in the study of understanding the mechanisms underlying the hydrogen effect on friction coefficients. The proposed collaboration with the University of Illinois on TEM studies of the friction/hydrogen interaction is a strong development for the project.
- The project team has a good understanding of coating technology and approach to assessing their performance in hydrogen atmosphere.
- This is a good project for studying ways to minimize hydrogen embrittlement in high-temperature, high-pressure environments.

Weaknesses

- There is a lack of connection/collaboration with infrastructure VT for samples and networking.
- The study has not advanced to the level of understanding the mechanisms that underlie the hydrogen effect on friction. However, the proposed FIB work will help toward this direction. Also, the dependence of the coefficient of friction on the relative velocity (motor speed) between the contacting surfaces has not been explained.
- The project needs better definition of applications and comparison with existing materials.
- Centrifugal compressors may not be the correct application for study at this time. More focus may need to be focused on direct displacement compression?

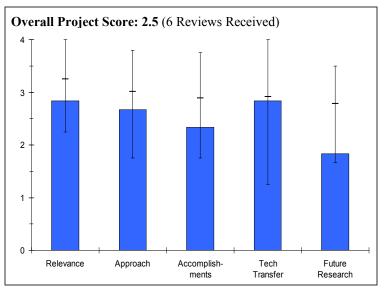
- It would have been useful to have this project and team as a material testing resource to the infrastructure projects.
- In the future, the project should be focused on understanding the mechanisms by which hydrogen affects the tribological features of interfaces.
- The project team should add direct displacement compression in scope

Project # PDP-26: Purdue Hydrogen Systems Laboratory

J. Gore, J. Patterson, R. Kramer, L. Pelter, and E. Ting; Purdue University

Brief Summary of Project

The objectives of the project are to 1) increase the production of hydrogen from the anaerobic fermentation of organic waste; 2) develop methods and techniques to maximize hydrogen production for a modular energy system for local energy production; 3) develop methods to optimize the value of the produced hydrogen for use in a modular system for local energy production; 4) develop a solar thermal energy system to pre and post process associated waste streams thereby reducing ancillary energy requirements and reducing potential environmental contamination issues for the final product; and 5) identify methods to separate hydrogen from biogas and investigate feasibility of using catalysis



to produce a marketable chemical product from the produced carbon dioxide.

Question 1: Relevance to overall DOE objectives

This project earned a score of 2.8 for its relevance to DOE objectives.

- The project objectives are very broad. The project focuses on hydrogen production from the anaerobic fermentation of organic waste; optimizing the value of produced hydrogen for use in a modular system for hydrogen production; and developing a solar thermal energy system to pre- and post-process associated waste streams; and identify methods to separate hydrogen from biogas.
- Interesting low-capital expenditure and yet energy efficient approach producing bio-hydrogen.
- This project supports the Hydrogen Program plan to identify renewable sources for hydrogen production.
- The concept of this project is to produce hydrogen through anaerobic fermentation of organic waste. This approach has been looked at and researched in the past. Without dramatic genetic engineering of existing organisms or the discovery of new organisms it is extremely remote that this could be a cost effective way to produce hydrogen. Only a fraction of the fermentation products are hydrogen.
- The anaerobic hydrogen production part in this project is relevant to DOE's objectives for biological hydrogen production. The part of "using catalysis to produce a marketable chemical product from produced carbon dioxide" is not clearly relevant.

Question 2: Approach to performing the research and development

This project was rated 2.7 on its approach.

- Purdue's approach is divided into eight areas. The approach seems reasonable considering the broad objective of the project.
- Overall, the project team uses a simple but elegant approach to producing hydrogen albeit with some kinetic limitation.
- The approach to hydrogen production by anaerobic fermentation of waste is well designed. The concept of using solar heating to supply process heat and heat for waste drying may enable the development of distributed systems which is a plus.
- No theoretical or technical basis is apparent to justify approach.

- The only somewhat novel part of this project is to try to use solar energy to pre- and post-process the waste systems.
- There is no work planned on genetic engineering of existing organisms never mind the dramatic alterations required for these organisms to have far better hydrogen production selectivity. The only work proposed to improve the hydrogen fermentation is to optimize the temperature and pH. There is prior work on this approach to hydrogen production that went beyond the work proposed for this project relative to the fermentation productivity with little success.
- The objectives include using anaerobic fermentation of organic wastes for a modular hydrogen energy system. The approach states this includes developing designs for implementation of this concept. The only thing mentioned about this is an energy balance that has been done. This concept needs a complete process design and cost analysis as well as the design and cost of obtaining enough organic waste, storage of that waste and the cost and method if getting rid of the wastes from the fermentation.
- The approaches used to maximize hydrogen production are good.

Ouestion 3: Technical accomplishments and progress toward project and DOE goals

This project was rated **2.3** based on accomplishments.

- The modular system developed for local energy production is good. Research to maximize hydrogen production through the use of a statistical experimental design is ongoing. The team has designed, constructed, and tested a solar thermal system.
- The progress towards the objective of identification of ideal process parameters is significant. However, more progress towards a continuous process (vs. batch process) will be necessary.
- There has been fermentation experimentation to try to optimize the hydrogen yield based on varying pH, temperature, and water content. Most of this type of work on anaerobic fermentation of wastes has been done by other researchers in the past.
- There has been work done with a vacuum tube solar collector and control system to determine the temperatures that could be achieved for pre and post processing of the organic waste as well as experiments to ensure this approach eliminates methanogens in the feed material and pathogens in the end waste material.
- The project began in September 2006. It did not make the planned contacts with industrial advisers until November 2008 and has had only one additional meeting with them since then. All of the other milestones shown are for 2008 and 2009. It would seem appropriate that there should have been milestones earlier during the project and that some or parts of the 2008 and 2009 milestones should have been completed earlier.
- All of the work done has been fairly elementary rather than breakthrough state of the art research.
- Progress seems slow. Two types of feedstock (food waste and distiller's grain) have been investigated. Water contents of the feedstock had opposite effect on hydrogen production, indicating that optimal parameters for hydrogen production could vary dramatically when different feedstock is used.

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated **2.8** for technology transfer and collaboration.

- Periodic advisory board meetings are held to gain input from industry (Cargill, Griffith Laboratory, BP, Advanced Power Technologies, and Innovene). Collaborative efforts with researchers at the Calumet campus are to be continued. Unfortunately the poster presenter (the PI was not present at the poster session) could not explain the nature of their collaboration.
- The project has assembled a very good advisory team and a collaboration with NREL but it is unclear from the presentation how much guidance has been used to direct the experimental program.
- The project lists several partners including Cargill, NREL, BP, Advanced Power Technologies, and Innovene. This is an impressive list and these organizations could offer a great deal to the project. However, it is not clear how these collaborations worked and were made useful other than through two advisory board meetings.
- Some collaboration was demonstrated in the project.

<u>Ouestion 5: Approach to and relevance of proposed future research</u>

This project was rated **1.8** for proposed future work.

- The future plan is fair. The project team will continue their efforts in various areas. It would be good to have some quantitative numbers to their planned future accomplishments.
- The future work seems to be a simple continuation of the current effort. There are no decision points or alternate development pathways.
- The project team plans to continue to try to optimize the fermentation by varying operating conditions, look at other inoculum, and look at other waste materials. Based on prior work in this area, it is very doubtful this can result in an attractive, cost effective approach for the production of hydrogen and energy.
- There is no cost analysis planned.
- Proposed future work is general and not focused.

Strengths and weaknesses

Strengths

- Professors' expertise and the availability of graduate students and post-docs to carry out this broad range of research are strengths. Purdue's effort will produce future hydrogen technology scientists/researchers.
- The is a simple and elegant method for making hydrogen.
- This is potentially one of the lowest capex and cheaper raw materials for making hydrogen.
- This is a solid, somewhat simple, experimental approach. The project goals are in alignment with the DOE Hydrogen Program goals.
- The one somewhat novel part of this project is to try to use solar energy to pre and post process the waste systems. The project has done work with a vacuum tube solar collector and control system to determine the temperatures that could be achieved for pre and post processing of the organic waste as well as experiments to ensure this approach eliminates methanogens in the feed material and pathogens in the end waste material.
- The idea of generating hydrogen through the anaerobic fermentation of organic waste is good.

Weaknesses

- The focus is too broad.
- The bio approach generally suffers from low kinetics and scale-up. Roughly 30% yield hydrogen (and rest CO₂) at ambient pressure may have some separation challenges.
- There is no clearly described vision for taking this technology forward into a commercially viable, scaleable process.
- The concept of this project is to produce hydrogen through anaerobic fermentation of organic waste. This approach has been looked at and researched in the past. Without dramatic genetic engineering of existing organisms or the discovery of new organisms it is extremely remote that this could be a cost effective way to produce hydrogen. Only a fraction of the fermentation products are hydrogen.
- There is no work planned on genetic engineering of existing organisms never mind the dramatic alterations required for these organisms to have far better hydrogen production selectivity to make this approach attractive for hydrogen production. The only work proposed to improve the hydrogen fermentation is to optimize the temperature and pH. There is prior work on this approach to hydrogen production that went beyond the work proposed for this project relative to the fermentation productivity with little success.
- The objectives include using anaerobic fermentation of organic wastes for a modular hydrogen energy system. The approach states this includes developing designs for implementation of this concept. The only thing mentioned about this is an energy balance that has been done. This concept needs a complete process design and cost analysis as well as the design and cost of obtaining enough organic waste, storage of that waste and the cost and method if getting rid of the wastes from the fermentation.
- All of the work done has been fairly elementary rather than breakthrough state of the art research.
- There is no cost analysis planned.
- Project goals are too broad and not focused on specific barriers.
- DOE targets for hydrogen production yield are listed. But, the yield, baseline, and benchmark of anaerobic hydrogen production are not reported. This issue was raised in previous review, but was not addressed by the investigator in this report.
- There is no consideration of cost.

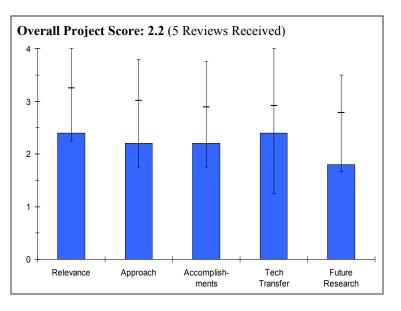
- The team should focus on increasing the hydrogen production by optimizing the anaerobic fermentation of organic waste. The team shouldn't spend effort on solar thermal energy system.
- It is recommended to have a preliminary scale-up analysis is performed and further analyze the economic potential of this approach.
- The project should focus on continuous, scaleable fermentation processes.
- Funds would be better spent elsewhere.
- This project should design a complete system including sourcing the organic waste feedstock and disposing of the remaining organic waste and do a cost estimate for the cost of the hydrogen produced and or the cost of the power produced.

Project # PDP-27: Developing Improved Materials to Support the Hydrogen Economy

Michael Martin; Edison Materials Technology Center

Brief Summary of Project

The objectives of this project are to 1) demonstrate feasibility with job creation potential; 2) cross-cutting breakthrough materials technology; and 3) stimulate nearterm manufacturing-based commercialization. Edison Materials Technology Center manages a program with a DOE Cooperative agreement in Hydrogen, Fuel Cells & Infrastructure Technologies. The program features 37 individual, topically related projects. Each project targets at least one DOE technical barrier. Successful projects generate jobs and marketable products or processes.



Question 1: Relevance to overall DOE objectives

This project earned a score of 2.4 for its relevance to DOE objectives.

- The project seems to be a random collection of tasks with no clear orientation toward the goals of the Production and Delivery Subprogram. It is unclear how these tasks were selected. More direction is needed from DOE to align the project with much needed work.
- This mix of projects associated with DOE goals that have near term commercial viability.
- Most of the projects supported by Edison Materials Technology Center (EMTEC) support DOE Hydrogen Program objectives.
- The project develops hydrogen and fuel cell technology, but seems to be focusing on helping businesses over come the "valley of death."
- The investigators are funding the state of Ohio only, which is not consistent with the DOE's nation wide mandate.
- This project, compared with other earmarks, tries to address Hydrogen Program goals. They attempt to address programmatic goals with the projects they fund, but the programmatic goals would likely have been better addressed with competitively bid projects.

Question 2: Approach to performing the research and development

This project was rated **2.2** on its approach.

- Giving money to random institutions for performing work unrelated to the Production and Delivery Subprogram is the worst possible approach. No progress can result from this.
- The team solicited projects for funding for near-term commercialization.
- There is no coherent picture as to the approach of the various projects.
- EMTEC's approach is to run solicitations and fund outside work. This is generally effective, but it is not clear why they should be running the solicitations for federal money instead of DOE. If the state of Ohio wants them to do this for state funds that is fine; however, it would seem to be more responsible use of federal money to have the DOE run the solicitations which will be funded with federal money.
- The actual project DOE is funding is a nonprofit that funds research projects. The EMTEC does not do any of their own research, so therefore personally does not contribute to overcoming the barriers to hydrogen commercialization. Some of the programs they have funded are addressing interesting questions, but direct funding of the research organizations would be more cost-effective.

Ouestion 3: Technical accomplishments and progress toward project and DOE goals

This project was rated 2.2 based on accomplishments.

- Some progress has been achieved, although the details are unclear from the presentation.
- R&D 100 award.
- No performance indicators are provided. A small number of the projects appear to be generating revenue which is a sign of technical success.
- Technical accomplishments seem to include starting two new projects- one for in-line PEM and electrolyzer monitoring and another for a multi-fuel SOFC.
- The PI reported progress from previous years as progress in the current year making it difficult to determine what has been done currently.
- The microballoon project should be ended. There are better technologies (metal and chemical hydrides) currently available.
- Their presentation only highlighted about 6 of their 38 projects. What are the other 30 projects on? What progress on the 6 projects was done in the last year? This was not clearly presented.

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated **2.4** for technology transfer and collaboration.

- There have been no collaborations outside the random institutions selected for conducting the work.
- Collaboration appears high.
- There appears to be no collaboration aside from direct support of partners.
- They seem to be working with a large number of partners.
- EMTEC brings various organizations together with their projects. They are actively pursuing commercialization of their work with industrial partners.

Question 5: Approach to and relevance of proposed future research

This project was rated 1.8 for proposed future work.

- It seems that fortunately the project is over.
- This project is complete. There is no additional funding.
- This project is 95% complete.
- The future of this project is unclear.
- Since the program ends in the summer 2009, their next steps are writing the reports for DOE as required. This is reasonable. Also, their plans to continue working towards commercialization with a few of their projects is admirable, as is their plan to apply for the R&D 100 award.

Strengths and weaknesses

Strengths

- There are some good skills from subcontractors.
- Several of the projects appear to directly support DOE Hydrogen Program objectives.
- This project has been very well funded.
- This project has many partners.
- Their effort to commercialize the projects they have funded is good. Also, some of their technical work is interesting. Partnershiping is an important part of their work and an important DOE focus.

Weaknesses

- EMTEC has made a poor selection of irrelevant tasks
- There is no basis for determination of technical success and apparently no accountability for the money given to project partners.
- This seems redundant with the federal DOE program.
- Primary participants have been limited to the state of Ohio.
- There has been a limitation to only support research being done in Ohio.

- We need to rework processes to permit more substantial DOE direction in projects like this to enhance relevance to the program
- This project should be run by the DOE Fuel Cells Subprogram. Useful "partner" projects should be continued by DOE and other projects (like the hydrogen balloon) should be ended.

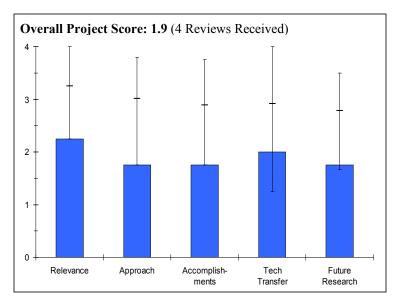
Project # PDP-28: Hydrogen Production and Fuel Cell Research

D. Yogi Goswami; University of South Florida

Brief Summary of Project

The objectives of this project are to 1) investigate the feasibility of the UT-3 thermochemical cycle theoretically and experimentally; 2) develop calcium oxide reactants with favorable characteristics and better performance; 3) conduct kinetic studies of gas-solid reactions to examine and improve cyclic stability and performance of solid reactants; and 4) lower hydrogen production cost by increasing hydrogen yield with an improved solid reactant.

<u>**Ouestion 1: Relevance to overall DOE**</u> <u>**objectives**</u>



This project earned a score of **2.3** for its relevance to DOE objectives.

- Task 1 is to investigate the feasibility of UT-3 thermochemical cycle. Task 2 is to investigate hydrogen production from biomass. Task 3 is on photoelectrochemical hydrogen production. Task 4 is on photo-catalytic hydrogen production. Task 5 on proton exchange membrane fuel cell (PEMFC) freeze degradation. Task 6 on the development of PEM electrolytes. The objectives are too broad.
- This project involves research exploring various hydrogen production paths (thermochemical, biomass, photoelectrochemical, and photocatalytic), in addition to research in PEM-based fuel cells.
- Particular research can give insight to which hydrogen-production processes are viable.
- Each of the six topics investigated have moderate relevance to DOE objectives.
- There is a total lack of focus. At this point, in its 5th year of funding, one would expect efforts having been focused on one particular and potentially promising technology. Instead, the University of South Florida (USF) group reports on a slew of technologies that include thermochemical H₂ Production, H₂ Production from Biomass, Photoelectrochemical H₂ Production, and Photocatalytic H₂ Production. These areas are obviously of relevance to DOE objectives. However, PIs contributions to-date have been meager, at best.
- For the hydrogen production part, it is not clear what they are doing. No answers to the questions given.
- This project has had no coordination with any of the DOE projects.

Question 2: Approach to performing the research and development

This project was rated **1.8** on its approach.

- UT-3 cycle has been studied for several decades. What is new here is not clear. The feasibility of the UT-3 process was done few years ago by researchers in three continents. It is not clear why are experiments are being performed to demonstrate feasibility. Are there any pitfalls in the earlier experiments? If so, the PI should explain what they were and clearly differentiate the present experiments from the past experiments. The other tasks for hydrogen production are going on in several institutions, and it is unclear how the USF approach is different from other on-going work.
- The approach is reasonable, focusing on some key gaps within each of the technologies addressed.
- The overall approach of having 6 separate research topics subdivides the efforts into small units and limits their capability to make significant progress.
- It is not clear why UT-3 cycle was selected for investigation. This cycle has been thoroughly studied in Japan and taken to the bench-scale closed loop demonstration stage. It is unclear what is it that they are doing

differently which is worth pursuing in the light of Japanese work (well over 30 papers going back to 1980). Thermal efficiency figures presented are questionable. No H2A cost analysis has been carried out for this or other hydrogen production methods investigated by the PIs.

- Again, no rationale has been given for the PIs' approach toward biomass-based hydrogen production via gasification in the presence of dolomite. The PIs reference the initial experimental studies that they carried out claiming significant improvement in hydrogen and overall gas yield in presence of sorbents. However, no gasifier data has been provided to support their claim. Information included in the poster is vague and superficial. The PIs seem to lack both understanding and knowledge required to tackle thermochemical conversion of biomass to hydrogen that is new or different than what has been done to-date or is not duplicative of already well-planed and executed effort funded by DOE.
- On photoelectrochemical (PEC) and photocatalytic water splitting the PIs present no rationale for their methods to improve performance. For example, their basis for nitrogen doping of titania for photocatalytic hydrogen production is unclear. N- and S- doping of TiO₂ (both rutile and anatase forms) have been investigated before. However, under visible light irradiation no hydrogen evolution occurs without the presence of electron donors or acceptors. Clearly, this not in accord with the DOE goal for direct water splitting using solar energy but without sacrificial reagents consumed.
- In general, the approach is still poorly defined and lacks sufficient detail. It is promising too much and unlikely to deliver.
- There is no clear project management organization.
- As noted above, most of the hydrogen production schemes attempted above have already been thoroughly studied.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated 1.8 based on accomplishments.

- There are six different tasks in this project. Technical accomplishments for each tasks is listed separately. It appears that this team has met their objectives.
- Task 1 (UT3 Thermocycle): Efficiency improvements are gained via heat recovery. However, it is not clear how thermal efficiencies are calculated. Hydrogen production must be about 284 kJ/mol. It is unclear what 593.5 kJ/mol refers to.
- Task 2 (hydrogen-production from biomass): No hydrogen yields, capital cost, or gasification efficiencies presented for this specific hydrogen-production process.
- Task 3 (photoelectrochemical hydrogen production): Improvement in window p-layer doping is stated but needs to relate Voc to efficiency.
- Task 4 (photo-catalytic hydrogen production): Optimum doping concentration profile is not given.
- Task 5 (PEMFC Freeze Degradation): The team needs repeat data on freeze/thaw testing to make a conclusion. The amount of water leading to degradation in PEM needs to be quantified during freeze/thaw cycling.
- Task 6 (Development of PEM Electrolytes): No conductivity vs. relative humidity data is given for membrane. This data is critical to make a reasonable comparison for membranes used in PEM-based fuel cells.
- Thermochemical H₂ Topic: UT-3 thermochemical cycle appears to be low efficiency and complex. One stated goal was to "improve the solid reactant's cyclic life, reaction rates and conversion". There is no evidence any of this was done just a lab experiment.
- Biomass Topic: Objectives are lengthy and grand, but actual work conducted appears basic and unremarkable.
- PEC Topic: Significance of achievements is not clear.
- Photocatalytic H2 Topic: Nitrogen dopant of TiO₂ appears to achieve a significant improvement in optical properties. Testing in an actual device should be conducted to quantify energy capture improvement.
- PEM Freeze Degradation Topic: Useful finding that blowing dry air over the membrane for 10 minutes prior to shutdown to remove water effectively allows low/no degradation freezing, but this finding has already been published by others.
- PEM electrolyte Topic: SPEEK membrane was prepared but not yet tested.
- The project team has very little to show after 5 years.
- The project team has made few publications.

<u>Ouestion 4: Technology transfer/collaborations with industry, universities and other laboratories</u>

This project was rated 2.0 for technology transfer and collaboration.

- The nature of collaboration was not explained. The mandatory slide on collaboration is missing.
- The collaboration between partners is not clearly defined.
- Collaboration appears to be limited.
- There is no evidence of broad collaboration with other DOE funded projects.

Question 5: Approach to and relevance of proposed future research

This project was rated 1.8 for proposed future work.

- Considering the broad scope of work, the plans for the future appear to be reasonable. It is impossible to judge the plans for the last two tasks (on PEM fuel cell).
- Future and current work needs to focus more on overcoming DOE barriers stated for each of the tasks.
- Some new avenues are planned on improving photocatalytic efficiencies.
- Improvement in photocatalytic efficiency of N-doped TiO₂ by Ag metal ion doping is not novel. The project team should check literature.
- The future plans lack of specificity, rationale, and detail to be compelling.
- This project is unlikely to meet DOE hydrogen production goals because very little has been accomplished as of 2005 start date.
- Statements about future activities were vague with no quantitative mileposts as to how the project will meet the DOE H₂ production targets and objectives.
- No H2A cost analysis of the production schemes has been mentioned.

Strengths and weaknesses

Strengths

- Knowledge and experience of the team members. Long list of publications/presentations.
- This project's strength is in involvement with several hydrogen production technologies.
- Each of the topics has worth, but having so many topics dilutes focus.
- None.

Weaknesses

- FY08 & FY09 funding numbers were not provided and therefore it is difficult to judge their accomplishments/performance. Nature of collaboration with partners is missing. The project focus is too broad.
- Discussion is needed on how DOE barriers are being overcome.
- The project team should interact with companies familiar with fuel cell testing and evaluation.
- The large number of mostly independent topics being investigated makes for an unwieldy presentation.
- There's no coherency and focus.
- Too many areas dilute the PIs' efforts and slow meaningful progress.
- Management and partnership have been very weak.
- The expertise of the PIs in all of these areas is highly suspect.

- The UT-3 process task can be dropped.
- It would be beneficial to make comparisons between the varying hydrogen production technologies (thermochemical, biomass, photoelectrochemical, photocatalytic), with respect to system efficiencies, capital and hydrogen production costs.
- The project team should focus efforts on a smaller number of topics to achieve more substantive progress.
- The budget for the actual activities being reported should be listed.

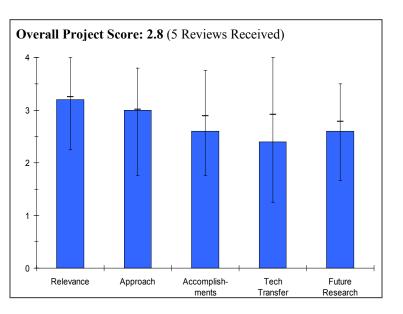
- The project team should narrow production scope to no more than one technology area that complements, rather than poorly duplicates other DOE funded activities.
- The project team should develop meaningful partnerships with experts in the field.
- The project team should let H2A cost analysis guide their hydrogen production R&D path and related decisions.
- Project management and coordination needs to be improved.
- The PIs should attend other PIs' presentations and network.

Project # PDP-29: Integrated Hydrogen Production, Purification and Compression System

Satish Tamhankar; Linde North America Inc. Tony Boyd and Ali Gulamhusein; MRT Mark Golben and David DaCosta; Ergenics Corp.

Brief Summary of Project

The overall objective of this project is to develop an integrated system that directly produces high-pressure, high-purity hydrogen from a single integrated unit. The specific project objectives are to 1) verify feasibility of the concept, perform a detailed techno-economic analysis and develop a test plan; 2) build and experimentally test a proof of concept (POC) integrated membrane reformer/metal hydride compressor system; 3) build and advanced prototype system with modification based on the POC learning and demonstrate at a commercial site; and 4) complete final product design capable of achieving the DOE 2010 hydrogen cost and performance targets.



Question 1: Relevance to overall DOE objectives

This project earned a score of **3.2** for its relevance to DOE objectives.

- The overall objective of this project is to develop an integrated system that directly produces high-pressure, high-purity hydrogen from a single unit. This project is in its first phase. The objective of Phase I is to verify the feasibility of the concept, perform a detailed techno-economic analysis, and develop a test plan. Another objective of Phase I is to build and experimentally test a POC integrated membrane reformer/metal hydride compressor system.
- This project has very high relevance to DOE objectives.
- An integrated production, purification and compression system has the potential to provide an efficient systems solution.
- An integrated system for hydrogen purification and compression is relevant to the DOE program goals.
- This project is relevant to DOE's forecourt hydrogen production program goals.
- This project does not address the greenhouse gas footprint of the technology and as such only partially meets DOE's overarching objectives for clean and renewable hydrogen production.
- Hydrogen from natural gas or other hydrocarbons using a Pd membrane reactor integrated with a metal hydridebased thermal compression device is a novel idea and has relevance to DOE's near term (transitional) hydrogen production and delivery objectives.

Question 2: Approach to performing the research and development

This project was rated **3.0** on its approach.

- The approach is to combine the membrane reformer developed by Membrane Reactor technology with the hydride compressor developed by Ergenics in a single package. This approach reduces capital cost and increases efficiency compared to conventional fuel processors. The membrane reactor technology and the hydride compressor are shown to work in separate tests. This team is focusing on issues involved in integrating these two technologies.
- Experimental proof-of-concept module is well suited to this project.

- It is not clear whether the engineering problems are simpler (solvable) when the processes are separated. A slide providing data on the engineering on the individual components would have been helpful.
- The team has a good overall approach, including POC for both the purification and compression system components, as well as the H2A analysis for evaluating cost effectiveness.
- The approach is credible as it combines good engineering with pilot scale testing.
- The team used innovative engineering of the metal hydride thermal compressor.
- The team used a methodical approach to the complex integration of the membrane reactor and multi-stage metal hydride thermal compressor.
- The approach is guided by cost analysis to reduce system components and improve reliability.
- It appears that PIs may have moved too quickly from optimization of individual subsystems (i.e. membrane reformer and thermal compressor) to integrated stage. Results to date point to possible interface issues affecting the overall performance of the integrated system.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated **2.6** based on accomplishments.

- Auto-thermal fluidized bed membrane reformer was tested. Membrane was operated at 550C and 25 bar. The team successfully tested a 15 micron thick membrane. Membrane foil quality diminished during testing. Hydrogen purity was an issue. After initial operation, leakage was observed in the metal hydride compressor.
- The project had moderate deficiencies in all areas:
 - Reactor: reduced catalyst activity, relatively low-methane conversion.
 - Membrane: permeance met expectations but leaks due to manufacturing quality led to low H₂ purity.
 - Compressor: leaks in tubing due to manufacturing defects led to substantially degraded performance.
- However, also had moderate successes:
 - Reactor: demonstrated tolerance to thermal cycling. Demonstrated production of high-purity gas.
 - Integration: demonstrated integration of reactor with compressor using waste heat to drive hydride compressor.
- The team has done solid work. The economics are promising but preliminary. More detailed information is needed for a real evaluation, but this is a good start.
- Progress has been on schedule, though unexpected problems in hydrogen leakage and performance degradation were encountered. The program appears to be adapting to the setbacks, and proposing reasonable paths forward to resolve the issues.
- Consider third party, unbiased testing and evaluation of the integrated system.
- Long-term verification testing needs to be conducted.
- There are no discussions with respect to operational safety issues, failure modes and consequences.
- What is the effect of impurities in the reformate/permeate on the metal hydrides used?
- No data have been presented for the factors influencing hydride bed operation and long-term stability. In other words, where is the weak link in the integrated chain of interconnected sub-systems and components? Can metal hydride beds be regenerated, if needed? If so, how?
- What is the effect of mercaptans and other sulfur organics on the long-term stability and conversion efficiency of the membrane reformer? Can landfill gas be used in this system? If so, what is the effect of silanes?
- PIs have shown continuous operation of a multi-stage, dual-line hydride bed heat exchanger successfully, albeit for a relatively short period of time. PIs report limited operational data to draw a solid conclusion as to the viability of this system, under extended operation.
- PIs need to address the issues related to Pd membrane stability, startups/shutdowns, and the ability to recover hydrogen from permeate and retentate steams to allow for 100 bar pure hydrogen delivery.

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated **2.4** for technology transfer and collaboration.

• MRT and Ergenics are key partners in this project. It is not clear what the other partners (University of British Columbia, National Research Council, and Noram Engineering) did for this project. The roles of partners were not presented.

- There appears to be very tight contact/collaboration between team members. The extent of collaboration with others in not known.
- It would be nice to see a formal university partner to ask questions around the periphery of the project and perhaps introduce a little more imagination.
- It is not entirely clear whether additional collaborations within industry or with academic institutions would be beneficial in helping to solve technical issues encountered.
- Good combination of industrial and university collaborators.
- There are no indications that the team has or has had interactions with other projects within this DOE program.
- Eventually need a third party, unbiased testing and evaluation of the integrated system performance and costs.

Question 5: Approach to and relevance of proposed future research

This project was rated 2.6 for proposed future work.

- Reduced catalyst activity, hydrogen purity, and MHC performance will be addressed during rest of FY09. Go/no-go decision will be reached by June 2009 (i.e. next month) regarding the next phase. Based on the information presented, to the team will probably not be in a position to make this decision.
- The future course of action is not well defined.
- A solid path forward was identified.
- The future work was well laid out for project continuation.
- The team presented clear future plans and go/no-go decision points.
- Go/no-go decision on next phase should also consider a safety audit of the system and detailed "what if" protocol.

Strengths and weaknesses

Strengths

- This is a strong team involving Linde, MRT, and Ergenics. The idea of combining membrane reactor with MHC is very good.
- The biggest project strength is its approach: experimental demonstration of an integrated reactor/membrane/hydride compressor is the appropriate course of action.
- Overall, and interesting approach to integration of hydrogen purification and compression; and an effective project for demonstrating the proposed system.
- Good transitional device for forecourt hydrogen production.
- Good collaborative work and mutually beneficial partnerships amongst participants.
- Innovative hydrogen compression engineering.

Weaknesses

- There is no clear plan to address the problem of reduced catalyst activity. It is unclear how they are going to improve the MHC performance? Membrane durability is an issue.
- Substantial problems in each of the major systems: catalyst activity, pin-hole free membranes, hydride leak-tightness.
- The cost analysis is weak. More needs to be done to support the cost projections.
- The problems encountered with hydrogen leakage and with unexpected performance degradation need to be better elaborated in terms of proposed solutions for future work
- Testing time is limited.
- System sensitivity to impurities is a weakness.
- Pd membrane and metal hydride materials stability and robustness are key to project success.
- The integrated system is more complicated.

- The team should have an independent third party look at the H2A results and try to use membranes made by Pall Corp.
- The hydride compressor is good in concept but, in additional to it leaking, seems to consume substantial energy thereby reducing the overall system efficiency. A careful examination of the hydride compressors net benefit to the system should be conducted. It should be compared to a well-understood/low-risk mechanical compressor to see if an advantage is really achieved.
- Cost analysis needs to be enhanced. My confidence in their estimates is low. The team should show much more detail/assumptions.
- The team should update H2A analysis with the most current estimates and clearly identify pathways to solving the encountered problems in leakage and reduced activity.
- The team should consider adding a safety audit of the system and detailed "what if" protocol.
- The team should identify sources, fate, and effect of all known and potentially present impurities in the feedstock on all subsystems in the hardware chain.

Hydrogen Storage Summary of Annual Merit Review Hydrogen Storage Subprogram

Summary of Reviewer Comments on Hydrogen Storage Subprogram:

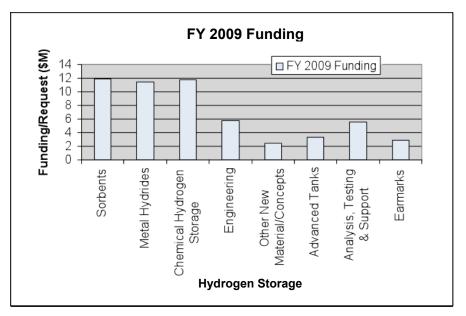
Reviewers indicated that the Hydrogen Storage subprogram area is focused, well managed, and effective; and has a diverse R&D portfolio addressing the technical system targets. Significant advances have been made for the various material systems, bringing materials closer to the vehicular system targets of the DOE Hydrogen Program. Effective communications and coordination between DOE, Center of Excellence (CoE) managers, and CoE partners, has allowed for cross-fertilization of ideas and focus of technical efforts. Although the subprogram strategy, goals, and achievements were well defined, some reviewers suggested that the remaining challenges were not adequately addressed and that greater attention to critical issues, obstacles, and challenges still facing each of the specific materials technology areas (i.e., chemical hydride, metal hydride, and sorbents) is needed to put progress to-date into proper context. It was also suggested that a "lessons learned" and gap analysis be performed to better assess progress made and the status of the portfolio. Some reviewers expressed concern regarding the 2010 Congressional budget request for the subprogram and the lack of clear future plans for Storage R&D.

In general, the reviewers thought that the revised vehicular performance targets, based on current fleet data and future projections, are an improvement and that re-evaluation of the hydrogen storage system targets was essential to both the real and perceived success of the Hydrogen Program. Some reviewers still had questions regarding the relevancy of the targets to the existing technical and economic challenges and recommended that further revisions be considered. The reviewers also urged DOE to identify storage systems and performance targets for early market applications.

Finally, the reviewers stressed the importance of the Hydrogen Storage Engineering CoE in providing feedback to the material research community regarding materials' characteristics critical for hydrogen storage and effective system design. This CoE can also provide valuable input on the important materials parameters in addition to gravimetric and volumetric capacities (i.e., heat capacity, thermal diffusivity/conductivity, packing geometries, agglomeration effects, etc.). Continued interactions between the Materials CoE partners and the Engineering CoE were strongly encouraged, and it was recommended that data generated to-date in the subprogram be properly recorded and archived to ensure conservation of the data and results from the Materials Centers.

Hydrogen Storage Funding by Technology:

The Hydrogen Storage subprogram portfolio remained focused in FY 2009 on materials-based R&D for onboard transportation applications. The primary goal has been development and demonstration of commercially viable hydrogen storage technology to enable greater than 300-mile vehicle driving range, while meeting safety, vehicular packaging, and cost and performance requirements. A new goal introduced in FY 2009 is to develop storage options to facilitate deployment and market growth of fuel cell power systems for early market applications. R&D efforts remained focused on applied, target-oriented research of materials systems including high-capacity metal hydrides, chemical hydrogen storage carriers, and high-surface area adsorbents with the potential to meet the vehicular technical targets. In addition, the subprogram continued to support advances in physical storage (e.g. compressed hydrogen gas) for nearer term applications. The initiation and funding of the Engineering CoE in FY 2009 reflects a growing programmatic emphasis on engineering and systems integration issues. The following chart illustrates the appropriated funding in FY 2009 for each major activity.



Majority of Reviewer Comments and Recommendations:

The Storage portfolio was represented by 34 oral and 46 poster presentations in 2009. A total of 60 projects (32 presentations and 28 posters) were reviewed. In general, the reviewer scores for the storage projects were good (1=poor, 2= fair, 3=good, 4=outstanding) with scores of 3.8, 3.0 and 2 for the highest, average, and lowest scores, respectively. The projects were reviewed by two (for one project) to six reviewers each with an average of 4.3 reviewers per project. Reviewers remarked favorably on the coordination and management of the Storage Materials Centers of Excellence. It was suggested that the Materials Centers focus on summarizing results, trends and lessons learned to-date, and on making recommendations for future hydrogen storage materials R&D. Key recommendations and major concerns for each project category are summarized below.

Chemical Hydrogen Storage: The chemical hydrogen storage R&D is conducted with a well-balanced approach, considering both material aspects and engineering issues, with good coupling between theoretical modeling and experimental activities, and is well focused on many DOE vehicle targets and technical barriers including cost. The chemical hydrogen storage material R&D has made good progress toward addressing issues related to ammonia borane (AB) by reducing foaming and release temperature, as well as increasing capacity and the kinetics for the release of hydrogen during the stoichiometric reaction. Continued R&D is required to further improve these AB release parameters as well as to address hydrogen purity, heterogeneous catalysis, liquid fuel formulation, and cost effective first fill. Recommendations were made to continue the down-select process with a focused effort on winning strategies, and to coordinate with the Engineering CoE to address onboard system requirements. Significant progress was made in AB regeneration chemistry and the associated cost analysis where separation steps were identified as the dominant cost factor and new approaches were developed to address the issue. It was recommended to further advance and complete the AB regeneration section be updated based on worldwide adoption of fuel cell vehicles.

Advanced Metal Hydrides: The overall goal of metal hydride materials applied research is to develop materials that can be charged with hydrogen on board the vehicle at conditions amenable to the vehicle environment. Key barriers to this goal are the hydrogen charge and discharge kinetics at acceptable temperatures and pressures and the thermodynamics of the reactions, which directly impact the net available capacity of the material. Since most of these materials may be embodied in a system as a packed powder, volumetric capacity of the material is also an issue. The Metal Hydride Center of Excellence

(MHCoE) was considered by the reviewers to be a well-managed and coordinated group of quality researchers focused on relevant research to the Hydrogen Storage subprogram. The MHCoE was commended for their flexibility and adaptability in refocusing on promising materials while moving away from less promising materials. However, the reviewers felt even further materials down-selection could be useful in some projects. In addition, reviewers recommended more communication and coordination between the MHCoE and the independent research projects on advanced metal hydrides to minimize duplication and maximize effectiveness of the program. The reviewers found the use of computation modeling to aid in materials research direction well coordinated and effective. The computational modeling efforts were also praised for incorporating gas phase species into their modeling. With the limited time remaining for most of the projects, it was recommended that the projects focus on the materials and activities that are expected to yield the most promising results and reduce efforts in higher risk areas.

Sorbent Materials: The goal of sorbent applied materials R&D is to develop materials with high hydrogen volumetric and gravimetric reversible net available capacities at closer to ambient temperature and at moderate pressure. The general approach is to identify and design (often via theoretical modeling) high surface area porous materials with increased hydrogen uptake capacities and higher binding energies for molecular hydrogen that will enable storage above cryogenic temperatures (e.g. 77K). The DOE portfolio for sorbent materials includes the Hydrogen Sorption Center of Excellence (HSCoE) and independent R&D projects. A number of new sorbent materials (i.e., various polymers, MOFs, COFs) have been synthesized and their hydrogen uptake capacity characterized. The reviewers noted that while many of these materials do show promise, issues still remain with achieving "net available" volumetric and gravimetric capacities that can meet DOE vehicular targets. "Net available" means that the temperature, pressure, energetics, and transient delivery/uptake rates are taken into account to determine the amount of fuel available to the power plant. Furthermore, retaining these properties at closer to ambient temperature/moderate pressure has proven difficult, as hydrogen/adsorbent site binding energies remain too low. Reviewers also pointed out the limited success for either or both the syntheses and experimental performance verification of improved storage from several materials that had theoretically predicted high capacities. The reviewers suggested more inputs from experimental results should be incorporated into the theoretical efforts in order to improve the latter's predictive potential. The reviewers remarked that while members of the HSCoE have provided some significant new theoretical insights into the mechanisms for hydrogen spillover behavior associated with selected metal dopants (i.e., Pt or Pd), issues remain with reproducibility in experimental studies of this phenomenon with often contradictory observations from different groups on hydrogen uptakes and the kinetics for adsorption and discharge. The reviewers emphasized that integrated efforts should be made by the researchers to prepare and process samples that can provide reproducible measurements of the reactions during hydrogen spillover to establish viable mechanisms that may enhance reversible uptake and increase the kinetics. The reviewers recommended that instead of using idealized (i.e., single crystal) densities to estimate material volumetric capacities greater efforts be made to consider powders or compacts/monoliths of porous sorbents as practically configured for vehicle storage. Down selection of sorbents from further evaluation should be based upon criteria rooted in laboratory measurements rather than upon theoretical predictions that had not been previously validated by experiments.

Advanced Tanks: The advanced tank R&D is conducted by a small but diverse group of researchers from industry, universities, and at national laboratories. Gradual progress has been made in conventional high-pressure tanks toward reducing cost, weight, and volume of the systems. However, this advancement has not been communicated in the clearest manner possible. Although Lawrence Livermore National Laboratory has made good technical progress in all the areas mentioned above, there are still concerns with respect to energy use, specifically for liquefaction. It was recommended that more than one OEM partner be included in this effort.

Analysis, Testing and Support: Reviewers noted that Argonne National Laboratory and TIAX LLC have made good progress this year. They are finalizing reports on systems that have been under evaluation since the beginning of the program. As in past years, the reviewers commented on the value of this work to an understanding of the relative merits of materials with respect to the requirements of the entire storage system. This work also allows screening of materials before the physical integration stage. This year the Engineering Center initiated complementary analysis work on integrating storage and fuel systems.

The National Testing Laboratory at Southwest Research Institute was considered to be essential for the National Hydrogen Storage Project; however the reviewers felt that more effort is needed to develop methods to verify extraordinary results, especially related to "spillover" effects and to understand the cause of irreproducible or spurious measurement results.

Notes on Storage Report Structure:

Chemical Hydrogen Storage

ST - 15 to 21 and STP - 17 to 20 are partners in the Chemical Hydrogen CoE STP - 21 is an independent project

Sorbent-based Materials and Other New Materials and Concepts

ST - 22 to 31 and STP - 25 to 29 are partners in the Hydrogen Sorption CoE ST - 32 to 33 (Sorbents) and STP - 2 and 3 are independent projects

Advanced Metal Hydrides

ST - 1 to 11 and STP - 36 to 42 are partners of the Metal Hydride CoE STP - 44 is an independent project

Advanced Tanks ST – 34, STP – 1, and STP – 4 (Advanced Tanks Projects)

Analysis, Testing and Support ST – 12 to 13, STP – 30 and STP – 45

Cross-Cutting STP – 22 to 23, 43, 46

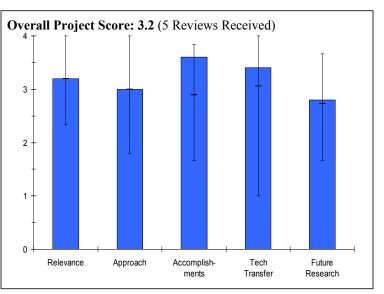
Project # ST-01: Metal Hydride Center of Excellence

Lennie Klebanoff and Jay Keller; Sandia National Laboratories

[NOTE: This presentation was to evaluate the entire Metal Hydride Storage Center of Excellence as a whole. A separate review form was used and can be found in Appendix C.]

Brief Summary of Project

The overall objective of the Metal Hydride Center of Excellence (MHCoE) is to research, develop and validate reversible onboard metal hydride storage materials and systems that meet the 2010 DOE system targets for hydrogen storage, with a credible path forward for meeting the 2015 DOE storage targets. The approaches to meet the hydrogen capacity targets of 6 wt%. 45 g·H₂/L volume density are to 1) synthesize and characterize hydride materials with high hydrogen capacity and favorable thermodynamics and 2) use stateof-the-art theory to guide the materials discovery effort. The approaches to meet the charge/discharge rate target of a 3-min system fill (5 kg) are to 1) develop materials



that are fully reversible, 2) develop catalysts that aid reversibility, 3) assess nanoengineering promotion of kinetics, and 4) investigate the role of contamination on reaction rates. The approach to meet the hydrogen purity target of 99.99% is to assess release of NH_3 , B_2H_6 and other volatile species from metal hydrides during desorption and cycling. The approach to meet the cycle life target of 1,000 desorption/adsorption cycles is to investigate durability of materials, cycling behavior, effects of contaminants, structural stability, and release of volatiles.

Question 1: Approach to performing the R&D including Center Management

This project earned a score of 3.2 for its approach to R&D and CoE management.

- The CoE is generally well managed. A lot of activities are directed to address the regeneration/reversibility issue of the materials.
- The overall impression of this CoE is good but not perfect.
- There are good connections between theory and experiment.
- The down-selection process is very impressive, but there are still a large number of materials being studied perhaps too many?
- The CoE is well focused on the many DOE targets and barriers.
- The CoE does not seem to be focusing enough on materials cost. This is not referring to systems cost, which is the proper domain of the new Engineering CoE; but to the absence of preliminary cost studies on the metal hydride materials being studied in this CoE by the materials experts that are best suited for this work, at least in a preliminary sense.
- The CoE appears to be well managed and has adapted over the years of the center's operation as progress has been made on various materials. Essentially, there have been continuous down-selections of different materials during the project.
- New center members have been effectively included. Extensive utilization of new member, UTRC, is particularly noteworthy.
- This is mostly basic research.
- The industrial partnership(s) is insufficient.
- Scalability of studied materials has not been established.

<u>Ouestion 2: Technical accomplishments and progress toward DOE goals</u></u>

This project was rated **3.0** on its accomplishments and progress.

- There have been some interesting basic results especially on boron-based materials.
- DOE targets have not been met yet; more work is needed to meet them.
- This task may require refocusing on alternative hydride systems such as carbon hydrides.
- The overall CoE activities showed good progress in overcoming the technical barriers.
- Very good technical progress has been made on many fronts.
- The down-selection process was nicely done.
- Good progress has been made this last year.
- Material properties for reversible materials to date continue to be problematic (e.g., enthalpy too high, kinetics slow, release of contaminant phases, less than complete rehydriding and/or loss of capacity).
- Good productivity based on papers and presentations.

Question 3: Proposed future research approach and relevance

This project was rated **3.6** based on future plans.

- Future work plans build on past progress, but more should be done to meet the DOE targets.
- With the remaining CoE life, the proposed future research is reasonably good; however, there is still no welldefined pathway to achieve DOE targets.
- The CoE has only a limited time remaining. In that sense, the list of remaining work is the best it can do. It cannot all be completed in time.
- Good planning.

Question 4: Coordination, collaboration and effectiveness of communication within the CoE

This project was rated 3.4 for collaboration and communication within the CoE.

- Collaborations within the CoE are excellent. This has improved over the years and has continued to improve this past year.
- Good coupling between modeling and experimental efforts in certain areas.
- Center partners have established reasonably good coordination within the CoE.
- The CoE seems to collaborate well internally, but it is hard to fully see this from the Director's presentation.
- Are the CoE members adequately open to each other? Are there any IP problems or conflicts that limit communication?
- It is not clear how much of the progress is synergistic (i.e., from internal CoE communications and collaborations rather that individual efforts). Is it clear to the CoE management that the overall progress of the CoE is more than the sum of the individual parts?

Question 5: Collaboration/Technology Transfer Outside the CoE

This project was rated 2.8 for collaboration and technology transfer outside the CoE.

- National and international collaborations seem to be very extensive and valuable, including joint
- publications.
- Good interactions with outside collaborators in certain areas (e.g., modeling).
- Limited interactions with other CoE.
- The Metal Hydride CoE contribution to the newly formed Engineering CoE will be critical.
- Industrial collaboration is limited.
- It is not clear how the progress outside of the CoE is filtered through the center activities

Strengths and weaknesses

Strengths

- Interesting basic research especially in the area of the solid-state chemistry of metal borohydrides.
- The CoE structure and materials down-select process are strengths.
- This is an excellent group of technically skilled individuals.
- This is a strong research team whose members complement one another in certain areas.

Weaknesses

- The focus has changed several times during the last few years. Unfortunately, these changes did not conclude in generating sufficiently new ideas.
- New approaches and non-trivial ideas could really benefit the research at the CoE.
- Poor collaboration with the industry is definitely a weakness.
- It is not clear how progress outside of the CoE addressing the same issues as the CoE is linked to the CoE plan.
- The material down-select criteria should be discussed with the Engineering CoE in order to incorporate the engineering input.
- The group may be a bit large for the most effective communication and interaction.

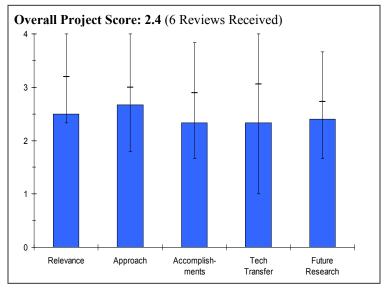
- Research on hydride materials as hydrogen sources should continue.
- Reconsider research directions toward non-conventional ideas and new approaches, which may include hydrogen storage in organic materials, combining photo-chemical generation of hydrogen with hydrogen storage, etc.
- Review the previous materials that did not make the down-select criteria based on the revised DOE target.
- Other than more cost thinking, no suggested changes for the duration of the effort.

Project # ST-02: Thermodynamically Tuned Nanophase Materials for Reversible Hydrogen Storage: Structure and Kinetics of Nanoparticle and Model System Materials

Bruce Clemens; Stanford University

Brief Summary of Project

The objectives of this project are to 1) develop a fundamental understanding of metal hydride reaction kinetics, 2) develop an understanding of metal hydride nanostructure thermodynamics, and 3) develop an understanding of metal hydride structures during phase change. Little is known about the kinetic mechanism present in many promising metal hydride material systems including Mg, Mg₂Si, Li₄Si, NaAlH₄, LiBH₄+MgH₂, etc. In order to improve the kinetics for any of these metal hydride systems, a sound understanding must be developed. Many systems suffer from inappropriate thermodynamics (equilibrium pressure) (e.g., Mg, Al), and continuum modeling suggests that reaction



thermodynamics should be modified by reducing particle size to the nanometer regime. Material structure can play an important role in reaction kinetics, especially during solid-state phase transformations such as those in metal hydride reactions. Understanding the interplay between material structure and reaction kinetics may provide insight on how to successfully engineer new materials with improved kinetics and storage properties.

Question 1: Relevance to overall DOE objectives

This project earned a score of 2.6 for its relevance to DOE objectives.

- The project is completely in line with and in full support of the DOE objectives. It aims to develop a fundamental understanding of reaction mechanisms in metal hydride transformations. It addresses the kinetic limitations that hinder the performance and hydrogen storage potential of metal hydride systems. This is of great value for the design of new materials with improved kinetics and storage properties with potential to meet the targets for the Hydrogen Program.
- One of the goals of this project is to develop an understanding of metal hydride reaction kinetics. This aligns well with DOE's goals because kinetics are an important aspect of the hydrogen storage element.
- Storage targets/barriers addressed include stored hydrogen gravimetric/volumetric capacity and reversibility.
- From a fundamental point of view, the work would help develop an understanding of the kinetic limitations of existing hydrogen storage systems; however, from an applied point of view, it does not strongly relate to the objectives because it utilizes highly ordered systems that might not relate to the bulk (real) materials.
- This project seems to be more like a Basic Energy Sciences (BES) effort. Focus on conventional metal hydrides has no direct connection to the complex hydrides being studied in the rest of the MH CoE. (Complex hydrides are not interstitial hydrides, at least some fundmental elements of the kinetics are expected to differ significantly between these materials.)
- This work is more fundamental in nature compared to the work of the rest of the CoE that is focused on developing high capacity hydride materials.
- Specific important contributions to the CoE efforts have not been demonstrated.
- This project does not appear to be well integrated into other CoE activities.

Question 2: Approach to performing the research and development

This project was rated **2.7** on its approach.

- The approach is well thought out, concentrating on modeling geometrically simpler systems and coupling theory with strong experimentation and verification. This work can contribute to a better understanding of the interplay between structural changes in materials and reaction kinetics and their limitations during hydrogen charging and discharging.
- In general, the approach seems to be well thought out; however, it is not clear why the PI is using thin films of Mg coated with Pd to model hydrogen absorption by Mg. Mg, more typically, might have an oxide coating on the surface, not Pd.
- The project develops the understanding of metal hydride reaction kinetics and thermodynamics at the nanostructure level and phase change/structure relationships.
- The project team employs microbalance, X-ray diffraction, and synchrotron X-ray methods.
- Experimental measurements and modeling are combined to resolve issues affecting hydrogen storage capacity, hydrogen diffusion limitations, and reaction kinetics during charge and discharge.
- Generally, work is on simple systems (i.e., single metal and binaries); work on more complex systems is planned.
- For a basic understanding it's definitely useful, especially for Mg-based materials; however, when it comes to more complex systems (i.e., Mg alanates), a thin film approach might be difficult based on the current results.
- Although the stated purpose of this project is to gain an understanding of hydride reactions and properties, the work has focused on thin films that have not been shown to be necessarily representative of other hydride structures.
- Work was continued on simple systems (e.g., MgH₂), which are very different materials compared to the complex hydrides studied by the rest of the center.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated 2.6 based on accomplishments.

- The project team has shown a satisfactory degree of accomplishments and good progress. The team developed model systems for seeing the hydrogenation reactions and successfully identified and modeled the hydride formation kinetics. This included determining the size of the critical dimensions for the structures (threshold) in order to improve kinetics and avoid the activation of a diffusion controlled hydride growth. Equally encouraging are the results from the quartz crystal microbalance (QCM) experimental setup while the neutron reflectivity data should be throwing more light into the thin film hydride growth model.
- The PI was successful in developing a model to describe the hydriding kinetics. This model needs to be backed up with further studies.
- Work on Mg₂Si showed that H₂ uptake is not H₂ diffusion limited, but rather that it is limited by Mg and Si diffusion.
- The Mg-Al system seems to be H₂ diffusion limited; Mg/Al layers inter-diffuse resulting in complex superlattice diffraction.
- The model was further developed to investigate hydride growth kinetics; application to experimental data indicates that there is a critical dimension (<120 nm) to avoid diffusion control. Examined transition from interface to diffusion limited growth.
- Observed loss of solid phase epitaxy on cycling for Mg/MgH₂ system.
- Postulated that for metal hydrides it is necessary to shift thermodynamics to add relative stability to metal phase. Initial attempts to demonstrate the effect with nano-level films were made. So far, no changes in thermodynamics.
- For Mg-Ti, a 10-fold increase in P_{eq} was observed with Ti addition.
- The neutron results with NIST are just now showing interesting results. What are they?
- There is one paper in press.
- For the MgH₂ system, this is a very good study and results.
- The publication of results has not improved since last year only one paper is mentioned as being in press after 4.5 years of effort.

<u>Ouestion 4: Technology transfer/collaborations with industry, universities and other laboratories</u>

This project was rated **2.6** for technology transfer and collaboration.

- The PI fully explores links within the MHCoE and gains access to unique facilities and expertise.
- Collaborations are reported with two CoE partners, but it is expected that they would have had a few more collaborators because this project is part of the MHCoE.
- Collaborators are listed as being HRL Laboratories, the University of Pittsburgh, and NIST.
- There is nothing significant shown regarding work with HRL Laboratories and the University of Pittsburgh; the NIST collaboration is a work in progress.
- Collaboration seems to be limited to working with HRL Laboratories' systems.
- Aside from the NIST work, connections to the rest of the CoE's work are not apparent.
- Some specific interactions on the Mg-Si system, but not much collaborations with others in the CoE.

<u>Ouestion 5: Approach to and relevance of proposed future research</u>

This project was rated **2.4** for proposed future work.

- The future research plan builds on current experience, and it is appropriately drawn for further progress toward reaching the objectives.
- It is good that the PI plans to develop a general model to describe the reverse reaction and phase growth with cycling. It would be interesting to see if the thin films can endure continued cycling. It would also be useful if the PI would compare the kinetics results of his thin film to kinetics studies done on bulk samples.
- Plans include continuing to study particle size effects.
- Plans include completing work on Mg/MgH₂, Mg-Al, and Mg-Ti.
- Plans are to continue work with NIST on neutron reflectivity study of Mg/MgH₂ thin films; model specifics of reaction kinetics and MgH₂ film growth.
- Plans to move to the complex hydrides systems, using the thin film approach could be difficult.
- With half a year left in this project, there is little in the proposed future work suggesting that a more relevant approach will be followed.
- Not applicable.

Strengths and weaknesses

Strengths

- Strong analytical/computational skills and development of potentially excellent experimental techniques and instrumentation.
- The PI seems to be well equipped to continue kinetic studies on thin films.
- The project team has carefully performed research at the nanoscale.
- The PI is knowledgeable.
- The project team has shown very good capabilities.
- Good capabilities have been employed to study material interactions in clean systems.

Weaknesses

- Need to demonstrate how representative the thin films examined are of the material systems which are of interest.
- The PI could develop additional collaborations with others in and outside the MHCoE.
- Progress seems slow and productivity could be better. The results so far are interesting but not compelling in terms of eliminating barriers.
- There is only one paper (in press); the publication record of this project still needs improvement. (This is the reason for the "Fair" score on Technical Accomplishments.)
- It is not obvious how collaboration with University of Pittsburgh played a role this past year.
- Also, it is not obvious how the results from this project are fed into MHCoE planning and decision making.
- The unclear relation to the bulk systems is a weakness.

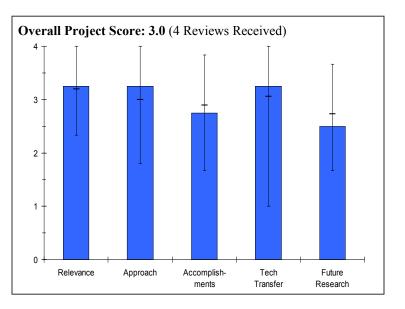
- So far, the approach has only focused on one partner system.
- The complex hydrides thin film approach might prove to be difficult.
- Efforts have not focused on materials of interest to the CoE or the program.

- The project should demonstrate how the thin film results and conclusions drawn from this work can be translated to the more advanced material systems examined within the Metal Hydride CoE.
- Nanoscale work needs to be validated on suitable nanostructured systems. The PI has also identified this as a critical assumption issue.
- The PI needs to justify key assumptions, such as why it's necessary to have a Pd coating on thin films.
- The PI should bring the work in progress to logical and meaningful conclusion, then publish it.
- In the time that remains, the PI should steer away from systems that hold no promise of meeting hydrogen storage system targets (e.g., Mg₂Si).
- The PI should emphasize how collaborations are enhancing the output of this project and how the project results are having an impact on the hydrogen storage element's quest to meet its goals.
- The project team uses a good approach to fundamental understanding, however, it seems that this type of research could fit better in the basic research program.

Project # ST-03: Discovery and Development of Metal Hydrides for Reversible On-board Hydrogen Storage *Mark Allendorf, Vitalie Stavila, and Eric Majzoub; Sandia National Laboratories*

Brief Summary of Project

The primary objective of this project is to discover new complex hydride materials. The experimental objective is to establish a synthesis route that combines high-energy milling followed by hot-sintering under high hydrogen pressures. The project works on improving kinetics, cycling life, and desorption properties by incorporating hydride materials in nanoframeworks. The theory objectives include employing the prototype electrostatic ground state (PEGS) technique for structure determination and hydrogen estimates to provide MHCoE partners with theoretical support regarding Al-N bond energies for AlH₃.



Question 1: Relevance to overall DOE objectives

This project earned a score of 3.3 for its relevance to DOE objectives.

- The discovery and development of reversible metal hydrides for on-board usage is very critical to the Hydrogen Program.
- Discovery of high potential materials with support of modeling is needed to help meet the DOE targets.
- This is a solid effort to solve a difficult problem (onboard reversible materials).
- The project basically supports DOE needs and targets.
- Although the key barriers are listed in slide 2, that list seems rather *pro forma* because there are almost no actual demonstrated relationships between the quantitative results of the project and the DOE system.
- There is a little on media gravimetric capacity, but almost nothing on any system targets (e.g., volume, cost, refueling times, quantitative purity of H₂).

Question 2: Approach to performing the research and development

This project was rated **3.3** on its approach.

- Good connections were made between modeling and experiments.
- Experimental work guided by modeling is a good approach.
- This solid approach combines excellent theoretical aspects with sound experimental efforts.
- The project is a complicated mix of candidate materials, theoretical (modeling), synthesis, and materials evaluation. It is not completely clear how this large spectrum of activities avoids overlap with other numerious groups from around the world working on similar techniques and materials.
- The various theoretical (modeling) activities seem especially complimentary and coordinated.
- The important experimental components of the project seem a bit haphazard and not as coordinated as the theoretical components.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated 2.8 based on accomplishments.

• It is clear that many good theoretical and fundamental understandings have been made on the borohydrides, alanates, amine systems, and etc.

- A lot of work has been completed in one year.
- It is necessary to incorporate all the phases possible to the modeling work to determine material suitability. However, it seems that only one system has been examined so far.
- Synthesis of the B₁₂H₁₂-anion-based compounds and comparison with theory is very helpful as it gives insight into the borohydrides decomposition intermediate to support a go/no-go decision.
- It is not at all clear how much (if any) progress has been made toward solving the system barriers. The large array of interesting results is simply not related to progress toward the DOE goals. One gets the feeling that little real (practical) progress has been accomplished during this project.
- The negative no-go on $Ca(BH_4)_2$ is nicely documented, clear, logical, and appreciated.
- There are some serious implications of theoretical and experimental results that are not fully discussed:
 - \circ Is the B₁₂H₁₂ intermediate going to be a potential barrier to most borohydride practical reversibilities?
 - Will the general presence of impurities (e.g., B_2H_6 , NH_3) mean the on-board purification will always be necessary, or is there any hope of the <10 ppb impurity levels required by proton exchange member fuel cells? In other words, there should be more in the way of practical implications of the results.

<u>Ouestion 4: Technology transfer/collaborations with industry, universities and other laboratories</u>

This project was rated **3.3** for technology transfer and collaboration.

- There has been good collaboration both within and outside of the CoE.
- There has been visible collaboration between theory and experiments.
- Collaborations are outstanding, and the many multiple-party publications clearly show that.
- What are the mechanisms of communications among the many collaborators?
- There are many collaborations within and outside of the CoE.

Question 5: Approach to and relevance of proposed future research

This project was rated 2.5 for proposed future work.

- The future work is planned reasonably well for the upcoming year.
- The new materials investigation path forward is rather vague. Is it screening-based, modeling-based, etc.?
- Strong focus on hydrides NH₃ stabilization, however, formation of NH₃ is likely.
- It's unclear why Ca(BH₄)₂ received a no-go, while Mg(BH₄)₂, which has the same thermodynamic decomposition issue, will be further researched wihin the CoE.
- The past modus operandi will continue.
- It is only partially clear why the future work activities selected are the most important to the overall objectives aimed at breaching of practical system barriers.
- The outline of proposed future work on slide 22 was somewhat vague.

Strengths and weaknesses

Strengths

- The experimental work is guided by theory.
- There are good connections between modeling and experiments.
- The project team has employed PEGS, and modeling in general.
- The project team has a good, comprehensive and coordinated understanding of the theory. Very good theoreticians have been involved.
- Attempts have been made to verify model calculations with experimentation.
- It is very nice to see the incorporation of gas-phase species into the computational predictions.

Weaknesses

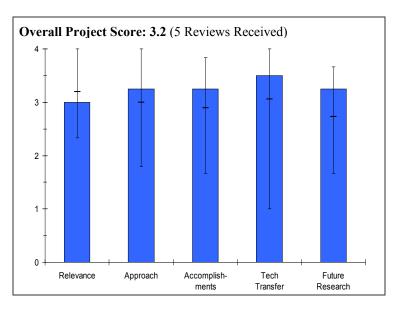
- There seems to be no theory prediction of what is the best nanoframework in terms of pore size distribution for incorporation of metal borohydride.
- There is almost a complete lack of effort to correlate theoretical and experimental results with their potential (or lack thereof) for meeting DOE system targets. Fundamentals should be better coordinated with practicals.

- With the remaining time left for this project, it is not clear why the team would like to further explore new mixed-metal borohydride systems.
- Modeling is needed to determine decomposition paths for the NH₃ stabilized systems.
- The project must invoke some practical systems thinking: mass, volume, cost, kinetics, reversibility, quantitative purity, etc. Some simple calculations on systems projections will suffice.
- There are too many materials being considered. More go/no-go decisions are necessary, particularly aimed at the many DOE on-board targets.

Project # ST-04: Chemical Vapor Synthesis and Discovery of H₂ **Storage Materials: Li-Mg-N-H System** *Z. Zak Fang and H.Y. Sohn; University of Utah*

Brief Summary of Project

The overall objectives of this project are to 1) discover new solid hydrides that meet reversibility and kinetics requirements, 2) develop chemical vapor synthesis process for production of nanosized solid metal hydrides, and 3) demonstrate the effectiveness and unique properties of nanosized solid hydride materials. Objectives for FY 2008-2009 were to 1) determine the thermodynamic properties of hydrogen storage using the ternary nitride material, LiMgN; 2) understand mechanisms of hydrogenation and dehydrogenation of LiMgN; 3) quantify NH₃ content during dehydrogenation of hydrogenated LiMgN; and 4) demonstrate effects of nanoscale particle size on properties of metal hydrides.



Question 1: Relevance to overall DOE objectives

This project earned a score of **3.0** for its relevance to DOE objectives.

- The research performed supports DOE RD&D objections.
- Very relevant work to DOE storage objectives.
- The PI has found a very good system in LiMgN that has the potential to meet DOE's short term goals for hydrogen storage.
- The PI and his group have performed a detailed hydrogen storage performance study of LiMgN; measured the thermodynamic properties, kinetics, and cycling properties; and explored the complex desorption process. They also have performed impressive cycling experiments on MgH₂ + TiH₂ nanoparticle system.
- Domain of materials was too narrow.

Question 2: Approach to performing the research and development

This project was rated **3.3** on its approach.

- The approach used is adequate.
- The approach of using "low-energy" ball milling to produce pure LiMgN, and thereby achieve reversibility, is a very good one.
- This is a good approach that uses multiple characterization methods.
- The approach uses more than one material preparation technique: both low-energy and high-energy milling techniqus, as well as chemical vapor synthesis.
- The approach looks at cycling properties as well as the first few cycle performances.
- The project team has considered a number of different material systems.
- The project team has demonstrated a number of reversible systems.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated 3.3 based on accomplishments.

- The PI has developed a method for making the LiMgN system absorb and release hydrogen reversibly and this is a significant accomplishment.
- An extensive amount of work has been completed on different material systems.
- Important progress has been in the understanding of the LiMgN system by focusing on pure material preparation. This is interesting fundamental research on a Li-Mg-N system.
- The understanding of mechanochemical reactions is incomplete.
- The results on the MgH₂-TiH₂ system are interesting.
- The PI measured enthalpy and kinetics of materials, which many PI's fail to complete.
- The PI measured impurity release (i.e. NH₃) in gas stream of LiMgN system.
- Stability was determined in the nanoscale Mg-Ti system after 100 cycles.
- This project has very good accomplishments and progress. However, it could be improved by 1) investigating the long-term cycling performance of LiMgN and 2) looking into particle size effects on the MgH₂+TiH₂ system.

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated **3.5** for technology transfer and collaboration.

- Collaboration with others is adequate.
- This project is well coordinated with other partners in the MHCoE.
- Good collaborations within the CoE.
- The project team has excellent collaborations with other groups in the CoE.

Question 5: Approach to and relevance of proposed future research

This project was rated **3.3** for proposed future work.

- The MgH₂+TiH₂ system is quite promising.
- The kinetics and cycling studies that were mentioned are crucial in determining if this material will be of use in practical applications. The cycling studies will help determine if the ammonia production leads to significant degradation of this promising material.
- The project team has a good plan for future work.
- For the future plan, there are few places that are not so certain:
 - The project team wants to use a nanoengineering method to change the structure of LiMgN to improve the hydrogen sorption performance and NH₃ release, but what would be the appropriate method they will use? High energy milling for MgH₂+TiH₂ system is not appropriate for the LiMgN system.
 - What will be the guideline for them to find additive to the LiMgN system to minimize NH₃ release?

Strengths and weaknesses

Strengths

- This is a good research that provides fundermental understanding of the material.
- There is adequate collaboration with others.
- The LiMgN system is a very promising "reversible" system that has the potential to meet DOE's short-term goals.
- This is a good project that is both broad in scope and in examining the details within given material systems.
- There is solid experimental data very relevant to DOE objectives.

Weaknesses

- The project is well designed; however, materials do not reach DOE targets.
- In the kinetics measurements, a better effort needs to be made to define the reaction conditions. Kinetics are strongly affected by pressure conditions, particle size, surface impurities, etc., and these need to be specified.
- To date, materials continue to have operating temperatures higher than the target.

• Some detailed experiments need to be carried out for structural and hydrogen sorption characterizations. For example, the detailed cycling performance of LiMgH and the structural characterization of MgH₂ and TiH₂.

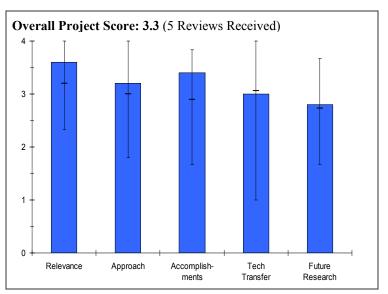
- This project should continue.
- Cycling studies should be a part of any future studies on this system.
- None.

Project # ST-05: Aluminum Hydride Regeneration

Jason Graetz, J. Wegrzyn, J. Reilly, J. Johnson, Y. Celebi, and W.M. Zhou; Brookhaven National Laboratory

Brief Summary of Project

The overall objective of the project is to develop a material that supports the 2010 DOE technical performance targets using aluminum hydride (AlH₃) by fully elucidating the nature of hydrogen desorption from AlH₃ and developing an efficient regeneration method. Objectives are to 1) develop new routes to prepare pure crystalline AlH₃ from Al (spent fuel) with minimal energy cost and 2) assist the engineering design for an off-board system based on AlH₃. The challenge is that AlH₃ is thermodynamically unstable below 7 kbar (300 K). In an AlH₃ system, H₂ evolution is controlled by temperature (rather than pressure) so the ability to tune decomposition kinetics are critical. Various



routes exist to adjust kinetics (e.g. size, coatings and catalysts). The key issue is regeneration (i.e., hydrogenation of Al metal), and multiple regeneration pathways are being investigated.

Question 1: Relevance to overall DOE objectives

This project earned a score of **3.6** for its relevance to DOE objectives.

- The regeneration of AlH₃ is very challenging and critical to the Hydrogen Program.
- The project is well aligned to the DOE objectives and is responsive to the goals of the Hydrogen Program because it addresses a number of key barriers.
- The challenge of off-board regeneration has been addressed, however the challenge of the instability of alpha AlH₃ for on-board storage did not receive as much attention.
- Particularly relevant to DOE objectives.
- Project seriously considers most DOE on-board system targets: weight, volume, regeneration efficiency, cost, refueling times, H₂ discharge rates, etc. This is an important approach for H₂ storage that should be further explored.

Question 2: Approach to performing the research and development

This project was rated **3.2** on its approach.

- The high-level electronic calculations and theory-guided approach achieved successful results.
- The ideas for low-energy regeneration routes are very good and effective.
- The project team employs a systematic, well thought out, and quite reasonable approach, which is guided by theory.
- There is very good synergy between calculations and adducts selection.
- Screening of the adducts was well done, but the separation of the pure alpha-AlH₃ remains a challenge. The overall efficiency of the alpha-AlH₃ formation should show superiority against the classical AlH₃ chemistry route.
- The use of AlH₃ liquid slurries for refueling, on-board H₂ generation and spent Al removal is innovative and has immediate practical engineering potential.

- The use of a slurry as an on-board storage medium presents engineering challenges; these challenges include: solvent presence causes the contamination of the fuel cell MEA, lowering of storage capacity in terms of weight percent, the need for continuous mixing in case of solid adducts, etc.
- The approach of low-pressure/temperature synthesis of AlH₃-adduct, followed by separation of the adduct to yield pure AlH₃ is very logical and innovative.
- Experimental work is well guided by theory.
- The approach leverages theory and experimentation.

Ouestion 3: Technical accomplishments and progress toward project and DOE goals

This project was rated 3.4 based on accomplishments.

- The BNL team has made excellent progress in 2009.
- Progress has been excellent, with the discovery of several new AlH₃ adducts and experimental verifications that some have the potential of practical off-board AlH₃ regeneration schemes
- The demonstration of DOE target discharge kinetics with a liquid AlH₃ slurry is of revolutionary importance and gives the potential for near-term practical vehicular systems.
- Satisfactory progress with respect to the objectives and the eventual improvement of the alane adduct separation and the most challenging step, its recovery. The project fully explores the possibilities for new, cost-effective and energetically efficient methods to regenerate aluminum hydrides and profits from the expertise within the CoE.
- Significant accomplishment with the verification/demonstration of all steps for the two complete regeneration pathways.
- There has been good progress and several new findings.
- The presentation of the results so far, is clear and easy to understand, even for a non-chemist.
- Good connections exist between theoretical adduct thermodynamics and experimental results.
- Nice work on the identification of additional adducts.

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated **3.0** for technology transfer and collaboration.

- The networking record is very good and guarantees access to a wide range of top-class expertise and therefore strengthens and greatly benefits the research.
- Some good collaboration exists, but there needs to be more discussion and input from the Engineering CoE.
- Collaboration is visible, especially with SNL.
- Good collaborations with several partners, but some of the results of those collaborations are not fully described.
- The collaboration with ANL for systems analysis has been excellent, and will continue to be important for the remainder of this project.
- Other than collaboration with the SNL modeling effort, there should be more apparent contribution from other partners.

Question 5: Approach to and relevance of proposed future research

This project was rated 2.8 for proposed future work.

- The future plans set clear and reasonable steps forward, getting the most out of experiences gained so far in the project.
- Further work plans need to take into account the energy balance of the overall regeneration process.
- Improving the efficiency of the alpha alane separation proposed is very good; the future work should include determining the superiority of this methodology versus other new synthesis and available methodologies.
- The focus on slurries is of concern due to the potential engineering challenges because even a liquid-state adduct still needs solvents present.

- The future work plan cannot be improved upon.
- The energy efficiency of the regeneration process should be assessed as early as possible so that efforts are not devoted to processes that have no reasonable hope of meeting targets.
- Consideration needs to be given to capacity penalties due to slurry formation.

Strengths and weaknesses

Strengths

- Excellent regeneration pathway design and good progress.
- Networking and pooling of expertise and resources.
- Very systematic and good visible progress.
- Excellent practical thinking and focus on virtually all DOE vehicle storage system targets.
- Productive, innovative R&D and positive results.

Weaknesses

- Additional input needed from the system engineering group.
- The engineering aspects and associated energy balance and regeneration costs are still an issue.
- Total energy analysis from Ti activation of Al to separation (for current adducts) is lacking.
- None.

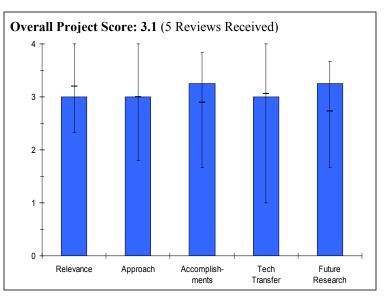
- Need to add quick and simple energy balance calculation before the closing of the project and include the calculation in the final report.
- Work together with the established Engineering CoE to investigate the feasibility of the "slurry solution" and all engineering aspects including regeneration energy balance.
- Incorporate efficiency analysis based on current systems and compare with other methodology.
- Slurry for on-board storage is not recommended as a focus.
- No changes are recommended for the remainder of this project; however given the positive potential for this project in reaching the ultimate DOE system targets (if confirmed by ANL systems analysis) a follow-on contract should be anticipated. The objectives of this new project should be the construction of a full-size demo vehicular system coupled with the selected off-board regeneration process.

Project # ST-06: Electrochemical Reversible Formation of Alane

Brenda Garcia-Diaz, Christopher Fewox, and Ragaiy Zidan; Savannah River National Laboratory

Brief Summary of Project

The overall objective of the project is to develop a low-cost rechargeable hydrogen storage material with cyclic stability and favorable thermodynamics and kinetics fulfilling the DOE on-board hydrogen transportation goals. This material is aluminum hydride (alane-AlH₃) that has a gravimetric capacity of 10 wt% and volumetric capacity of 149 g/L hydrogen and desorption temperature: ~60 to 175°C (depending on particle size and the addition of catalysts) which can meet the 2010 DOE targets for desorption. Specific objectives of the work include: 1) avoid the impractical high pressure needed to form AlH₃, 2) avoid chemical reaction route of AlH₃ that leads to the formation of alkali halide salts such as



LiCl, and 3) utilize electrolytic potential to translate chemical potential into electrochemical potential and drive chemical reactions to form AlH_3 .

Question 1: Relevance to overall DOE objectives

This project earned a score of **3.0** for its relevance to DOE objectives.

- The project is dedicated to the low-temperature/low-pressure, electrochemical reversible formation of alane a material with a high storage capacity and its regeneration is crucial to its viability as a hydrogen storage medium. The project is therefore focused on the Hydrogen Program goals and addresses key targets of R&D objectives.
- This project addresses one of the critical issues of efficient regeneration of the most promising solid state H₂ storage materials.
- The alane system has very good potential to meet DOE's short-term objectives for hydrogen storage. It has good hydrogen-holding capacity and kinetics.
- This project addresses hydrogen storage system weight, volume, cost, and efficiency, as well as storage material regeneration processes.
- This project is focused on the development of an efficient, low-pressure, low-cost route to regeneration of alane (AlH₃).
- This work supports the regeneration efforts of a promising storage material.

Question 2: Approach to performing the research and development

This project was rated **3.0** on its approach.

- Very well-thought-out, clear, systematic approach focused on overcoming the initial barriers to electrochemical formation of alane and making significant steps forward.
- The project team demonstrated excellent innovation to overcome the barriers to recover alane with very high energy efficiency using electrochemistry and capture of AlH₃ formed.
- The electrochemical approach to producing alane is a very good one; it is far more realistic than trying to use high-pressure formation. The fact that LiCl production can be avoided is significant. The fact still remains that regeneration must presently be done off board, which is less than ideal.
- Electrochemical recharging of alane $(Al \rightarrow AlH_3)$ in a non-aqueous electrolyte.

FY 2009 Merit Review and Peer Evaluation Report

- Recent emphasis has been on bench-scale electrochemical generation of AlH₃ from pure Al in H₂ atmosphere and on harvesting of pure (adduct free) AlH₃.
- The project includes modeling of electrochemical behavior and process efficiency.
- The electrochemical approach is an important alternative to the study for regenerating spent alane. It eliminates the need for very high-pressure charging.
- The approach considers energy utilization as well as material yield.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated **3.3** based on accomplishments.

- The project team has made significant accomplishments through a robust approach. The project demonstrated, for the first time ever, a reversible cycle using electrochemistry and direct hydrogenation, with high yield of, isolated and characterized, gram quantities of alane produced under mild conditions.
- The fact that gram quantities of alane have been produced electrochemically is significant. This could lead to more cost-effective ways of producing this material commercially.
- This is the first time alane has been isolated for the reaction system in gram quantities. It is suggested that the project team try and release hydrogen directly from the adducts, bypassing the pure alane recovery and eliminating the need for the slurry.
- The project team demonstrated production of high-purity AlH₃ in gram quantities.
- The project team has produced a model for the electrochemical generation of AlH₃.
- The team succeeded in isolating AlH₃ and confirming purity.
- The results are encouraging in terms of an efficient closed cycle for "release/regeneration" using AlH₃.
- Alane is formed effectively using the electrochemical approach developed in the course of this project.
- Significant progress has been made in harvesting alane from an electrochemical cell and gram quantities of alane have been successfully formed. This is an important achievement.

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated **3.0** for technology transfer and collaboration.

- Close collaborations exist between SRNL and many of its Center partners. This has proven to be very beneficial for this project.
- The project team has made excellent interaction with BNL and University of Hawaii groups.
- The project team has collaborated with BNL, University of Hawaii, University of New Brunswick, and ANL.
- The project team has collaborated closely with alane researchers in the center.
- There is good coordination with ANL analysis.
- The project belongs to the Metal Hydride CoE. There is some collaboration and partnership with BNL (on the alane-TEDA formation issue) and also others contributors are mentioned; however, the extent of the coordination of these activities during this reporting period was not entirely clear.

Question 5: Approach to and relevance of proposed future research

This project was rated **3.3** for proposed future work.

- The future plans are sound and build on current experiences with attention to the determination and optimization of the process efficiency.
- The future plans are built on the results already obtained and no new initiatives are planned. The collaborations that have worked so well will continue.
- The PI should provide data that ANL will use to determine and optimize efficiency.
- The researchers should work with BNL and SNL to identify better separation solvents.

- The researchers should work with the University of Hawaii to explore new solvent(s) that promise higher efficiency.
- The PI should determine if there are other complex hydrides that can be regenerated in similar manner.
- The project team has a good plan for future work.

Strengths and weaknesses

Strengths

- The project team has a solid understanding of electrochemistry.
- The results are very encouraging (on a promising hydrogen storage material) for meeting the capacity targets of the program.
- The PI and his colleagues are well qualified to carry out this research. The close collaborations with CoE partners are working well. The project is well focused and has led to a method of producing gram quantities of alane.
- The emphasis is on a storage material that has a chance of meeting the DOE targets.
- This project seemingly had a very successful year.
- The objective of producing AlH₃ of reasonable purity in a moderately efficient manner was met.
- Collaborations clearly helped and should continue to help this project.
- The future plans are well thought out and sensible.

Weaknesses

- Scalability could be an issue and practicality and cost effectiveness of the process could be prohibitive for its application.
- This project is not likely to lead to an "on-board" method of regenerating alane, however there are no other projects that are close to achieving this goal
- Some electrochemical engineering is needed to optimize the cell design. Based on the pictures of the very simple cell embodiment used, it is clear that there is much room for improved electrochemical regeneration performance (e.g., improved current efficiency), product recovery, and dendrite abatement.

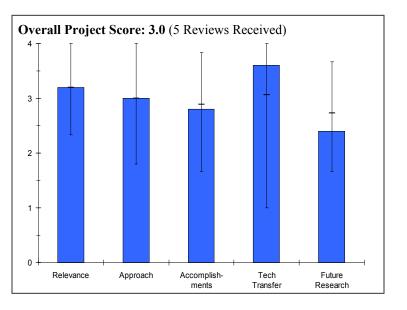
- The project team with its partners and with the support of the Engineering CoE should evaluate the lifecycle system costs and its potential for practical commercialization.
- A more practical electrochemical cell design (e.g., involving the implementation of concentric, rotating electrodes) might work nicely for this application.
- The project team should intensify the interactions with the alane regeneration experts.

Project # ST-07: Fundamental Studies of Advanced, High-Capacity Reversible Metal Hydrides

Craig M. Jensen; University of Hawaii Sean McGrady; University of New Brunswick

Brief Summary of Project

The objectives of this project are to 1) develop new materials with the potential to meet the DOE 2010 kinetic and system gravimetric storage capacity targets, such as novel borohydrides that can be reversibly dehydrogenated at low-temperatures and Al and Mg nano-confined in carbon aerogels, 2) determine the mechanism of action of dopants for the kinetic enhancement of the dehydrogenation and re-hydrogenation of complex hydrides, and 3) develop a method for the hydrogenation of Al to alane, AlH₃ at moderate pressures in hydrogen containing supercritical fluids.



<u>Ouestion 1: Relevance to overall DOE</u> <u>objectives</u>

This project earned a score of 3.2 for its relevance to DOE objectives.

- This project addresses hydrogen storage system gravimetric and volumetric targets and barriers to meeting those targets.
- The PI seemed to be working on several aspects at the same time, all of which align with the Hydrogen Program.
- Hydrogen discharge/recharge rates and storage system thermal management issues are addressed in a substantive manner.
- Some aspects of the project contribute to an improved understanding of hydrogen chemisorption and physisorption.
- The project has partial relevance to DOE on-board storage goals. It does focus on weight, kinetics, and process efficiency.
- Work is relevant to DOE RD&D objectives.
- Project does not focus adequately on volume, cost, and H₂ purity which relate to the fuel cell needs.
- This project is clearly relevant.

Question 2: Approach to performing the research and development

This project was rated **3.0** on its approach.

- The general approach is effective to address the barriers.
- The approach is to develop new classes of reversible complexes that have the potential to meet the DOE 2010 kinetic and system gravimetric storage capacity targets.
- The project team tries to pursue too many directions at the same time and thus stretches themselves too thin.
- Systems of current interest include:
 - Al and Mg nano-confined carbon aerogels.
 - o Borohydrides that can be reversibly dehydrogenated at low-temperatures.
 - Unconventional solvents for the hydrogenation of Al to AlH₃ and/or LiH/Al to LiAlH₄ at moderate pressures.
- The approach is scientifically interesting, but somewhat unfocused because it deals with three rather distinct efforts.

- The science is not always clearly extrapolated to technological (engineering) potential for a practical vehicular system, refueling modes, and spent product regeneration. Some engineering implications are perhaps easy to see, but the PI needs to more clearly state them.
- In some cases, it is not obvious how the scaffolding work is distinct from similar efforts within the CoE.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated **2.8** based on accomplishments.

- For three projects with total funding of approximately \$400K, the project team is making reasonable progress in developing the basic understanding of high-capacity, reversible metal hydrides.
- The project team has made progress with nanoconfined Mg in carbon aerogels:
 - High (9-16 wt%) MgH₂ loadings of carbon aerogel without host degradation were obtained using an organo-metallic method. Higher MgH₂ loadings were obtained with materials that have larger pore sizes.
 - Nanoconfinement of MgH₂ was found to improve kinetics (by a factor of 5 over the previous best result) but did not appear to effect the dehydrogenation of MgH₂.
- Progress with anionic borohydrides.
 - Full hydrogenation of MgB₂ to Mg(BH₄)₂ was achieved in the presence of a catalyst at pressures as low as 120 atm.
 - \circ NMR spectroscopy confirmed that the product of the hydrogenation is Mg(BH₄)₂.
- Progress was shown with hydrogenation in non-conventional solvents.
 - Fully charged, Ti-doped LiAlH₄ was obtained in major yields from the direct hydrogenation of Ti-doped LiH/Al in liquefied dimethyl ether (DME) at room temperature in 100 bar of Me₂O/H₂.
 - Well-To-Tank (WTT) efficiency analysis of a LiAlH₄-based hydrogen system utilizing liquid DME as a rehydrogenation medium showed that the system approaches the 60% target value.
- The number of positive results is significant.
- It is not clear that the nanoconfined MgH₂ (in aerogels) can meet the systems targets.
- The best loadings are 17-23% MgH₂ and thermodynamics have not been significantly improved. In response to the question, the PI stated that MgH₂ insertion in C-aerogel was preliminary model work and the solution work will move on to materials with more hope of meeting DOE needs.
- The catalyzed synthesis of Mg(BH₄)₂ from MgB₂ and transition metal (TM) borides seems promising, but the present pressures and temperatures (900 atm and 500°C) seem daunting. The PI's hope of achieving milder conditions may be too optimistic. Like the BNL AlH₃ work, the use of solvents such as DME to synthesize LiAlH₄ seems promising. It sounds as if this has to be an off-board regeneration process if it is going to meet the 3 minute refueling goal.
- It is disappointing not to see a few fundamental calculations carrying this materials synthesis and property work toward the many DOE system targets. Some simple calculations would have been appreciated. By doing a little "back-of-an-envelope" calculations, it seems that nothing reported herein has much intermediate-term chance of overcoming the present DOE barriers.
- The presentation was inconsistent regarding the reversibility of $Mg(BH_4)_2$. Slide 20 states that reversibility is at 120 atm, but does not state the temperature, while slide 11 suggests reversibility at 950 bar and 400°C.
- Bu₂Mg is hardly the most efficient reagent. Cp₂Mg or t-Bu₂Mg may be considered as potential precursors for MgH₂.
- The formation of MgB₁₂H₁₂ during continuous operation of Mg(BH₄)₂ is not addressed. The question if Mg(BH₄)₂ behaves differently from Ca(BH₄)₂ is also not addressed.
- The role of the Ti catalyst in Li-Al-Ti-H system was not addressed effectively and does not seem to be well understood.
- The direct synthesis of LiAlH₄ in polar solvents has already been reported in the past and DME is a known process.

<u>Ouestion 4: Technology transfer/collaborations with industry, universities and other laboratories</u></u>

This project was rated **3.6** for technology transfer and collaboration.

• There is good collaboration with other partners.

- This project's collaborations are indeed extensive, however how each contributed was not obvious in the presentation, but it is clear that collaboration did occur.
- The list of collaborators includes California Institute of Technology, HRL Laboratories, National Institute of Advanced Industrial Science and Technology, PNNL, University of Rome, University of Geneva, Institute for Energy Technology (Norway), Jet Propulsion Laboratory, UOP, KEK (High Energy Accelerator Research Organization), Tohuku University, University of Illinois, SNL, NIST, and the University of New Brunswick.
- The University of Hawaii work involves many good collaborations. It is an excellent example of collaborations within the Hydrogen Program.
- There is a lot of good collaboration.

Question 5: Approach to and relevance of proposed future research

This project was rated 2.4 for proposed future work.

- Interesting basic research is planned; however, it does not offer a way of meeting the DOE targets within a reasonable period of time.
- Given that the upcoming year will be the last year of the program, the plan should focus on a few specifically defined objectives. The current plan has too many tasks to perform in one year.
- Future work on nanoconfined Mg in carbon aerogels includes:
 - $\circ~$ Determine dehydrogenation and rehydrogenation kinetics of aerogels loaded with both MgH_2 and Ti catalyst.
 - Prepare nanoconfined MgH₂ from the hydrogenation of dimethyl magnesium intercalated aerogels as a means of increasing loadings.
 - Determine pressure-composition-temperature (PCT) isotherms to elucidate the effect of nanoconfinement on the dehydrogenation of MgH₂.
- Future work on anionic borohydrides includes:
 - Explore variations in reaction conditions to improve yield from low-pressure hydrogenation of MgB₂ to Mg(BH₄)₂.
 - \circ Continue the studies of the catalyzed and un-catalyzed hydrogenation of MgB₂ to elucidate the mechanism and possibly learn how to improve the kinetics.
- Future work on hydrogenation in nonconventional solvents include:
 - Maximize the extended cycling capacity of Ti-doped LiAlH₄ through variation of the dopant concentration and recharging conditions in liquid dimethyl ether.
 - Continue exploration of methods to improve the levels of hydrogenation of alane using alternative supercritical fluids (SCFs) and a variety of initiators/catalysts.
 - \circ Explore SCF synthesis of Mg(AlH₄)₂.
 - $\circ~$ Proceed with further evaluations of WTT efficiency of the DME/LiAlH_4 system in collaboration with ANL.
- Future work proposed on anionic borohydrides and hydrogenenation in nonconventional solvents is worthwhile.
- There are not plans to focus on overcoming the many system property barriers.
- The scope should be narrowed from the past year to address fewer key areas in greater detail.

Strengths and weaknesses

Strengths

- There is good collaboration with various DOE and non-DOE research groups including international collaborations.
- There is good collaboration with other CoE partners.
- The PI and his co-workers seem to have good instincts about how to improve things. In the past they have tended to stay focused on systems with a reasonable chance of meeting DOE hydrogen storage targets.
- The collaborations are extensive and seemingly effective.
- Stepping away from the supercritical CO₂ effort was a good decision.
- Good, innovative chemistry.
- Excellent collaborations.

Weaknesses

- The group tries to pursue too many directions at the same time, thus being unfocused and skipping essential details.
- There are too many research areas that are not related in the project.
- Some of the approaches are not well explained.
- The project may be going in too many directions with the available funding and possibly limited time.
- While the results from the work on aerogels are interesting, it appears that the dilution factor makes the hydrogen storage targets unachievable. The presenter referred to it as a "model approach," but it seems to have little chance of meeting the targets.
- The connection to on-board system end points and associated DOE barriers is poor.

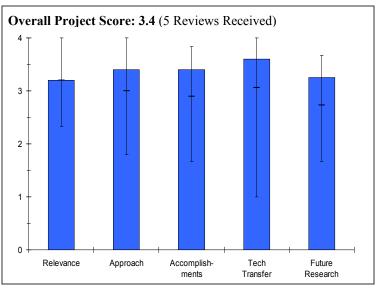
- The PI should reduce the number of research topics/directions.
- The project should focus on directions with the highest potential for meeting DOE targets.
- More attention to the science behind the many informative research accomplishments and fewer sidebars about factors outside the control of the PI would help the project to end on time and produce a better appreciation of the significance of the results.
- The PI should end all work on nanoconfined MgH₂ in carbon aerogels and move to better materials with more potential.
- Given the poor results to date, it is suggested that PI and University of New Brunswick partner terminate further work on rehydriding Al in SCFs. The approaches in the BNL and SRNL projects seem much more promising from technical and cost angles.
- The project team should begin cost projections and systems target calculations.

Project # ST-08: First-Principles Modeling of Hydrogen Storage in Metal Hydride Systems

J. Karl Johnson and David S. Sholl; University of Pittsburgh/Georgia Institute of Technology

Brief Summary of Project

The overall objectives of this project are to 1) compute the thermodynamics of metal hydride systems, 2) compute interfacial properties of hydrides, and 3) address fundamental processes in hydrogenation. Specific objectives for FY 2009-2010 are to 1) complete reaction screening, including multistep and metastable reactions and new additions to the database; 2) finalize work on thermodynamics of multiple, gas-phase species; 3) include thermodynamics of amorphous and crystalline closo-borane structures such as $MgB_{12}H_{12}$ and related materials in the screening of candidate reactions; and 4) finish work on mixed metal hydrides.



Question 1: Relevance to overall DOE objectives

This project earned a score of 3.2 for its relevance to DOE objectives.

- Material modeling has become an important tool in the development of storage materials, both in guiding experimentalists toward promising materials and in understanding the behavior of complex material interactions.
- This project addresses issues/barriers associated with meeting DOE's hydrogen storage system gravimetric and volumetric targets, as well as factors affecting charging/discharging rates (e.g., kinetics).
- Theory is a powerful tool for screening candidate materials, but needs to tie-in with experimental work.
- This project addresses the lack of understanding of hydrogen physisorption and chemisorption.
- Overall this project is highly relevant.

Question 2: Approach to performing the research and development

This project was rated **3.4** on its approach.

- The PIs have been leaders in developing techniques for modeling complex material behavior using first principles calculations. Entropy is not included in the energy calculation, without this it will not give the information necessary to tell if a phase is stable or not.
- The project team uses first principles density functional theory (DFT) to compute structures and energies of solid phases and gaseous species.
- The project team uses phonon density of states calculations for determinations of finite temperature thermodynamics.
- Free energy minimization methods are employed for screening mixtures suitable for promising reactions.
- Surface energy calculations are used to assess the influence of nanoscale structures on the thermodynamics.
- The project now includes the application of first principles molecular dynamics to generate and study amorphous phases.
- The project team employs transition state theory to characterize surface reactions and diffusion mechanisms.
- It is suggested that the project team downplay the effort on amporphous phase calculations. The energy differences between these systems and their crystalline counterparts will be small and there will likewise be a small impact on reaction energetics.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated 3.4 based on accomplishments.

- The project team has made good progress.
- The project team has made sizeable additions of thermodynamic data to key databases used by the Hydrogen Storage Program.
- Computational methods were used to generate and characterize 200 amorphous structures (100 atom assemblies).
- The project team computed diffusion barriers for charged defects and showed evidence that diffusion can be controlled by doping.
- Free energy calculations now include multiple gas phase species.
- New mixed metal borohydrides were characterized.
- Now that the kinetics calculations have been performed for MgH₂ (a baseline system), it would be good to see this effort extended to materials of current interest.
- It is nice to see the thermodynamic models include the formation of gas phase species. This will be a big help in improving the predictive accuracy of these methods.
- A clear description of what structures have been added to the metals hydrides database is needed.

<u>Ouestion 4: Technology transfer/collaborations with industry, universities and other laboratories</u>

This project was rated **3.6** for technology transfer and collaboration.

- The project team has shown good collaborations.
- The project team collaborates broadly throughout the Metal Hydride CoE program. Collaborating institutions that benefit from working with the Pittsburgh group include California Institute of Technology, HRL Laboratories, University of Hawaii, Jet Propulsion Laboratory, University of Missouri, NIST, SNL, Stanford University, University of Illinois at Urbana-Champaign, and University of Utah.
- There is coordination of theory work within the Metal Hydride CoE through the theory working group.
- The PIs continue to have close collaboration with others and are responsive to input from experimentalists.

Question 5: Approach to and relevance of proposed future research

This project was rated **3.3** for proposed future work.

- Proposed future work included:
 - Carry out analysis of multi-step reactions and submit paper for publication.
 - Finish calculations for updated database reactions and carry out screening.
 - Analyze the thermodynamics and structure of amorphous MB₁₂H₁₂ systems for M=Ca and Mg.
 - Examine diffusion through void spaces in metal hydrides, as prompted by experimental observations.
 - Implement fast reaction screening with multiple gas phase species for as many cases as possible.
- The listed approach for proposed future research was too vague to be meaningful.

Strengths and weaknesses

Strengths

- This project is good for screening candidate materials.
- The PI is knowledgeable and enthusiastic. This is a force in the theory community working on hydrogen storage issues.
- Good choices have been made regarding computational methods and research thrusts.
- This project provides a lot of useful data to the Hydrogen Storage Program community.
- The PI is clearly responsive to prior reviewer comments and recommendations.
- There is strong coupling of experiment and theory.
- This is a strong collaborative effort.

Weaknesses

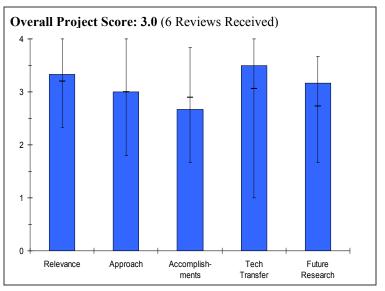
- Inclusion of entropy into energy calculation is lacking.
- Some aspects of the work on amorphous materials calculations need shoring up. A determination should be made of what happens as one varies the number of atoms. These types of calculations definitely need some form of experimental corroboration.
- There have been a relatively small number of publications.

- The project team should continue the good work.
- The project team should tighten up their work on amorphous phases. The results are interesting, but they need to be validated.

Project # ST-09: Thermodynamically Tuned Nanophase Materials for Reversible Hydrogen Storage *Ping Liu and John Vajo; HRL Laboratories, LLC*

Brief Summary of Project

The overall objective of the Metal Hydride CoE is to research, develop, and validate reversible onboard metal hydride storage materials and systems that meet the 2010 DOE system targets for hydrogen storage, with a credible path forward for meeting the 2015 DOE storage targets. The approaches to meet the hydrogen capacity targets of 6 wt% and 45g H_2/L volume density are to 1) synthesize and characterize hydride materials with high hydrogen capacity and favorable thermodynamics and 2) use stateof-the-art theory to guide the materials discovery effort. The approaches to meet the charge/discharge rate target of a 3 min system fill (5 kg) are to 1) develop materials that are fully reversible; 2) develop catalysts



that aid reversibility; 3) assess nanoengineering promotion of kinetics; and 4) investigate the role of contamination on reaction rates. The approach to meet the hydrogen purity target of 99.99% is to assess release of NH_3 , B_2H_6 and other volatile species from metal hydrides during desorption and cycling. The approach to meet the cycle life target of 1,000 desorption/adsorption cycles is to investigate durability of materials, cycling behavior, effects of contaminants, structural stability, and release of volatiles.

Question 1: Relevance to overall DOE objectives

This project earned a score of **3.3** for its relevance to DOE objectives.

- The development and demonstration of a safe and cost-effective light-metal hydride material system is critical to the Hydrogen Program.
- Lower dehydrogenation temperatures of LiBH₄/MgH₂ were achieved in scaffolds, but cycling properties still need to be improved. The search for new borides containing light transition metals for H₂ storage purposes is a valuable objective, but a major breakthrough in that field is uncertain.
- The PIs investigated the LiBH₄/MgH₂ destabilized system, and looked into how nanostructured carbon scaffolds affect the thermal dynamic property of the system.
- The scaffold approach has hydrogen capacity penalties inherent to it.

Question 2: Approach to performing the research and development

This project was rated **3.0** on its approach.

- The general approach is novel and effective.
- Examining a new system in addition to the LiBH₄-MgH₂ system is a good approach, given the lack of success in LiBH₄-MgH₂.
- The use of scaffolds is turning out to be more difficult than expected, but it still warrants further study.
- The project team uses a good approach: it is fairly well integrated with other efforts and contributes to overcoming some barriers.
- The overall approaches are appropriate; however the project team needs to design experiments to understand how the carbon scaffolds change before and after hydrogenation, after storage material is incorporated and even after cycling. Structural, volume, and composition change could reveal fundamental processes that govern the hydrogenation performance. This is important to the performance as well as the final loading.

Ouestion 3: Technical accomplishments and progress toward project and DOE goals

This project was rated 2.7 based on accomplishments.

- Lower dehydrogenation temperatures of LiBH₄/MgH₂ were achieved in a scaffold, but cycling properties need to be improved.
- Given the fact that the funding level was the same in 2008 and 2009, this year's progress is less impressive compared to last year.
- There is no explanation for the mechanism of reaction between LiBH₄ and MgH₂ in carbon aerogel.
- The investigated materials exhibit relatively poor cycling behavior.
- The LiBH₄-Mg₂NiH₄ system has desorption temperatures that are still too high.
- The LiBH₄-MgH₂ system in the carbon aerogel exhibits capacity problems with cycling.

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated 3.5 for technology transfer and collaboration.

- Collaboration appears to be very good in terms of key interactions with LLNL on carbon aerogels and University of Hawai'i on incorporation techniques for hydrides into aerogels.
- Good collaboration within the CoE.
- Professor Jensen of the University of Hawai'i seems to be making a solid contribution to this work.
- Collaborations are appropriate.

Question 5: Approach to and relevance of proposed future research

This project was rated **3.2** for proposed future work.

- This project is 80% complete, so the future work needs to be well focused.
- The search for new borides containing light transition metals for hydrogen storage seems to be a valuable objective, but the possibility of a major breakthrough is uncertain.
- It would be helpful to understand why the scaffold helps the hydrogenation performance. There are many parameters that play important roles such as scaffold structure, the filling of the storage materials, the structure and mechanical changes during the hydrogenation process, the real diffusion length, etc. A possible physical-chemical model on the hydrogenation and dehydrogenation process should be proposed.

Strengths and weaknesses

Strengths

- Work is focused on new destabilized systems and nanoporous scaffolds and is therefore likely to yield new valuable insight into thermodynamics and kinetics of hydrogen storage materials
- A novel technical approach and the outcomes can be utilized by other partners.
- Good collaboration with other partners.
- A variety of experimental techniques are utilized in research.
- The destabilization approach is generally a good one.

Weaknesses

- There is a lack of strategic planning in the experimental design. There is too much effort on optimizing LiBH₄/MgH₂ in scaffolds.
- Mechanisms of reported transformations remain unclear.
- There is no evidence that pure hydrogen is released.
- Gas analysis would be a useful tool to utilize.
- It appears that the destabilization approach does not work well for the LiBH₄-MgH₂ system.
- Incorporation of an aerogel framework to accelerate kinetics possesses a hydrogen capacity penalty.
- It may be difficult to overcome barriers for practical applications.

FY 2009 Merit Review and Peer Evaluation Report

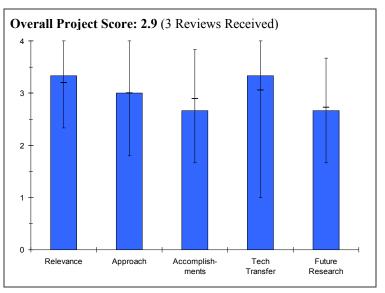
- With the time remaining for this project, it is suggested that the PIs drop the "search for other ternary systems with high capacity and low reaction temperatures" in their future work plan and allocate the available resources to achieve a more fundamental understanding of the current system.
- In the time left, this project should probably focus on characterizing and understanding the LiBH₄-MgH₂carbon-aerogel and LiBH₄-Mg₂NiH₄ systems as completely as possible in order to provide guidance for future hydrogen storage materials that might adopt this approach with better success.
- It seems that the LiBH₄/MgH₂ system cannot meet the targeted goal, therefore another potential system should be examined. Further fundamental understanding of the role the scaffolds is needed.
- If possible, there should be a theoretical estimation of similar systems.

Project # ST-10: Catalyzed Nano-Framework Stabilized High Density Reversible Hydrogen Storage Systems *X. Tang, D. Mosher, S. Opalka, X. Tang, T. Vanderspurt, B. Laube, and R. Brown; United Technologies Research Center*

E. Rönnebro and T. Boyle; Sandia National Laboratories F.-J. Wu and J. Strickler; Albemarle Corporation

Brief Summary of Project

The first objective of this project is to design and synthesize hydride/nanoframework combinations to improve reversible capacity, desorption temperature, and cyclic life. The second objective is to build upon successes previously demonstrated in the community and extend to a wider range of doped, functionalized and catalyzed framework chemistries in order to 1) advance the understanding of behavior modification by nanoframeworks, 2) obtain/maintain nanoscale phase domain, 3) tune hydride/framework interactions to decrease desorption temperature for highly stable compounds, stabilize high capacity compounds (resulting in ligand elimination) and influence desorption product formation,



and 4) activate H₂ dissociation on highly dispersed catalytic sites.

Question 1: Relevance to overall DOE objectives

This project earned a score of 3.3 for its relevance to DOE objectives.

- The concept of using frameworks to reduce the hydrogenation/dehydrogenation temperatures for high capacity reversible metal hydrides is relevant, provided that the hydrogen capacity penalties associated with the framework are not prohibitive.
- Work on calcium borohydride does not appear to be the most straightforward way to support the goals and objectives, but is likely to yield valuable insight into basic research issues such as hydride/nanoframework interactions.

Question 2: Approach to performing the research and development

This project was rated **3.0** on its approach.

- Both carbon and oxide framework materials are being examined, the metal hydride materials being studied are relevant and the materials modeling work is supportive.
- The project is well designed and well integrated with other efforts, but it may contribute only indirectly to overcoming technical barriers.
- The PIs combined both theoretical work and experimental results, which is very good. Questions: For the molecular modeling, both the host and the guest are in an open space (i.e., not confined to a nanosized pore). Would that affect the calculation results? Especially when compared to the experimental results?

Ouestion 3: Technical accomplishments and progress toward project and DOE goals

This project was rated 2.7 based on accomplishments.

- The project has made significant progress towards objectives and some barriers (e.g., high loading of borohydrides in silica gel).
- The team made very good progress.
- The project does not appear to have produced any significant positive results.

<u>Ouestion 4: Technology transfer/collaborations with industry, universities and other laboratories</u>

This project was rated **3.3** for technology transfer and collaboration.

- Good collaborations in attempting to try various routes to obtain a positive result.
- Collaborations exist and partners have contributed fairly well to the project.

Question 5: Approach to and relevance of proposed future research

This project was rated 2.7 for proposed future work.

- The proposed work on calcium borohydride does not appear to be the most straightforward way to support goals and objectives but is likely to yield valuable insight into basic research issues such as hydride/nanoframework interactions.
- There are three questions that should be addressed in the proposed future research:
 - 1. How would the filling of the metal hydride affect the hydrogenation property in the nanopore framework?
 - 2. Does the volume change of the metal hydride that occurs during hydrogenation and dehydrogenation have an effect on the property?
 - 3. Why would the doped framework, rather than a catalyst-decorated inner surface of the framework, give better results?
- There does not seem to be a clear path forward to achieve positive results.

Strengths and weaknesses

Strengths

- The project combines computational and experimental methods to design hydride-nanoframework composites.
- This project did not exhibit any strengths.

Weaknesses

- The modeling work is secondary to the experimental achievement of positive results.
- The project concentrates on a system (calcium borohydride) that has been down selected by other groups.

Specific recommendations and additions or deletions to the work scope

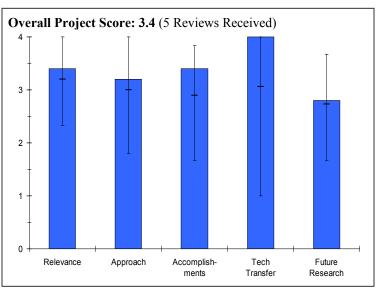
• A no-go decision should be made for this project.

Project # ST-11: Neutron Characterization and Calphad in Support of the Metal Hydride Center of Excellence

Terrence J. Udovic and Ursula R. Kattner; National Institute of Standards and Technology

Brief Summary of Project

The overall objectives of this project are to 1) support the development of hydrogenstorage materials by providing timely, comprehensive characterization of CoEdeveloped materials and storage systems using state-of-the-art neutron methods and Calphad and 2) help speed the development and optimization of storage materials that can meet the 2010 DOE system target of 6 wt% and 45 g/L capacities. Objectives are to 1) characterize structures, compositions, hydrogen dynamics, and absorption-site interaction potentials for candidate storage materials and 2) provide Calphad calculations of phase relationships of potentially promising hydrides.



Question 1: Relevance to overall DOE objectives

This project earned a score of **3.4** for its relevance to DOE objectives.

- The nature of the results, particularly those from neutron experiments, is unique to the program in that the information generated cannot be obtained (or easily obtained) by other available methods.
- NIST boasts a high performance neutron scattering facility and its scientists in charge of research are among the best worldwide, at least from a European perspective. The facility and its scientists are critical assets for the Hydrogen Program, in particular for the Metal Hydride CoE, and this project fully supports DOE RD&D objectives. A reduction of DOE RD&D funding for hydrogen research would annihilate years of successful buildup of R&D knowledge and endanger the competitiveness of U.S. industry in the long run.
- Neutron characterization is the best tool for the Hydrogen Program.
- Neutron characterization is important to support the development of hydrogen storage materials.
- This project addresses issues that relate to hydrogen storage system gravimetric and volumetric targets and barriers to reaching those targets.
- The results provide new understanding of hydrogen physisorption and chemisorption phenomena.

Question 2: Approach to performing the research and development

This project was rated **3.2** on its approach.

- The Neutron and Calphad methods are both effective at addressing the technical barriers and the project is well designed.
- The PI should get a better picture of the overall approach to the direction of research than just characterizing the materials.
- Neutron methods are used to elucidate hydrogen diffusion mechanisms and determine the following:
 - Elemental compositions of materials;
 - Location of hydrogen atoms in storage materials; and
 - Resolve crystal structures of materials and the nature of bonding of absorbed hydrogen on surfaces and in bulk structures.

- Application of Calphad methods contributes to the development of a thermodynamic database from the available literature and from first principles calculations, including the incorporation of database information into an overall temperature-pressure-composition framework for multicomponent metal-hydrogen systems.
- The very nature of the work performed (neutron scattering on a great variety of new hydrogen storage materials for various research groups) contributes to a sharp focusing on technical barriers.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated 3.4 based on accomplishments.

- Progress towards objectives is truly outstanding. The location and dynamics of hydrogen atoms have been successfully studied for a great variety of new hydrogen storage materials, including the M_xB₁₂H₁₂ intermediate, and a very useful diagnosis of a practical hydrogen storage bed has been performed by neutron imaging.
- The neutron imaging of hydrogen-storage beds is new this year.
- There needs to be more directed progress to see a clear path.
- Structures of Li₂B₁₂H₁₂, Na₂B₁₂H₁₂, and CaB₁₂H₁₂ were solved by a combination of X-ray diffraction (XRD), neutron vibrational spectroscopy (NVS), and density functional theory (DFT) calculations.
- It was found that only partially filling a 13 nm carbon aerogel with LiBH₄ increases the fraction that exhibits non-bulk-like BH₄-reorientation dynamics. Results indicate preferential filling of smaller pores and/or surface film formation.
- Neutron imaging techniques, employed to provide in-situ, real-time diagnostics of practical hydrogen-storage beds, illustrated how the use of deuterium instead of hydrogen enables the imaging of thicker beds.
- A Calphad database for H-Li-Mg-Ca-B-Si-N with thermodynamic descriptions of the constituent subsystems is being developed from literature data for the binary solution phases and intermediate compounds and from first principles calculations.
- The project team used the modified Neumann-Kopp rule for rapid prediction of the heat capacities of complex metal hydrides.
- It was found that confinement of Li₃BN₂H₈ in nanoporous carbon materials renders it partially reversible.
- NVS and prompt-gamma activation analysis (PGAA) indicated non-trivial amounts of residual hydrogen in carbon aerogels.

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated **4.0** for technology transfer and collaboration.

- This project exhibited very good and close collaboration with CoE partners.
- A regular meeting with collaborators is fruitful to streamline the direction of research.
- This program provides unique neutron-based experimental data that can only be measured in a select few places. The collaborators that have received these data include California Institute of Technology (Caltech), General Motors, HRL Laboratories, Jet Propulsion Laboratory (JPL), LLNL, University of Maryland, University of Michigan, University of Missouri-Columbia, Ohio State University, University of Pennsylvania, SNL, and Stanford University.
- The Calphad work is done in collaboration with Georgia Institute of Technology, University of Illinois, University of Missouri-St. Louis, University of Pittsburgh, and SNL.
- NIST works in a coordinated manner with the Metal Hydride CoE and the Hydrogen Sorption CoE lead laboratories.
- Due to the very nature of its work (neutron scattering studies in collaboration with other research groups) the project is well integrated with other research efforts.

Question 5: Approach to and relevance of proposed future research

This project was rated 2.8 for proposed future work.

- The plans are built on past progress and sound effective. Proposed future work includes: to
 - Continue structural and spectroscopic characterizations of dodecahydro-closo-dodecaborates (M_xB₁₂H₁₂) (with SNL, Caltech, University of Maryland, University of Missouri-St. Louis, and Ohio State University);
 - Continue rotational dynamics investigations of nanoscaffolded borohydrides (with HRL, LLNL, Michigan State University, Caltech);
 - Continue Mg thin-film characterizations using neutron reflectometry (with Stanford University);
 - Perform neutron scattering characterizations of new materials in conjunction with the needs of the other partners, including borohydrides and nanoscaffolded materials of interest;
 - Continue feasibility studies using neutron imaging to probe hydrogen distribution and transport in storage beds for candidate materials (with JPL, University of Maryland);
 - \circ Develop Calphad description of the Ca-B-H and Mg-B-H systems including the Ca(BH₄)₂ and Mg(BH₄)₂ compounds (with MHCoE Theory Group); and
 - Continue to expand Calphad database (evaluate literature for data, identify data needs and systems with Metal Hydride CoE partners for future database development).
- Future work should address issues listed in the *Project Weaknesses* section below.
- The investigations planned for the future have been built on past progress and are well focused on barriers, and the systems for future research are well chosen. However, an unexpected need for studying new systems may arise at short notice and should be accounted for in the planning.
- Future work was not proposed.

Strengths and weaknesses

Strengths

- Neutron characterization is the most critical tool for the Hydrogen Program.
- Neutron characterization is important.
- The project provides unique capabilities that employ neutron-based measurement methods.
- The project also provides experienced access to a useful database (Calphad) and also contributes to the building of that database.
- The results have a broad impact on the progress of the hydrogen storage CoEs.
- The work is skillfully done.
- This is excellent work.
- There are numerous collaborations.
- There has been a large amount of presentations and publications.
- This project provides the most basic and complete information on the structure and dynamics of solid hydrogen storage materials.

Weaknesses

- There is a lack of novelty.
- Close collaboration with a sample provider is lacking.
- There is concern about the attitude with respect to future plans. The PI left an impression that NIST is opening
 itself up to being treated like a job shop within the Hydrogen Storage Program. See the statement:
 "Perform neutron scattering characterizations of new materials in conjunction with the needs of.....partners..."
 This is okay, but threads of continuity (leading to focused pieces of research) should run through the work plan.
 With limited time and resources, the emphasis should be on the storage system materials with the best chance of
 meeting the DOE targets.
- The Calphad calculations do not appear to have reached their full potential yet.

Specific recommendations and additions or deletions to the work scope

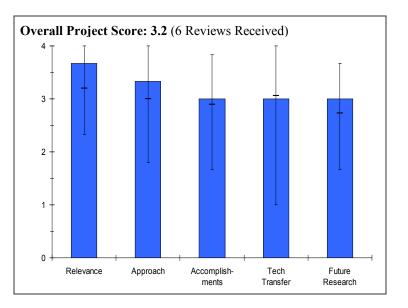
• The remaining work should be organized in such a manner so that the project is focused on specific science issues for hydrogen storage.

Project # ST-12: Analyses of Hydrogen Storage Materials and On-Board Systems

Stephen Lasher, Kurtis McKenney, Jayanti Sinha, and Paul Chin; TIAX LLC

Brief Summary of Project

The overall objective of this project is to help guide DOE and developers toward promising R&D and commercialization pathways by evaluating the status of the various on-board hydrogen storage technologies on a consistent basis. The onboard assessment objective is to evaluate or develop system-level designs to estimate weight, volume, and bottom-up factory cost for the on-board storage system. The offboard assessment objective is to evaluate or develop designs and cost inputs to estimate refueling cost and well-to-tank energy use and greenhouse gas (GHG) emissions for the fuel chain.



<u>**Ouestion 1: Relevance to overall DOE**</u> <u>objectives</u>

This project earned a score of 3.7 for its relevance to DOE objectives.

- The economic analysis of various storage option is a vital and critical element in determining the path forward.
- The project is highly relevant and critical to the Hydrogen Program.
- These types of cost estimations are necessary.
- On-board storage is one of the two or three most critical areas of R&D necessary for hydrogen fuel cell vehicles to be successful. This project analyses the well-to-whells (WTW) costs and performance of potential on-board storage technologies and compares the results to the DOE targets. This is essential to screening out storage technologies that cannot achieve the targets and highlight the critical areas for R&D for promising storage technologies.
- The presentation was clear and focused, and solid improvements were shown over the years. The analyses are clearly relevant to DOE objectives on various pathways for storage in vehicles.
- Good balance of on-board versus off-board (regeneration) system costs and barriers.

Question 2: Approach to performing the research and development

This project was rated **3.3** on its approach.

- The approach includes bottom-up design and cost estimation, use of the H2A Production and Delivery tools as appropriate, seeking information and input from a broad rangeof stakeholders and experts, as well as a thorough a WTW approach to costs. The work being done is excellent.
- The approach is consistent and well established, albeit requiring considerable feedback from the PIs and thus the need to decouple the cognitive biases.
- The media and storage tank assumptions are clearly stated.
- TIAX, LLC is collaborating directly with ANL who performs the WTW energy efficiency and GHG analysis for the storage technologies. Between TIAX and ANL, a complete analysis of WTW costs, energy efficiency, and GHG emissions can be obtained.
- TIAX and ANL presentations should be integrated into one or each should show the total WTW results including costs, energy efficiency, and GHG emissions in a summary slide.

- It is not clear if the H2A Delivery Components and Carier Components models being used are up-to-date with the latest H2A Delivery efforts. It is not clear if these component model tabs are being properly used and pulled together for a particular delivery scenario.
- Solid; however the projections to high-volume (500,000 vehicles per year) are not credible without transparent comparisons to *current* costs.
- It should be made clear up front that assumptions regarding liquid carriers are based primarily on Air Products and Chemicals, Inc. (APCI) inputs. Are there other investigators or end-users interested in this approach to storage? The use of the n-ethylcarbazole systems is not feasible due to toxicity and will not be a long-term storage choice. N-ethylcarbazole serves as a stand in material while the reactor is developed in this project and other material carriers are developed in other parts of the program.

Ouestion 3: Technical accomplishments and progress toward project and DOE goals

This project was rated **3.0** based on accomplishments.

- The project is on target with the set objectives and deliverables.
- Given that this is the last year of the program, most of the on-board and off-board assessments are complete.
- Ammonia borane on-board analysis could have been a higher priority than LCH₂ given the effort and focus at the Chemical Hydrogen CoE, however automanufactuers have shown more .interest in LCH₂.
- Good progress in terms of completing the analysis of the liquid carrier technology, and updates of compressed hydrogen gas technology.
- Too much time and effort was spent on fine tuning the compressed gas technology analysis.
- Considering the FY 2008 budget, more analyses of different storage technologies could have been achieved.
- New DOE storage targets should be used for comparisons.
- Solid year-after-year improvement and presentations are now crisper. While the effort is primarily modeling, there must be simultaneously some "qualitative" assessment or ranking of such alternatives relative to practicality (beyond cost).
- Excellent breakdown of materials versus equipment costs, but when one has glaring sensitivity to one material (e.g., Pd for the carrier system) should there not be an attempt to project Pd demands under a 500,000 units/year scenario? Are we exchanging one vulnerability for another (beyond Pt)?
- Why the high losses for the carrier material and what are the costs of environmental impact of such losses?
- It is suprising that the ownership impact variations are so minimal among the carrier, Compressed H₂, and liquid H₂ options. What is the conclusion if this analysis is correct and how do we rank these for applicability (based on geography)?

<u>Ouestion 4: Technology transfer/collaborations with industry, universities and other laboratories</u>

This project was rated **3.0** for technology transfer and collaboration.

- There is excellent collaboration with ANL, the Storage CoEs, and key hydrogen storage tank vendors which together cover a large portion of expertise in storage technology and analysis.
- Naturally, this project has to develop a working relationship with the PIs and also coordinate efforts with ANL system analysis.
- It is stated that TIAX interacted with the FreedomCAR Technology Teams, but only the Delivery Technology Team meeting is mentioned specifically. More interaction with the auto original equipment manufacturers (OEM) and energy companies could be helpful.
- There has been good collaboration with Air Products and Chemicals on carrier materials, but where are the cross-checks with other industrial gas companies? This should be done to ensure due diligence.

<u>Question 5: Approach to and relevance of proposed future research</u>

This project was rated **3.0** for proposed future work.

• The future plan is detailed, constructive and will add additional important results as well as detailed report documentation of results to date.

- Given that the project is almost completed, it is not clear when all the reports will be available to partners and general public.
- DOE is directing TIAX on what storage technologies to analyse. A thorough WTW analysis of a potential onboard "sorption" technology that operates at a variety of temperatures and pressures (-100°C to room temperature) and charged with cold H₂ gas (-150° to -50°C) would be very beneficial to the HFCIT Program. This would include looking at different sorption characteristics, including those achieved to date and potential ones. This is a very promising storage technology and would give DOE a clear picture of what sorption characteristics and other parameters are needed for this approach to meet DOE targets.
- Not clear what the final recommendations would be to the Engineering CoE for storage.
- There needs to be a more definitive chart for recommendations or very clear, focused suggestions for the discrimination of the different approaches.

Strengths and weaknesses

Strengths

- Consistency and experience are the two strengths.
- The cost analysis is one of the most critical aspects in evaluating the feasibility of hydrogen-based transportation system.
- Cost analysis is necessary to identify technology viability.
- On-board storage is one of the two or three most critical areas of R&D for hydrogen fuel cell vehicles to be successful. This project analyses the WTW costs and performance of potential on-board storage technologies and compares the results to the DOE targets. This is essential for screening out storage technologies that cannot achieve the targets and highlight the critical areas for R&D for promising storage technologies.
- The approach being taken includes bottom-up design and cost estimation, use of the H2A Production and Delivery tools as appropriate, seeking information and input from a broad range of stakeholders and experts, as well as a thorough a WTW approach to costs. The work being done is excellent.
- TIAX is collaborating directly with ANL who performs the WTW energy efficiency and GHG analysis for the storage technologies. Between TIAX and ANL, a complete analysis of WTW costs, energy efficiency, and GHG emissions can be obtained.
- The future plan is detailed, constructive, and will add additional important results as well as detailed report documentation of results to date.
- Different hydrogen storage technologies have been evaluated.
- Very comprehensive, detailed approach in attempt to settle on recommendations for action; however there is not clear pathforward in the end.

Weaknesses

- Lack of secondary analysis of the results and their implications. There needs to be further assessments of the bottlenecks in cost reduction. In short, is this pathway ever going to result in a decrease in cost? If so, what should happen and what is the likelihood of it happening?
- There is limited collaboration between this project and other projects in hydrogen storage and delivery team.
- The communication seems to be primarily with telecons. Face-to-face workshops would be helpful to ensure mutual understanding.
- It would be better if the TIAX and ANL presentations were integrated into one or if each showed the total WTW results including costs, energy efficiency, and GHG emissions in a summary slide.
- Considering the FY 2008 budget, more analyses of different storage technologies could have been achieved.
- It is stated that TIAX interacted with the FreedomCAR Technology Teams, but only the Delivery Technology Team meeting is mentioned specifically. More interaction with the OEMs and energy companies could be helpful.
- DOE is directing TIAX on what storage technologies to analyse. A thorough WTW analysis of a potential onboard "sorption" technology that operates at a variety of temperatures and pressures (-100°C to Room Temperature) and is charged with cold H₂ gas (-150° to -50°C) would be very beneficial to the HFCIT Program. This would include looking at different sorption characteristics, including those achieved to date and potential ones. This is a very promising storage technology that would give DOE a clear picture of what sorption characteristics and other parameters are needed for this approach to meet DOE targets.
- What is the best approach given the work, thus far?
- What key analyses are needed to break the logjam of viable options?

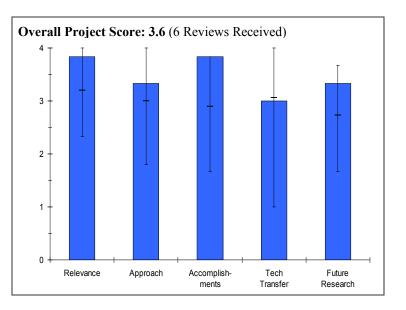
- While it may be a little out of scope, it is useful to start looking at the core issue(s) of each technology being analyzed. The objective should be to determine the major bottleneck of each technology and under what conditions they will be able to solve problems.
- Analysis should cover materials focused on within the DOE program, such as the the on-board storage material AlH₃ and its off-board regeneration.
- A thorough WTW analysis of a potential on-board "sorption" technology that operates at -100°C to Room Temperature at different temperatures and pressures and charged with cold H₂ gas (-150° to -50°C) at different temperatures, would be very beneficial to the HFCIT Program. This would include looking at different sorption characteristics including those achieved to date and potential characteristics. This is a very promising storage technology and would give DOE a clear picture of what sorption characteristics and other parameters are needed for this approach to meet DOE targets.
- More focus should be placed on key issues uncovered by the analysis and specific recommendations going forward.

Project # ST-13: System Level Analysis of Hydrogen Storage Options

R.K. Ahluwalia, T.Q. Hua, J-K Peng, and R. Kumar; Argonne National Laboratory

Brief Summary of Project

The objectives of this project are to 1) perform independent systems analysis for the DOE, 2) provide input for go/no-go decisions, 3) provide results to CoEs for assessment of performance targets and goals, 4) model and analyze various developmental hydrogen storage systems, and 5) identify interface issues and opportunities and data needs for technology development. ANL will develop thermodynamic and kinetic models of processes in cryogenic, complex metal hydride, carbon, and chemical hydrogen storage systems. Additionally, improvements needed in material properties and system configurations necessary to achieve hydrogen storage targets will be assessed.



Question 1: Relevance to overall DOE objectives

This project earned a score of **3.8** for its relevance to DOE objectives.

- This is a critical project to the overall Storage Program. It has consistently provided valuable information on the overall storage system requirements.
- On-board storage is one of the two or three most critical areas of R&D needed for hydrogen fuel cell vehicles to be successful. This project designs and analyzes the performance of potential on-board storage technologies and compares the results to the DOE targets. It is also responsible for well-to-wheel (WTW) energy efficiency and greenhouse gas (GHG) emissions of on-board storage technologies. These analyses along with WTW cost analyses done by TIAX are essential to screening out storage technologies that cannot achieve the targets and highlight the critical areas for R&D for promising storage technologies.
- This work is well balanced and has clear objectives.
- This is a highly relevant project for providing system-level analysis of hydrogen storage options for materials developed in the CoEs and independent projects.
- This is one of the core projects that make the DOE Hydrogen Storage Program such a well-run ship

<u>Ouestion 2: Approach to performing the research and development</u>

This project was rated **3.3** on its approach.

- The approach is technically sound, albeit somewhat optimistic. In this case, the built-in optimism is required for the current approach.
- ANL does its own on-board storage system design, modeling, and analysis and is quite skilled at this. In some cases, it could be more efficient to work with vendors and/or original equipment manufacturers (OEM) or others to obtain guidance and/or designs of certain components rather than always developing their own designs and models from scratch.
- The PI needs to be clearer about which DOE storage targets they are comparing to on any given slide. It would be best to always use the new DOE storage targets.
- Moving forward, it is unclear what the roles and responsibilities of ANL will be versus those of the new Engineering CoE (in terms of designing and evaluating on-board storage systems for various storage

technologies). The WTW analyses assume hydrogen is made from natural gas. This may not be the best choice as a baseline for production. It has relatively large GHG emissions, and it is intended as a means for hydrogen production only in a distributed manner at refueling stations and only during a transition period.

- The flow is appropriate and systematic including incorporation of alanes, metal organic frameworks (MOF), and ammonia borane (AB). The connection to science-based understanding is appropriate, but the options may be too broad or too comprehensive. Meaning, if budgets are being trimmed, are there options that are closer to reality for transfer to the Engineering CoE for execution?
- The project is well designed and addresses important technical barriers for different groups of materials with potential for meeting the DOE targets.
- The approach is thorough.
- It is suggested that the PI exert more effort to highlight important aspects of the analysis. It is easy for important data to be lost among other less relevant information.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated **3.8** based on accomplishments.

- The project team has delivered on all the assignments.
- ANL has made a great deal of progress over the past year and has done some excellent storage system design and performance analysis. This includes alane slurry system performance and well-to-tank (WTT) efficiency, MOF system design and performance with liquid-N₂ cooling, WTT efficiency for amino-borane systems with two regeneration schemes, and WTT efficiency of lithium allanate with a new regeneration scheme.
- The value of the work being done by ANL and TIAX on storage systems analysis would be much clearer if the last two graphical slides in the ANL back-up slides were put into their presentation. Other summaries of WTW cost, energy efficiency, GHG emissions, and performance for various storage technologies that have been analyzed would be very beneficial to the stakeholders at the Annual Merit Review.
- Solid accomplishments were seen in each of the areas, but there is no clear resolution or indication as to which are the closest to practicality. For example, are MOFs truly viable (at this stage of development) or is an ammonia borane system safe enough for the general public?
- This year's presentation (focused on MOFs and ammonia borane) must be put into the larger context of previous conclusions and suggestions.
- What stands out for transfer to the Engineering CoE?
- It was noted that the PI was flexible enough to include and perform an analysis on a very recent material from University of New Brunswick/University of Hawaii (i.e. a method for regenerating LiAlH₄). This task has been focused upon in the past without finding a satisfying solution, but now there is more promise.
- The 5.9 wt% estimate for 350 bar is much higher than what is seen in any existing 350 bar tank.
- Important analyses of AB regeneration and cryogenic MOF tanks were provided.

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated **3.0** for technology transfer and collaboration.

- There is strong collaboration with TIAX, the Storage Systems Analysis Group, and the Storage CoEs. Together, these cover a large portion of expertise in storage technology and analysis.
- It is stated that ANL interacted with the FreedomCAR Technical Teams but there is nothing specific about this in the presentation. Much more industrial company interaction with the auto OEMs, energy companies, vendors, etc. would be very helpful.
- Some collaborations were mentioned but not fully fleshed out during the presentation. In some cases, roles could be implied, but for others (e.g., FreedomCAR) they were unclear; these roles needed to be explained.
- It is not clear if there are any interactions with the Hydrogen Sorption CoE. This project builds on communicating with materials researchers; thus being update on new findings is crucial. It is also important that the results from this project are promptly provided to the experimentalists. A good discussion forum is the materials CoEs and communications could be facilitated by attending meetings with them.

Question 5: Approach to and relevance of proposed future research

This project was rated **3.3** for proposed future work.

- The future plan is detailed, constructive, and will add additional important results. The choice of storage technologies to be analyzed is well thought out.
- It would be better to make it clear that the ANL work is part of the overall Storage Systems Analysis Group and that the net result of the total effort will include the all important WTW cost, energy efficiency, GHG emissions as well as performance characteristics of the storage technologies that will be analyzed.
- Not very clear or definitive.
- Materials from different groups are being pursued, however, within the Metal Hydride CoE, there is much research focusing on borohydrides and amides, besides alane and the alanates. Are there any plans on assessing these materials? This would be useful in helping guide the materials scientists on what materials to continue developing.
- Would like to see AB analysis updated based on the new hydrazine pathway.

Strengths and weaknesses

Strengths

- Strengths include consistency, experience, a strong technical approach, and careful analysis.
- On-board storage is one of the two or three most critical areas of R&D for hydrogen fuel cell vehicles to be successful. This project designs and analyses the performance of potential on-board storage technologies and compares the results to the DOE targets. It is also responsible for WTW energy efficiency and GHG emissions of on-board storage technologies. These analyses, along with WTW cost analyses, are essential for screening out storage technologies that cannot achieve the targets and highlighting the critical R&D areas for promising storage technologies.
- ANL has made a great deal of progress over the past year and has done some excellent storage system design and performance analysis.
- There is strong collaboration with TIAX, the Storage Systems Analysis Group, and the Storage CoEs, together these cover a large portion of expertise in storage technology and analysis.
- The future plan is detailed, constructive, and will add additional important results. The choice of storage technologies to be analyzed is well thought out.
- The project team has been strong in describing work on MOFs and ammonia borane.
- The strength of this project is the feedback provided from the system analysis of different materials to the experimentalists, which is important to better understanding the potential of the materials of interest as well as improvements necessary to meet the DOE targets.

Weaknesses

- Moving forward, it is unclear what the roles and responsibilities of ANL will be versus those of the new Engineering CoE (in terms of designing and evaluating on-board storage systems for various storage technologies).
- It is stated that TIAX interacted with the FreedomCAR Tech Teams, but there is nothing specific about this in the presentation. Much more industrial company interaction between the automobile OEMs, energy companies, vendors, etc. would be very helpful.
- It would be better if it was clear that the ANL work is part of the overall Storage Systems Analysis Group and that the net result of the total effort would include the all important WTW cost, energy efficiency, GHG emissions, as well as performance characteristics of the storage technologies that will be analyzed. ANL presentations should include summary slides of the total analysis of WTW cost, energy efficiency, GHG emissions as well as performance characteristics of the storage technologies that will be analyzed.
- One of the barriers (Barrier B: system cost) is not addressed in the presentation for any of the systems.
- Recent work is not cross-referenced well with earlier work and conclusions.

- This project has been a critical element of the storage research. In view of the new engineering center and the potential duplication of effort, it is highly recommended to keep this project and preserve the institutional memory and experience.
- The project team should find a way to better connect their work with past presentations and future work, and should strive to develop more definitive recommendations.
- The project team should consider including other groups of materials that are currently focused on within the community.

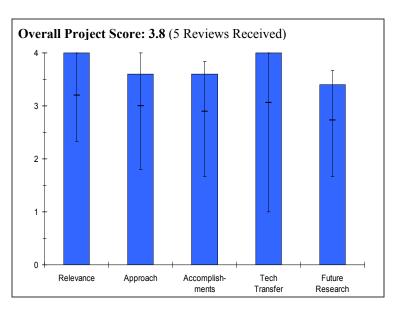
Project # ST-15: 2009 Overview - DOE Chemical Hydrogen Storage Center of Excellence

Kevin Ott; Los Alamos National Laboratory

[NOTE: This presentation was to evaluate the entire Chemical Hydrogen Storage Center of Excellence as a whole. A separate review form was used and can be found in Appendix C.]

Brief Summary of Project

The overall objective of this project is to identify, research, develop and validate advanced on-board chemical hydrogen storage systems to overcome technical barriers and meet 2010 DOE system goals with the potential to meet 2015 goals. The specific goals are to 1) develop chemistries, materials, catalysts, and new concepts to control thermochemistry and reaction pathways for hydrogen release; 2) develop and demonstrate chemical steps leading to off-board regeneration of fuel from spent fuel; 3) assess concepts and systems using engineering analysis and studies using DOE targets as guidance; 4) down-select the most promising chemical systems for more detailed work and engineering development; and 5) develop life cycle analysis.



Question 1: Approach to performing the R&D including Center Management

This project earned a score of 4.0 for its approach to R&D and CoE management.

- The CoE has been one the most coordinated teams.
- The CoE directly attacks the primary barriers to success for this method of storage. Recycling is a key challenge and they have highest focus there. Design is a challenge, and they have resources there. The use of theory to guide experiments is essential in areas of focus where data does not exist. Also, the center is looking at business-related questions that should be answered up front, which is important. For example, is there enough boron in the world?
- Overall, the CoE is very well focused on achieving a material that will meet the DOE targets.
- The CoE strategy considers engineering aspects as well as material properties (e.g., emphasis on liquid systems and Rohm and Haas engineering and analyses).
- This CoE is obviously well managed, communicates well internally, and is unusually well focused on virtually all DOE targets and technical barriers.
- There is excellent support between modeling and experimental efforts.
- The center is very well managed.
- There is good communication and interaction between CoE participants.
- There is good coordination between PIs on specific topic areas.

Question 2: Technical accomplishments and progress toward DOE goals

This project was rated 3.6 on its accomplishments and progress.

- The overall productivity of this CoE is high.
- Progress has been excellent on all three fronts: ammonia borane (AB) decomposition kinetics and thermochemistry, new materials, and regeneration of AB-based materials.

- There are several meaningful progress items, plus help for Metal Hydride CoE. Kinetics is improved in high capacity material. While new processes are good and give the center a better chance to find a regeneration scheme, the raw number of things tried is not progress. However, the reduction in the number of steps reported by the center clearly is progress. Improved efficiency is good progress, too. Also, down-selecting effectively to focus on winning strategies, which is an administrative progress in my view, is still a good way to meet targets that have not yet been attained, but that may be met with continued funding.
- The down-selection process was logical with good quantitative and qualitative criteria.
- Metal aminoborides are offering interesting new potentials.
- Important progress was achieved on improvements in the regeneration process for AB.
- The engineering cost and energy efficiency analysis of AB processing is a significant achievement.
- The \$7-8/kg H₂ regeneration cost calculations are promising relative to DOE cost targets.
- The simplified AB regeneration approach is promising. The wider issue facing this process is the infrastructure and total cycle energy efficiency.
- In terms of on-board properties, AB is close to, or can meet, some of the DOE target values simultaneously: wt. density, vol. density, operating temperature, and kinetics.
- Compared to the other CoEs, this effort seems to be technically closest to achieving a practical on-board system, given that off-board regeneration is acceptable.
- The CoE continues to make significant progress on the development of a high capacity chemical hydrogen storage material.
- Improvement continued in the properties of various forms of AB.
- The team has continued to explore other materials as well.

Question 3: Proposed future research approach and relevance

This project was rated **3.6** based on future plans.

- Given the past results, the proposed future work is logical and reasonable.
- Proposed future work builds on achievements to date and shifts focus toward identifying properties and issues relevant to engineering issues.
- The CoE has good plan but it was presented more or less as, "We will figure out what is needed and do it." The regeneration plan is right: there is a need to lower steps and global energy input to system. The center should work with ANL on what needs to be done on engineering support and address it. If history is a guide, good work will be done, but it could be better planned in this single area.
- All of this planned work cannot be completed by the March 2010 end of the CoE.

Question 4: Coordination, collaborations and effectiveness of communications within the CoE

This project was rated 4.0 for collaboration and communication within the CoE.

- This CoE has always had close coordination internally, as well as externally.
- There is a clear mechanism for formal communication, but it is also clear that the partners talk "offline" a lot. Collaboration is frequent and effective. Virtually every program references a theory group project. Most of the engineering is attached to a material person or two to help inform and improve it. Personnel exchanges are key to accomplishing these goals.
- Organization and communications are models of what a CoE should be.
- Contributions to the new Engineering CoE will be very valuable.
- As mentioned earlier, there is excellent communication and coordination within the CoE, resulting in true synergism.
- The modeling support of experimental efforts is noteworthy.

Question 5: Collaborations/Technology Transfer Outside the CoE

This project was rated **3.4** for collaboration and technology transfer outside the CoE.

- Collaboration is frequent and effective. Continue to help Metal Hydride CoE. Worked with New Energy and Industrial Technology Development Organization (NEDO) in workshop. Also, DOE partners (e.g., TIAX and ANL), are part of the International Partnership of the Hydrogen Economy exchanges and linked to the Engineering CoE as they are required to be.
- Outside collaborations are reasonably extensive and good.
- Collaborations with ANL, TIAX, and the Storage Systems Analysis Working Group (SSWAG) are especially useful.
- I would have liked to see some comments as to how useful, in fact, the international collaborations (e.g., LANL/AIST and IPHE) have been.
- Interactions with the other CoEs have not proved to be fruitful; however, this may not be due to the CoE's efforts, but rather related to differences in expertise, approach, or focus.

Strengths and weaknesses

Strengths

- There is outstanding team coordination and approach to the development of chemical hydrogen storage materials. The results from the CoE are outstanding as well.
- The CoE exhibits strong technical competency.
- There is an excellent spectrum of R&D relative to DOE needs and targets.
- The CoE effectively down-selected materials.
- The CoE is focusing on high capacity material.
- There is a good mix of theory and experimentation.
- Overall, the CoE is well managed.
- Coordination and communication are excellent.
- The CoE maintains close collaboration internally and externally.
- The people are great.
- Organization and communications are also top notch.

Weaknesses

- The chemical (off-board regeneration) hydrogen storage is arguably the largest departure from the existing transportation energy economic model. While this is not (and should not be) the focus of the CoE, it has to be addressed technically, if at all.
- There is a tough challenge to face regarding energy efficiency.
- There is uncertainty regarding the funding level or whether there will be funding at all.
- None.
- None.

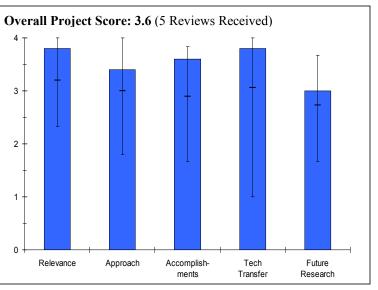
- It would be useful to consider forecourt models for the chemical hydrogen storage materials.
- Find budget to continue this work after the CoE charter is complete.
- Keep them aligned to old targets (as they intend), because they can do it. Allow them to maintain focus on regeneration.
- None.
- None in these closing days.
- Strongly consider renewal of CoE.

Project # ST-16: Amineborane-Based Chemical Hydrogen Storage

Larry Sneddon; University of Pennsylvania

Brief Summary of Project

The overall objectives for this project are to 1) develop methods for on-demand, low temperature hydrogen release from chemical hydrides that can achieve DOE targets and 2) develop high conversion off-board methods for chemical hydride regeneration. In collaboration with CoE partners, the goal of this project is to develop new methods for hydrogen release and spent fuel regeneration that will enable the use of amineboranes for chemical hydrogen storage. The University of Pennsylvania will use the activating effects of ionic liquids, chemical promoters, and/or metalcatalysts to enhance the rate and extent of hydrogen release from amineboranes.



Question 1: Relevance to overall DOE objectives

This project earned a score of **3.8** for its relevance to DOE objectives.

- Work on high-capacity liquid systems that release H₂ below 100°C can significantly improve the ability to meet targets and commercial viability for the transportation sector.
- The project is aligned with Hydrogen Program objectives and addresses key issues for one of the more promising hydrogen storage options.
- This project is closely aligned with the DOE objectives stated in the multi-year RD&D plan. The ammonia borane (AB) system has considerable potential as a high-capacity hydrogen storage material. The strong emphasis of this project is on novel methods for enhancing hydrogen release and for improving the efficiency of spent fuel regeneration in support DOE objectives. Further, it complements related activities within the Hydrogen Sorption CoE.
- This project is highly relevant. It has the potential for the development of high hydrogen gravimetric and volumetric hydrogen storage capacities and rapid release rates.
- The project aspects are generally well aligned with DOE goals and objectives for vehicular storage systems. Weight, volume, release rates, and practical regeneration of storage material are nicely addressed.
- Cost is not significantly addressed. At this rather advanced stage of the project, not to mention the strong partnership with Rohm and Haas, it would seem that preliminary costs would begin to be addressed.
- Hydrogen purity targets are not adequately addressed at least not in this presentation.

Question 2: Approach to performing the research and development

This project was rated **3.4** on its approach.

- A multi-faceted approach employing the use of ionic liquids, proton sponge additives, and metal catalysts is resulting in significant improvements in hydrogen release rates. Although the halide-based approach to regeneration is intriguing and appears to relatively straightforward and scalable, the efficiency of the spent fuel digestion step remains a serious challenge.
- The ionic liquid approach is excellent because liquids rather than solids are preferred for vehicular applications. Because of the high capacity of ammonia borane, the weight penalty associated with the ionic liquid still leads to materials with high capacities.

- The project team is thoroughly and effectively looking at three approaches for fast release of H₂ from AB: ionic liquids, chemical promotion and metal catalysts.
- Practical off-board regeneration of AB is effectively studied from both theoretical and confirming experimental chemical perspectives.
- Considering the project is in its final stages, the PI should consider making down-selects from the three approaches to concentrate on one. If no down-select is possible at this time, the PI should establish down-select criteria to help direct the work and avoid diluting his efforts.
- Work is focused on addressing key issues for the AB systems including optimizing capacity, hydrogen release kinetics, and regeneration of AB.
- The use of ionic liquids and catalysts to increase H₂ release rates is promising.
- The project team has looked at dehydrogenated AB product without IL or catalyst present. It was unclear whether this was material dehydrogenated from AB/IL or without IL. It has been suggested that the products are different. Dehydrogenated product with IL and/or catalyst present should be investigated because regeneration chemistry may be affected (positively or negatively) since they are believed to affect degree of cyclization and dehydrogenation mechanism. Initial cost studies of the regeneration scheme have identified separations as a major cost factor. It is not clear if catalysts and ionic liquids need to be separated from dehydrogenated AB for regeneration. If they do, what is separation technique, and how is it expected to affect cost of regeneration? Rhodium and ruthenium catalysts would likely need to be reclaimed during regeneration cycle also.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated **3.6** based on accomplishments.

- Progress toward the goals has been very good on all three fronts. Much new and good data has been generated during the last year.
- Impressive increases in H₂ release rate have been accomplished using ionic liquids and catalysts. A system which releases 2 equivalents of H₂ in 9 min at 110°C has been demonstrated. A system has been demonstrated with >11 wt% H₂, 0.089 kg·H₂/L (material); this exceeds DOE system targets significantly, suggesting system targets may be reached.
- Good progress is being made on parametric studies designed to improve release rates using different combinations and amounts of ionic liquid additives, proton sponge compounds, and metal catalysts at different temperatures. Although some questions about the temperature-additive-concentration behavior remain unanswered, an improved overall understanding of the factors that control hydrogen release from AB is emerging from this work.
- It was mentioned that AB-20% ionic liquid system is a solid, whereas the AB-50% ionic liquid system is a liquid. The overall characteristics of the hydrogen release kinetics would be expected to be significantly different for those two cases. It is unclear why dramatically different trends in the H₂ release characteristics are not observed experimentally.
- Significant progress has been made in reducing the amount of ionic liquid required for good hydrogen capacities and reasonable release rates.
- It seems that the recent material weight, volume, and discharge rates are close to being successfully extrapolated to DOE system targets. It would have been nice to see a little of that in the presentation.
- There are many seemingly promising AB decomposition approaches demonstrated. Which will be the most promising from a cost point of view?
- Less promising results are apparent in the area of spent fuel conversion. It is not apparent what aspects of the regeneration mechanism are limiting the efficiency of spent fuel digestion in the halide-based regeneration process.
- The super-acid regeneration approach appears to have run into a significant problem with the low yield of BX₃.
- Regeneration of AB work demonstrated BX₃ reduction. Digestion work less successful.
- Great progress on rate and equivalence continues. At this time, the PI should consider performing a rate vs. capacity comparison to determine the optimum level. Perhaps this work could be coordinated with the Engineering CoE on a system-level analysis.

<u>Ouestion 4: Technology transfer/collaborations with industry, universities and other laboratories</u>

This project was rated **3.8** for technology transfer and collaboration.

- Collaboration with other CoE members is apparent.
- Extensive interactions and collaborations with other participants in the Chemical Hydride CoE (especially with PNNL and Rohm and Haas) are evident. This contributes greatly to the overall success of project and the CoE in general.
- There are very strong collaborations between the University of Pennsylvania, PNNL, and Rohm and Haas.
- Collaborations are excellent.

Question 5: Approach to and relevance of proposed future research

This project was rated **3.0** for proposed future work.

- The project is nearing completion; it is highly recommended that the PI establish some down-select criteria.
- The focus for future work on this particular project appears to be mostly on optimizing H₂ release. Need to make sure that those working on regeneration schemes include the effects of catalysts, IL, and other additions to the system in their regeneration work.
- Speaker mentioned the need to do work to try to maintain dehydrogenated AB product in the liquid phase. That work would be very beneficial. For this project, focus can be on optimizing H₂ release if the CoE as a whole is more focused on regeneration, which is still the major hurdle for these systems.
- The approach(es) for achieving efficient hydrogen release at acceptable temperatures have been largely validated in the last two years. A solid plan is in place to develop a comprehensive understanding of the dependence of hydrogen release rate on additive type, concentration, and sorption temperature. A critical remaining hurdle to the overall success of this project is improvement in the efficiency of the spent fuel digestion to BX₃. Based upon the information provided in the presentation, the cause of the low efficiency remains an outstanding question. A sharply focused effort on understanding the rate-limiting steps should be major part of the future plan in order to develop a coherent experimental for improving the efficiency.
- The future work is directed at all of the key remaining issues.
- Plans generally aim at continued work on all the decomposition approaches. Is it time to down-select the least promising one or two approaches?
- Down-selection will require some cost and engineering considerations of the competing processes, especially decomposition.

Strengths and weaknesses

Strengths

- The PI and his colleagues constitute a very strong research team, and they are addressing the challenging issues that underlie the development of ammonia borane using novel and scalable approaches. Use of ionic liquid additives and proton sponge materials for enhancing release rates and reducing foaming are especially interesting and important.
- Use of the AB liquid phase system is highly desirable. In addition to obvious practical benefits of on-board vehicle application, it allows combinations and concentrations of reactants and additives to be readily evaluated at different temperatures.
- Use of ionic liquids should help reduce volatility of undesirable compounds and could lead to a scalable process.
- Materials being investigated have high H₂ storage capacities and good release rates at appropriate temperatures.
- Good collaboration with other CoE members.
- An understanding of the reaction chemistry is being developed.
- The PI and project approach are excellent. The PI's record of achieving significant results is also excellent.
- Excellent, innovative chemistry.

Weaknesses

• The PI should make every effort to keep desorption temperatures under 100°C. Continuous 120°C operation is unlikely in the near- to mid-term for fuel cell systems.

- Over the last two years, a clear pathway to improving the efficiency of spent fuel digestion and conversion to BX₃ has not emerged. Future plans for dealing with this critical issue are not developed particularly well.
- The regeneration approach appears to have run into a roadblock.
- At this stage, the project is a bit far from cost and practical engineering considerations. Other than the positive system implications of weight, volume and kinetics, how close are these materials to other system targets regarding cost, H₂ purity, transfer of spent product/regeneration/refilling scenarios, control considerations, etc.?
- There is potential weakness due to the complexity of the reactor system that will be required to control the reaction.

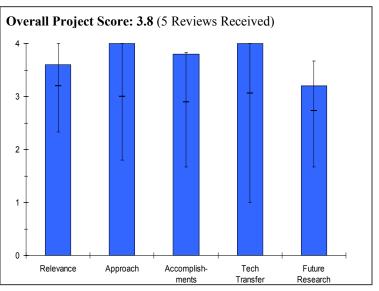
- Future work should look a little more at composition of the gas phase during H₂ release experiments in order to determine what routes avoid or minimize potentially problematic species like ammonia and borazine. Work to retain products in liquid phase for removal would be very valuable.
- Given the fact that the project is nearly complete (<20% funding remains), it is highly unlikely that all of the proposed future work on hydrogen release and spent fuel regeneration can be completed. A focused effort on the most critical issues is needed so that sufficient information is available to support a meaningful down-select of the processes and materials being investigated here.
- Since this project is 80% complete, perhaps it should focus its remaining efforts of non-precious metal catalysis for improving hydrogen generation and on alternative methods of producing BX₃.
- Given the impending time limit, the PI should focus on the best one or two decomposition approaches.
- The PI should continue to look at digestion schemes that avoid formation of B-O bonds.
- Use preliminary cost and impurity studies to aid the down-selection process.
- Begin the rough, conceptual chemical engineering design of an on-board system in relation to the required regeneration processes.
- The PI should work with the Engineering CoE to establish a rate vs. capacity comparison. As the rate of the reaction increases, the potential complexity and mass/volume of the "balance of plant" could decrease, thus saving weight (i.e., less buffer tanks, reactor volume, etc.) However, if the rate increase comes at the cost of a material weight decrease, a tipping point may occur where a further increase in rate may lead to a heavier overall system.

Project # ST-17: Chemical Hydrogen Storage R&D at Los Alamos National Laboratory

Roshan Shrestha, Ben Davis, Himashinie Diyabalanage, Anthony Burrell, Neil Henson, Michael Inbody, Kevin John, Troy Semelsberger, Frances Stephens, John Gordon, Kevin Ott, Andy Sutton, and Koyel Bhattacharyya; Los Alamos National Laboratory

Brief Summary of Project

The objectives for this project are to 1) develop and demonstrate heterogeneous catalysts and continuous flow reactor operation for hydrogen release, 2) develop liquid ammonia borane (AB) fuels and increase rate and extent of hydrogen release, 3) identify and demonstrate new materials and strategies for near-thermoneutral hydrogen release, 4) demonstrate all chemical steps and conduct engineering assessment for energy efficient AB regeneration process (high yields, rates and energy efficiency, integrate steps when possible), 5) develop materials and processes to minimize gas phase impurities and demonstrate adequate purity of hydrogen stream, and 6) provide materials



chemistry support for the Pennsylvania State University work on electrochemical conversion of B-O to B-H.

Question 1: Relevance to overall DOE objectives

This project earned a score of **3.6** for its relevance to DOE objectives.

- Aminoborane materials are potentially very important towards achieving the DOE objectives.
- The project is well aligned with key problems of AB regeneration, hydrogen gas impurities, low system penalty in use, and the need for better materials. Also, the overall goal of chemical hydrogen storage is aligned with meeting the needs of the vehicle H₂ system.
- Chemical hydrogen storage approaches have the potential to achieve high hydrogen storage gravimetric and volumetric capacities with rapid hydrogen release rates, in a liquid form that is amenable for vehicular applications.
- This project is unusually relevant to almost all of the DOE on-board targets and perceived barriers.
- The work covers multiple aspects, relating to both engineering and materials, of the use of AB as a hydrogen storage material.

<u>Ouestion 2: Approach to performing the research and development</u>

This project was rated **4.0** on its approach.

- LANL, as the CoE lead for chemical hydrogen storage materials, is working on all necessary fronts to make AB materials achieve targets (e.g., catalysis, hydrogen gas impurity reduction, AB regeneration). They are coordinating heavily with all the necessary partners and experts.
- The effort is rather highly funded, but correspondingly covers many useful technical areas. Looking at Msubstituted AB, liquid AB forms, heterogeneous catalysis, and thermodynamic control are all well-placed directions.
- A simplified "single pot" AB regeneration process is the ultimate goal for realizing commercial AB use.
- The materials examined are appropriate; the work to reduce energy intensity and number of steps is spot on; and the catalyst work is also aimed squarely at kinetic and H₂ purity challenges. Science guided by a combination of theory and engineering is the appropriate approach.

- Science guided by theory and engineering is the best approach for the DOE portfolio.
- The approach is targeted at all the key issues.
- The approach covers both on-board H₂ release and AB regeneration, both very important.
- The effort is unusually well focused at the ultimate application (e.g., engineering, cost, impurity) factors.
- The effort on regeneration is very logical and thorough.
- This is a good approach covering new materials exploration and development, as well as specific aspects of AB.
- The focus on targets is maintained when exploring new materials and their properties.

<u>Ouestion 3: Technical accomplishments and progress toward project and DOE goals</u></u>

This project was rated **3.8** based on accomplishments.

- The project team has made many significant accomplishments.
- The project was well presented, and it is obvious that much excellent progress has been made on many fronts.
- The catalysts shown reduce impurity production and raise rate.
- Important contributions were made toward individual process steps in AB regeneration.
- Development of a 1- or 2-step regeneration process for AB is an important development.
- The project team had the guts to scrap a working regeneration system and come up with one that avoided highenergy mass movement and reduced total steps to gain efficiency.
- The project team managed to find a simpler and more efficient regeneration method even when it had a process that worked before.
- Important contributions were made toward cost analysis of AB regeneration.
- There are interesting differences in kinetics and thermodynamics as a function of metal substitution.
- The project team managed to reduce the exothermic nature of the reaction (a necessary step towards simplified systems). The results varied significantly, and the PI needs to continue efforts to understand why. The PI should be coordinating with the Engineering CoE to determine the optimal exothermicity of the system.
- What effect on material density is incurred by the addition of salts to the AB in order to reduce the thermodynamics?
- KAB material gives sub-100°C one-step release, which is very nice. It would be better if a similar, lighter material could be crafted based on what was learned here.
- The project team has made significant progress toward characterizing and understanding impurity release from AB.
- Catalysts seem to be a key variable in reducing impurity emissions from decomposing AB; however, can the impurity levels ever be reduced to the levels required for fuel cells or will an on-board purifier always be required?
- There are so many promising results that down-selection of the best possibilities will be difficult.
- The project team found promising alternatives to Pt for heterogeneous catalysts.
- The project team examined a number of AB liquid alternatives in terms of impurity release.

<u>Ouestion 4: Technology transfer/collaborations with industry, universities and other laboratories</u>

This project was rated **4.0** for technology transfer and collaboration.

- The collaborations with Rohm and Haas, ANL, TIAX, etc., are nicely getting to the bottom of cost, practical reactor designs, and practical regeneration processes. These are impressive group efforts.
- Outstanding the project team works with everyone in the CoE and many outside too. The team got significant value from ANL collaboration. The IPHE partnership may answer some key questions, and it is nice to see that initially politically driven activity bear technical fruit.
- Collaborations are excellent and are targeted at key issues.
- There are many excellent collaborations within the Chemical Hydrogen Storage CoE and outside.
- The project team is working with all the relevant material partners. The team should now coordinate with the Engineering CoE to understand the system.
- The planned connection to the new Engineering CoE will be very valuable.
- Work includes effective collaborations and interactions with others inside and also outside of the CoE.

Question 5: Approach to and relevance of proposed future research

This project was rated **3.2** for proposed future work.

- The project is near completion.
- This project should work with Engineering CoE to both address system-related requirements of materials and begin transferring knowledge to the Engineering CoE.
- Future plans are in right areas (i.e., AB regeneration, enough engineering to guide mechanism selection, and storage stability). Future plans seem well conceived, though details are scant.
- The future work is comprehensive and targeted at the key issues.
- In general, the plans listed are logical and needed.
- Given only 20% remaining in the project duration and funding, it is hard to see that so much can be done.
- Some near-term down-selection is needed.
- Proposed focus on the new AB regeneration process should be an important contribution to the development of an effective storage material.

Strengths and weaknesses

Strengths

- This is a very well-coordinated effort aimed at almost all the DOE targets and barriers.
- This is a strong team.
- The project team has good approaches.
- Connections have helped the team make progress.
- High capacity material to develop.
- The project team is organized.
- The project team has made the hard choices.
- There is a potential for high hydrogen gravimetric/volumetric capacities and rapid hydrogen release rates.
- Aminoborane-based materials are targeted for a liquid form, which is more amenable for vehicular applications.
- Ultimate thinking is practical and realistic.

Weaknesses

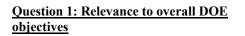
- The barrier to meet on AB regeneration efficiency and yield at the same time is high.
- The funding is uncertain.
- The cost of regeneration is the key issue going forward.
- None.

- Keep these guys working in 2010, and try to fund them afterwards.
- None.
- Other than careful down-selections and focus for the project duration, no real changes are recommended.

Project # ST-18: PNNL Progress as Part of the Chemical Hydrogen Storage Center of Excellence *Tom Autrev: Pacific Northwest National Laboratory*

Brief Summary of Project

The CoE's objectives for this project are to 1) develop methods for on-demand, low temperature hydrogen release from chemical hydrides that can achieve the DOE targets and 2) develop high efficiency off-board methods for chemical hydride regeneration. PNNL's goal is to meet the CoE objectives through studies and development of high capacity chemical hydrides that increase kinetics while maintaining high capacity.



Overall Project Score: 3.6 (5 Reviews Received)

This project earned a score of **3.8** for its relevance to DOE objectives.

- The project addresses the DOE objectives, targets, and barriers very well.
- This work is highly relevant to the development of high capacity hydrogen storage materials.
- Regeneration of, and low temperature and high purity hydrogen carriers are good foci. These materials are likely to bear fruit, and are thus good choices.
- Ammonia Borane (AB)-based materials have the best combination of hydrogen gravimetric/volumetric capacities and rapid hydrogen release rates.

<u>Ouestion 2: Approach to performing the research and development</u>

This project was rated **3.2** on its approach.

- The approach is very well balanced to include experimental work, theoretical modeling to support the experimental work, and engineering activities.
- The project is very well focused on developing high capacity materials for hydrogen storage.
- The project team is using the right tools and studying suitable hydrogen storage materials (AB variants), guided by internal and external theory.
- The approach is heavier on experimental than theoretical. This is appropriate given the complexity of the chemical systems.

This is a relatively large effort, by DOE standards, and generally addresses many important subjects both in the H_2 generation and storage material regeneration directions.

- The project focuses somewhat more on fundamental mechanisms and reaction pathways than the LANL effort. Also, the AB regeneration approach is apparently somewhat different from that of LANL's and UPenn's. As such, the PNNL work seems to be generally complimentary to that of the other CoE partners.
- It is not completely clear how the metal amino borane (e.g., LiNH₂BH₃) differs from the large effort in this by LANL. Is there some duplication?

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated **3.6** based on accomplishments.

- A wealth of new and positive data has been generated in the last year.
- Stabilizing AHBH in solution is important step.
- An approach was developed to mitigate foaming during pure AB hydrogen release.

- Antifoaming agents are a big step, though much of it previously reported.
- Clever process to activate the hydrogen so it will react more easily with spent fuel.
- Tuning the BOX species being regenerated is important, and the further tuning most likely lowers energy requirements.
- The PNNL regeneration approach seems to be approaching a final state (i.e., beginning cost and engineering modeling [with ANL, Rohm and Haas, etc.]). It will be interesting to soon make the final comparison with the somewhat different LANL (Pennsylvania) regeneration approach.
- Many significant accomplishments have been made. The room-temperature-stable ammonium borohydride is very interesting.
- Progress has been made in morphology control (antifoaming), thermodynamic manipulation, decomposition kinetics quantification, and impurity control.
- The relatively new work on NH₄BH₄ (ABH₂) is to be highly praised. It will be difficult to safely apply, but offers some fantastic vehicular possibilities in terms of weight and volume.
- The project team made important contributions to understanding impurity release from AB variations.
- The work has expanded to investigate M-NH₂-BH₃ materials.
- The project team developed capability to make lab-scale amounts of AB for use in its experimental studies.
- The project team completed a number of kinetic studies on materials and improved release properties in some cases.
- The project team developed a way to improve stability of NH₄BH₄ at room temperature.
- Work to determine hydride transfer reactions for various metal hydrides was continued.

<u>Ouestion 4: Technology transfer/collaborations with industry, universities and other laboratories</u>

This project was rated **4.0** for technology transfer and collaboration.

- Good communication and collaboration inside and out of the CoE to achieve value in the work. Examples include University of Alabama, etc. collaboration on theory for cost and efficiency and work with the International Partnership for the Hydrogen Economy (IPHE) and others.
- PNNL is covering solid aminoborane, while LANL is covering aminoborane in liquid form.
- There are many good collaborations, which are generally well explained.
- Other than mentioning the area of M-substituted AB, the exact nature of the IPHE collaboration is not well documented. At this stage, what can be said about the synergism of the IPHE effort and its likely benefit to the United States and DOE? Is there potentially more benefit coming out of the International Energy Agency collaborations?
- There have been effective collaborations with CoE participants and with other researchers.
- There have been a broad number of partnerships.

<u>Ouestion 5: Approach to and relevance of proposed future research</u>

This project was rated **3.2** for proposed future work.

- Future work covers all of the key areas.
- The proposed future work seems like a logical and reasonable extension of the past work and results. Batch reactor work is appropriate as is cost analysis.
- Impurity reduction is appropriate.
- AB Regeneration plan is appropriate.
- It seems very unlikely all this work can be reasonably completed by March 2010 the project's end.

Strengths and weaknesses

Strengths

- Strengths of this project include:
 - A strong team.
 - The right material.

- o Strong method.
- Excellent benefit from collaboration.
- High hydrogen gravimetric and volumetric capacities.
- o Rapid hydrogen release rates.
- Excellent understanding of what is needed for the chemistry of AB decomposition and regeneration.

Weaknesses

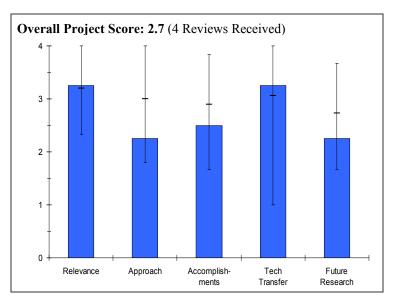
- Weaknesses of this project include:
 - Funding at risk.
 - Solids handling for vehicular applications.
 - Efficiency and cost of AB regeneration.
 - o None.

- The project team would benefit from the same engineering guidance LANL uses at this point. The team may be planning to do that sort of review, but this was not clear.
- The project team should follow up on NH₄BH₄ stability work because of the high capacity, but should eliminate the use of the NH₃ stabilizer as they see fit.
- Phase 2 (if it is justified and funded) should be completely consolidated with LANL. Two parallel efforts cannot be afforded. Down-selections will have to be applied.

Project # ST-19: Main Group Element and Organic Chemistry for Hydrogen Storage and Activation Anthony J. Arduengo and David A. Dixon; University of Alabama

Brief Summary of Project

The objectives of this project are to 1) develop promising approaches to chemical hydrogen storage for current and future DOE targets using computational chemistry and synthetic organic/inorganic chemistry and 2) provide computational chemistry support (i.e., thermodynamics, kinetics, properties prediction) to the experimental efforts of the DOE CoE for Chemical Hydrogen Storage to reduce the time to design and develop new materials that meet the DOE targets. Experimental focus is on organic and main group chemistries which may be able to perform better for release and regeneration by improving the energy balance. This will provide longer term alternatives.



Question 1: Relevance to overall DOE objectives

This project earned a score of **3.3** for its relevance to DOE objectives.

- This project fully supports DOE program objectives. The computational approaches are yielding results on thermodynamic properties, hydrogen release, spent fuel regeneration pathways, and discovery of new compounds with improved sorption characteristics. Those results are vital to the overall success of the Chemical Hydride CoE, and the work is directly relevant to DOE RD&D objectives for hydrogen storage.
- The project aims to develop new approaches for meeting DOE targets for H₂ storage using computational chemistry; it is well aligned with the DOE objectives.
- The PI's efforts seem to be valued by the experimental members of the CoE.
- This project couples strongly with many activities in the Chemical Hydrogen Storage CoE, and is helpful in understanding experimental results. However, the overarching goals of this effort are not entirely clear. What exactly are they looking for? The results seem somewhat scattered and not focused on a specific goal.

Question 2: Approach to performing the research and development

This project was rated 2.3 on its approach.

- A comprehensive computational effort comprising multiple approaches is being used to predict thermodynamic properties and reaction pathways for candidate chemical hydrogen storage systems. Experimental validation of these predictions is made both within the project and through extensive collaborations with CoE partners. The molecular orbital and density functional theory approaches are powerful adjuncts to the experimental efforts in the CoE, and they are being used to determine thermodynamic properties and to identify new compounds with improved sorption properties.
- Kinetics issues have received less attention in the project. Accurate predictions of reaction rates, identification of transition states, and elucidation of elementary steps in reaction mechanisms remain important challenges.
- The PI has expertise in quantum chemistry calculations, and it shows in the choice of problems that are included in the project. The calculations are restricted to liquids and gas phase molecules, but there is no work on solids; this is an obvious shortcoming of the approach and scope of research.

- The project uses an "enumerative" approach to calculating thermodynamics of all imaginable reactions (>500); a more systematic approach to identifying desired reactions with targeted thermodynamics would be preferable to what is currently a computational "trial-and-error" technique.
- Overall, a large number of molecules are being considered, and the project seems a bit unfocused.
- Relevance of gas phase calculations to real solid-state materials has not been established. This comment was made previous Reviews but has not yet been addressed.
- For the amidoborane work, the PI is starting with the molecular state, and says that this will help them when they move to the solid state. However, for several years, this PI has been saying that they will move to solid-state calculations, but it never seems to happen. In this case, how will they obtain the crystal structures for the metal amidoboranes? When they have them, how will they do the quantum chemistry calculations? (The methods used by this PI are only applicable to molecules and clusters, but not solids.) There are a lot of literature of solid-state calculations in these and related (e.g., complex hydride) systems for consideration.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated 2.5 based on accomplishments.

- A significant database on the thermodynamics of hydrogen release and regeneration from candidate compounds has been generated. This is very useful for guiding experimental work both within this project and by CoE partners. A large number of potentially useful systems are being explored in this project. This is a useful and important complement to the sharply focused efforts on ammonia borane (AB) being conducted elsewhere within the CoE.
- Although new systems are being investigated, there are several important outstanding issues concerning the efficient regeneration of ammonia borane that are also being addressed. The work on this project is providing information that will undoubtedly be important overcoming existing obstacles to efficient conversion of spent reactants.
- It would be helpful if more information could be provided concerning the predictive accuracy and reliability of the kinetics calculations. The project has amassed a large amount of data on reaction kinetics and thermodynamics. However, there does not seem to be many breakthroughs in materials, regeneration reactions or theoretical methods that show promise for making significant progress towards meeting the DOE goals.
- Not clear that the experimental portion of this project is really producing useful results. They had a no-go on the main experimental chemistry they were pursuing, but it's not clear what they are doing now or whether they are making progress. For a program in its fourth year, this is quite disappointing. The budget is just far too large to justify the results obtained.

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated **3.3** for technology transfer and collaboration.

- The collaborations have been extensive, especially with experimentalists within the Chemical Hydrogen Storage CoE are evident.
- The computational effort in this project is fully integrated with other projects in the CoE, and the collaborations are yielding positive results.
- The project has a very well-developed collaborative network. This is an area of strength.
- Collaboration seems to be a strong suit of this project.
- There is a good connection between the computational effort and the CoE and other partners. The connections between the experimental efforts and other collaborators are less clear.

Question 5: Approach to and relevance of proposed future research

This project was rated 2.3 for proposed future work.

- Reliable thermodynamics predictions for "thousands of compounds" have been made in this project.
- Given the existence of that vast database, it is not entirely clear why additional predictions are needed. On the other hand, if new work is warranted, it would be helpful to understand what rationale is being employed to identify and explore other systems.
- What approaches will be used to predict kinetics of the key steps in the regeneration process? How is the reliability of model predictions for hydrogen release kinetics and rates of selected steps in the regeneration process being established?
- The very broad scope of the proposed future work is inconsistent with the time and funding available for the project. A thoughtful examination of the most critical remaining issues is needed, and the future work should be prioritized to reflect those considerations.
- The project will continue using the same methods as previously; there does not seem to be a clear path to success that could improve future accomplishments.
- Many (eight) routes listed in future work slide, with limited remaining time in the CoE, suggest focusing efforts on a smaller number of avenues for study.
- Far too much future work is proposed given that only one year of funding remains. The work needs to be prioritized, and it is unclear which work is the most important and which work will not be completed.

Strengths and weaknesses

Strengths

- The computational work on this project is a critical element of the overall technical effort within the Chemical Hydrogen Storage CoE. Valuable information concerning reaction thermodynamics and the identification of improved storage compounds has been generated in the project.
- The PI and his colleagues are highly qualified to conduct this project. The computational approaches they have employed and the results that have been obtained thus far have greatly aided the search for improved candidate storage systems.
- The project team has shown expert use of computational chemistry tools to study gas phase molecules and liquids. The collaborative network has been well developed. The project team has accumulated a large amount of computational chemistry results for molecular reactions.

Weaknesses

- There are many directions being pursued in this project. It is not clear which barrier or problem is considered to be the most challenging and should therefore receive the most attention. At this point in the overall technical effort, it would seem that a more focused effort on only a few critical issues is needed.
- This project needs a stronger focus. It would benefit from developing systematic computational framework for finding new, attractive reactions. There are no realistic plans to extend calculations to solid phases.

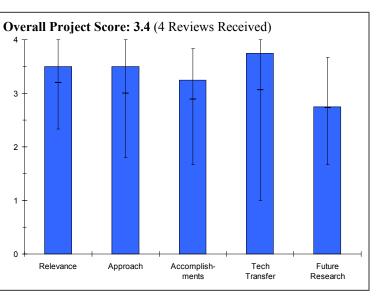
- Improving the efficiency of spent fuel conversion is the most critical remaining issue facing the Chemical Hydrogen Storage CoE. Recommend a sharply focused computational effort in close collaboration with experimentalists to address the regeneration issue.
- The experimental effort of this project does not seem to be producing useful results. It appears as though it could be deleted from the project scope without significantly affecting the overall project goals.

Project # ST-20: Low-Cost Precursors to Novel Hydrogen Storage Materials

S. Linehan, N. Allen, R. Butterick, A. Chin, L. Klawiter, F. Lipiecki, S. Nadeau, and S. November; Rohm and Haas Company

Brief Summary of Project

The overall objectives for this project are to 1) develop and advance novel hydrogen storage materials that meet the DOE 2010 targets and with the potential to meet 2015 targets, 2) leverage expertise and experience across the CoE, and 3) support the DOE Chemical H₂ Storage Systems Analysis Sub-Group. The Phase 2 goal is to identify cost- and energy-efficient pathways to "first fill" and regeneration for ammonia borane (AB) and other borane materials, define and evaluate novel chemistries, and process for producing chemical hydrides.



Question 1: Relevance to overall DOE objectives

This project earned a score of **3.5** for its relevance to DOE objectives.

- The project is quite relevant to the DOE storage mission. Low-cost precursors to NaBH₄ are necessary not only for the chemical center but can also have application for the metal hydride center.
- The work has high relevancy and is consistent with the overall CoE direction.
- The project addresses the critical issue of cost for first fill and cost for AB regeneration of one of the most promising hydrogen storage options.
- Reducing the cost of NaBH₄ is crucial to reducing the cost of ammonia borane for chemical hydrogen storage.

Question 2: Approach to performing the research and development

This project was rated **3.5** on its approach.

- The project team is very well focused on the key issues in its approach.
- The approach is working along three paths: 1) cost analysis for regeneration of AB, 2) a first fill AB process analysis, and 3) low-cost NaBH₄ for the first fill. The approach is good in that several different strategies are being investigated. The low-cost NaBH₄ process work is looking at different routes for converting B-O bonds to BH bonds.
- Considerable expertise and knowledge in the area including commercial application and scale.
- The project is focused on costs of producing NaBH₄ cheaply for first fill and AB regeneration. A company with extensive experience in chemicals market should provide a reliable cost estimate with good credibility.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated **3.3** based on accomplishments.

- Reactive milling and solution-based systems for reduction are progressing well. Estimates of more than an order of magnitude reduction in NaBH₄ cost leads to substantial savings in first-fill cost.
- Separations have been identified as being responsible for a huge portion of costs for regeneration. In the LANL AB regeneration route, areas for significant cost savings have been identified.
- First fill and regeneration costs of amido borane have been estimated with a high degree of confidence.

• The project is 80% complete and a decision between borohydride production via a chemical route versus a carbothermal route has not been made. Similarly, a replacement for tin in the chemical route has not been found. Remaining effort should be directed toward one route so that there are time and resources left for a meaningful contribution from this project. The time remaining on this project is relatively short; it is difficult to see that all the process development work will be far enough along to provide a comfort level that the process(s) is feasible.

<u>Ouestion 4: Technology transfer/collaborations with industry, universities and other laboratories</u>

This project was rated **3.8** for technology transfer and collaboration.

- As part of the overall structure of the CoE, this work is well integrated with the rest of the program. Understanding that the scopes may change quickly, it would have been useful to look at the two-step regeneration process.
- Collaboration within the CoE appears to be working well. There is collaboration with TIAX on cost analysis; TIAX well established in the Hydrogen Program for cost estimates.
- Excellent collaborations are taking place.
- There has been excellent collaboration within the Chemical Hydrogen Storage CoE. The Rohm and Haas work is well integrated within the center.

Question 5: Approach to and relevance of proposed future research

This project was rated 2.8 for proposed future work.

- Proposed down-selection between carbothermal and metal reduction is appropriate. Plans to investigate cost of AB first fill using alternative routes (PNNL and Shore schemes) are appropriate.
- Future work is directed at the key issues.
- Is the plan to repeat the same process for the two-step AB process?
- The project is scheduled to end in March 2010 and may end prematurely depending on available funding. The future work plan should include some down-selection points.

Strengths and weaknesses

Strengths

- Dow Chemical's experience is a strength.
- The project team has an excellent strategy and approach for manufacturing cost estimates.
- It is good to investigate multiple routes to lower-cost precursors. Analysis tools appear to be effective in guiding the work. Rohm and Haas brings industrial process development expertise to the team.

Weaknesses

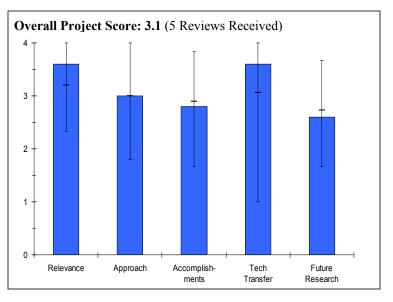
- None.
- Little data has been shown on the carbothermal route. In fact, earlier work at INL cannot be reproduced. It is not clear how much longer this path should be continued if the results are poor. Suggest that this path have a near-term go/no-go decision point.
- Process efficiency for either route is low. Projections appear to point to routes with higher efficiency, but this has not been demonstrated.

- It would be useful to also consider the business model implication for this technology. The PIs have considerable knowledge in the commercialization. One of the weaknesses of this route is the question of competitive distinctions among the manufacturers if there are to be multiple providers of AB. It is not clear how this market functions aside from being a monopoly. If so, is this a feasible approach? Why should there be additional effort or resources devoted to this route? (Granted the proposed technology has many more immediate challenges.)
- Perhaps the carbothermal approach for NaBH₄ production should be discontinued, since the initial results have not been promising.

Project # ST-21: Ammonia Borane Regeneration and Market Analysis of Hydrogen Storage Materials David Schubert, Jonathan Owen, Duane Wilson, and Larry Harrower; U.S. Borax

Brief Summary of Project

The objectives of this project are to 1) meet the need to maximize efficiency of offboard regeneration of ammonia borane (AB) fuel and 2) provide an understanding of global supplies of boron ore resources required for hydrogen storage. This project will 1) find recyclable thermodynamically favorable intermediates, 2) collaborate with PNNL and other CoE partners to maximize efficiency of AB regeneration, 3) tune chemistry of borate esters as hydride acceptors in PNNL's AB regeneration cycle, 4) develop a better understanding of global supplies of boron ore resources required for hydrogen storage, and 5) develop a resource model applicable to other materials of interest for hydrogen storage (e.g., lithium and magnesium).



Question 1: Relevance to overall DOE objectives

This project earned a score of **3.6** for its relevance to DOE objectives.

- The project is quite relevant to the objectives of the Chemical Hydrogen Storage CoE, which is focusing on ammonia borane as the storage material with the most promise. A sufficient source of boron is necessary if this fuel will be a large-scale substitute for gasoline.
- Study of borate resources important in establishing long-term feasibility of chemical hydrogen storage with ammonia boranes as well as several borohydride systems proposed in the Metal Hydride CoE for large vehicle fleets.
- AB Regeneration is currently the major hurdle for materials being investigated in the Chemical Hydrogen Storage CoE.
- The issues/barriers addressed in this project include hydrogen storage system cost, efficiency, AB regeneration, and system life cycle assessment (i.e., availability of boron and other constituent elements).
- The FY 2009 focus was on maximizing efficiency of off-board regeneration of AB fuel and on determining the size of present day, known, global borate resources.
- The viability of boron sources is critical to the AB chemical hydrogen storage approach. It is also important for a number of metal hydrides.

Question 2: Approach to performing the research and development

This project was rated **3.0** on its approach.

- The project team is looking at borate esters for AB regeneration based on guidance by theory at PNNL. Borate esters are being prepared guided by theory, with experiments feeding back to help validate theory.
- The model for Boron reserves is less conservative than that of the U.S. Geological Survey, and likely more realistic. Estimating future boron demands is a good approach, but has considerable uncertainty.
- The project team is using alcohols for digestion of spent ammonia borane to produce borate ester intermediates.
- Properties of aryl borate esters have been tuned to yield thermodynamically favorable AB regeneration intermediates and validating computations. (The overall approach focuses on tuning the chemistry of the critical digestion and reduction steps of the AB regeneration process.)

- Established global reserve estimates through review and analysis of publicly available information sources to quantify borate resources.
- The assumption of 15% hydrogen storage in ammonia borane used for boron demand may be a bit on the optimistic side.
- U.S. Borax (USB) most likely is the best source of information regarding world borax reserves. They have a good understanding of the global economics of the boron industry. They are looking at boron resources in the context of other competing economic uses of the ore.
- They are also looking at synthesizing several aryl borate esters that may lead to thermodynamically favorable regeneration intermediates that the CoE can use to validate computations for the AB regeneration process with metal hydrides.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated 2.8 based on accomplishments.

- This is a new project. The project team has had a good start on obtaining significant results.
- The project is still in early stages.
- Several borate esters have been prepared for AB regeneration testing by PNNL.
- U.S. Borax is proceeding with the synthesis of a large set of borate esters of several types to be supplied to PNNL for experimental validation of theory/basis for proposed AB regeneration process. U.S. Borax has begun sending borate esters to PNNL for testing.
- Several esters have been synthesized and provided to PNNL to validate some of the reaction steps in AB regeneration.
- The project is new. Borate reserves work indicates there are sufficient borate resources in the United States to meet U.S. demand for H₂ storage in the U.S. vehicle fleet in 2050.
- First order estimation of U.S. and global borate reserves has been completed by U.S. Borax. In this analysis, account is taken of consumption by competing applications through initial fill timeframe for the first fleet of fuel cell vehicles (FCV). A key finding is that present day known U.S. borate resources are sufficient for projected U.S. FCVs and competing boron needs through 2050.
- The initial assessment of boron resources indicates that there are sufficient supplies of boron to accommodate the widespread introduction of FCVs, as well as meet the current demand for boron-containing chemicals.

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated **3.6** for technology transfer and collaboration.

- Collaboration with PNNL is apparent and appears to be working well.
- The project claims to be highly collaborative and is. The collaborators are PNNL, LANL, and Rohm and Hass. There is a clear role for each member institution.
- This seems to be an effort that is being taken very seriously by the Chemical Hydrogen Storage CoE.
- This project team appears to have excellent collaborations with PNNL, LANL, and Rohm and Haas.
- Collaboration is excellent within the Chemical Hydrogen Storage CoE.

<u>Ouestion 5: Approach to and relevance of proposed future research</u>

This project was rated **2.6** for proposed future work.

- The future work covers the appropriate bases.
- The project team plans to:
 - Synthesize a larger set of borate esters of several chemical types for AB regeneration studies at PNNL.
 - Perform spent fuel digestion studies.
 - o Participate in AB regeneration cycle validation in collaboration with PNNL.
 - o Provide analytical support, safety analyses, and other required consultation.
 - Further refine boron global reserve data.

- Analyze important questions regarding industry impacts of hydrogen storage technologies and market parameters, including impacts on competing uses and impacts on borate prices.
- Ramping up production to meet first fill requirements could result in excess capacity as spent AB will likely be recycled back to AB.
- It is not clear how the new acetate development will help the overall project.
- The project team could provide more details on future work.

Strengths and weaknesses

Strengths

- U.S. Borax represents a knowledgeable partner for AB regeneration process development and borate resource assessment.
- U.S. Borax's cost share is a relatively large fraction of the total budget.
- Close collaboration appears to exist between U.S. Borax, Rohm and Haas, PNNL, and also LANL.
- The project team is working with the major U.S. supplier of boron.
- U.S. Borax brings extensive knowledge of the boron industry to bear on the production and regeneration of ammonia borane. They are a good addition to the center team.

Weaknesses

- There are no obvious weaknesses.
- None.
- Market projections would be more comprehensive if worldwide demand for boron were estimated assuming FCVs are widely adopted throughout the rest of the world and not only in the United States.

- It seems from the funding numbers presented by U.S. Borax that the project was perhaps slightly under-funded by DOE in FY 2009. This project needs to receive the full amount of the requested budget. As that budget is understood, DOE is putting up \$300K total and U.S. Borax is putting up ca. \$350K.
- Perhaps there should be a little more emphasis on helping to reduce the cost of AB regeneration.

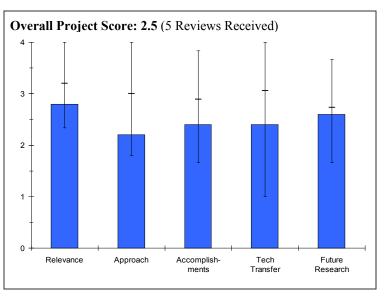
Project # ST-22: Overview of the DOE Hydrogen Sorption Center of Excellence

Anne C. Dillon and Lin J. Simpson; National Renewable Energy Laboratory

[NOTE: This presentation was to evaluate the entire Hydrogen Sorption Center of Excellence as a whole. A separate review form was used and can be found in Appendix C.]

Brief Summary of Project

The overall goals of the DOE Hydrogen Sorption CoE are to 1) discover and develop high capacity sorbent materials that can operate near ambient temperatures and at moderate pressure and be efficiently and quickly charged on board with minimum energy requirements and minimum penalties to the hydrogen fuel infrastructure and 2) overcome barriers to 2010 DOE system goals and identify pathways to meet 2015 goals. Objectives are to 1) develop materials which utilize mechanisms that bind hydrogen with an optimal energy for near room temperature operation (15-20 $kJ/mol \cdot H_2$; 2) rapidly correlate capacity, structural, and energetic information to reduce time between discovery, assessment.



and down-select; 3) integrate experiment and theory seamlessly in both "feedback" (explanation) and "feedforward" (discovery) modes; 4) devise facile synthetic routes using low-cost approaches; and 5) create a nimble, flexible yet structured, teaming environment to accelerate discovery, evaluation, and selection of promising development directions.

Ouestion 1: Approach to performing the R&D including Center Management

This project earned a score of 2.8 for its approach to R&D and CoE management.

- A broad-based R&D effort is being conducted by the Hydrogen Sorption CoE. The CoE is managed well, and the use of research clusters is a useful approach for subdividing the comprehensive technical effort and avoiding duplication. Close attention is being paid to down-select criteria, and that is providing a straightforward, efficient way to focus the technical work within the Center.
- There is a good balance between universities, national labs, and industry, as well as between computational and experimental efforts within the CoE.
- The research cluster (RC) approach for organizing project topics is appropriate and efficient and the CoE resources (i.e., task mix) are well balanced. Moreover, the specific topic breakdown by sorption mechanism is productive for fostering collaboration by grouping projects that tend to have common synthesis, characterization, and motivation.
- The complementary "clusters" research approach is good in general. However, there is a real need for close coordination among all the clusters.
- The technical barriers appear to be hard to overcome based on the current progress. The CoE relied too much on theoretical estimation rather than using it in a supportive role.
- The approach seeks to develop materials that operate from "100K to 350K with no significant thermal management issues to efficiency [to] meet DOE targets." Given the recent energy efficiency analysis of liquid nitrogen (LN₂) cooling of a cryogenic storage medium by Argonne (ANL) (for metal organic framework [MOF]-177), is the CoE going to focus on reducing this relatively large energy input? Similarly, if the intention is to raise the temperature in the storage bed in order to access lower pressure (below the 3 bar min. delivery pressure), how would this mode of operation (P & T swing) compare with an isothermal mode of operation (e.g. only P swing) from efficiency and dormancy perspectives?

- It is nice to see focus on volumetric capacity (e.g., Argonne (ANL) volumetric capacity, gravimetric capacity, material density plot). The gravimetric versus volumetric capacity plots in future accomplishments slides are very insightful for demonstrating progress. However, are these volumetric capacity values based on single crystal materials densities or based on that for powders, tablets, etc.?
- It is not clear what metrics and decision-making tools are used to down-select various research directions.
- The director says that sorbents meet 13 of 16 targets, but this is somewhat irrelevant. First of all, the most important 3 targets are the ones that are not met and secondly, the targets must all be met *simultaneously*.
- It was stated that there are viable paths to achieve the "ultimate" targets (all of them). However, the issue of volumetric densities is still a real concern. There should be serious attention paid to this issue. What is the highest (measured not inferred) volumetric density ever shown for a sorbent material?
- Far too much emphasis seems to be placed on highly speculative predictions coming from theory. The theoretical calculations predict nanostructures which are predicted to store H₂ with more favorable binding energies. But more often than not, these predictions involve things that seem to be impossible to synthesize.

Question 2: Technical accomplishments and progress toward DOE goals

This project was rated 2.2 on its accomplishments and progress.

- New results on boron-substituted materials (notably porous BC₃), high specific surface area (SSA) MOFs, and new materials containing metal centers capable of multiple H₂ binding at higher energies are promising. A focused effort among multiple CoE partners on understanding spillover effects and competing processes, as well as on increasing hydrogen uptake rates is yielding valuable information.
- A great deal of progress is clear in the area of "optimized binding sites". This work seems to be diverse (with no apparent overlap), novel, and promising.
- Overall, results on substituted MOFs and covalent organic frameworks (COF) for cryoadsorption tanks and high SSA BC₃ appear to be most promising for meeting DOE targets.
- One of the approaches stated by the CoE is that optimized pore sizes can greatly improve volumetric capacities and therefore can help meet DOE targets. However, it seems like each of the CoE partners are defining their own optimized size without a common understanding.
- There is still no baseline checking and confirmation of the reported measurement results from last year.
- Last year spillover was a key topic (Southwest Research Institute and University of Michigan results) so the CoE decided to refocus its efforts and resources on spillover. This year spillover is not a strong role. The CoE did well in checking the data reproducibility, but it is left with progress based on theory estimations that does not warrant a real material.
- Good progress has been made by all clusters on improving volumetric and gravimetric capacity, especially for cryo-adsorption applications. In contrast, high capacity storage at temperatures compatible with fuel cell operation remains problematic for all approaches, and at this late stage in the project, poor reproducibility in spillover studies is a serious issue.
- Given the length of time and resources that have been devoted to spillover, it is imperative to resolve reproducibility issues and achieve consistency of experimental results across CoE partners.
- The "closed loop" between theory and experiment is great to see in this CoE, which previously seemed to lack such a connection. In this area what is the "ideal" % boron content and SSA determined from computation and how does that compare with current experimental values? What methods have been identified for bridging this gap?
- In the area of spillover it should be of high(est) priority to demonstrate robust reproducible results across the Sorption CoE (i.e., akin to a round-robin testing). It is imagined to be very difficult to validate theory, down-select or discontinue materials, and/or have confidence in individual results if synthesis and measurements are not currently capable of being reproduced by different researchers.
- The accomplishments are not very strong. Much of the highlighted accomplishments either has to do with spillover materials (where the results are not very compelling and clouded by issues of irreproducibility and inconsistency) or theoretical or idealized models of sorbent materials. This CoE was largely founded on ideas of the theorists in this field, and unfortunately, the experimental efforts simply have not been able to verify a large number of these theoretical calculations. So, the number and impact of accomplishments having to do with real, measured materials of high capacity is quite limited.

Question 3: Proposed future research approach and relevance

This project was rated 2.4 based on future plans.

- The future work plan is well formulated and addresses the critical issues identified in the RCs.
- Good use is being made of down-select criteria to focus the technical effort in the future.
- Go/no-go criteria were detailed and RC-specific. However, given the limited remaining timeframe of the current Sorption CoE and the initiation of the Engineering CoE, it might be more instructive to have more stringent criteria or a additional categorizing of down-selected materials (e.g., priority level 1, 2, 3, etc.). If there are already 40 materials (with more anticipated), that may be too much information to sort through for the Engineering CoE.
- There has been too much effort on spillover materials without a fundamental understanding.
- The creation of the down-selection criteria and road map is very important at this stage. Real measurements at the higher temperature in the down-selection criteria would be necessary.
- The majority of the focus should be on reproducing/understanding spillover results given the amount of resources being devoted to this topic.

Question 4: Coordination, collaborations and effectiveness of communications within the CoE

This project was rated 2.4 for collaboration and communication within the CoE.

- The management approach adopted by the CoE is facilitating good communication among the participants. Theory and experimental studies are well integrated. This is essential for addressing the serious technical challenges (e.g. temperature, binding energy, capacity) faced by the Hydrogen Sorption CoE.
- It is clear that there is a great deal of collaboration and coordination both within and between the CoE projects.
- There should be a concerted effort (e.g., round-robin testing) with regard to spillover validation.
- The CoE seems to be reasonably coordinated.
- There has been insufficient communication within the CoE.

Question 5: Collaborations/Technology Transfer Outside the CoE

This project was rated **2.6** for collaboration and technology transfer outside the CoE.

- Collaborations with other CoEs (e.g., aerogel work with Metal Hydride CoE) and with other institutions are in place and are yielding positive results.
- The excellent publication and presentation record is validating the broadly based technical contributions being made by participants in the CoE and is an effective means of disseminating results to the scientific community.
- One area of suggested improvement is to strengthen communication and collaboration with independent researchers (e.g., Long & Yaghi) where there is logical overlap and expertise that could aid, for example, with sample/synthetic reproducibility for spillover in MOFs.
- There has been insufficient communications with other CoE partners.

Strengths and weaknesses

Strengths

- The approach to develop structures with a high number of sites with enhanced enthalpies of adsorption and optimized pore sizes can greatly improve the materials properties for on-board application.
- A highly qualified and well-managed research team is conducting first-rate R&D work that is focused on DOE objectives. Good communication and collaboration is facilitating progress across all research clusters.
- This is a strong, capable team and leadership.
- Resources have been appropriately dispersed.

Weaknesses

- There have been insufficient communications with other CoE partners.
- There is still no baseline checking and confirmation of the reported measurement.

- The CoE relied too much on theoretical predictions based on non-existent materials to design the sorption material. So far synthesis of these materials has been very difficult or even not impossible (i.e., down-selected NREL's metal-decorated C60). However, the CoE continues to follow the same track with current materials (i.e., boron-carbon [BC] systems synthesis with different approaches, yet the theory has not been validated).
- A straightforward statement or exposition of the critical issues faced by the CoE and whether those issues can be addressed in a timely and successful way is needed. Although there is a great deal of useful information being generated within the CoE, potential problems and "show-stoppers" need to be highlighted and a straightforward and transparent plan for addressing the problems should be provided.

- The center should refocus and reduce the number of materials systems based on the down-selection criteria provided. The results for the down-selection have to be based on the experimental results, not the theoretical estimation.
- The key advantage of sorption over other H₂ storage systems is the fast release and sorption of H₂, therefore spillover of H₂ proves to be at a huge disadvantage and its deletion is subsequently recommended.
- Lack of reproducibility in the spillover studies at different Hydrogen Sorption CoE laboratories is an important issue. A strongly focused effort is recommended in order to understand the origins of the reproducibility problem so that a down-select decision on spillover materials can be made in a timely way.

Project # ST-23: A Biomimetic Approach to Metal-Organic Frameworks with High H₂ Uptake Hong-Cai (Joe) Zhou; Texas A&M University

Brief Summary of Project

The objective of this project is to design, synthesis and characterize MOFs with active metal centers aligned in porous channels and accessible by hydrogen molecules. Through optimized, cooperative binding, the MOFs are expected to have enhanced affinity to hydrogen. These MOFs can help to reach DOE 2010 goals, and ultimately the 2015 hydrogen storage goal.

Ouestion 1: Relevance to overall DOE objectives

This project earned a score of 3.3 for its relevance to DOE objectives.

- If MOF materials can be developed with significant hydrogen storage capacities at room temperature it will have a large impact.
- The project's aim at better uptake and retention at room temperature is a very well-aligned goal. Use of biomimetic concepts would be novel and diversify the portfolio, but they are not at all evident in this project.
- Further exploration of high surface area materials with enhanced physisorption binding potential is an important and viable approach toward meeting the DOE targets. In particular, MOFs offer vast opportunities to chemically engineer a broad range of physisorption binding mechanisms while maintaining accessible surface area. This project is currently focused on surveying a wide variety of open metal sites with which dihydrogen's polarization can be affected to a significant degree.

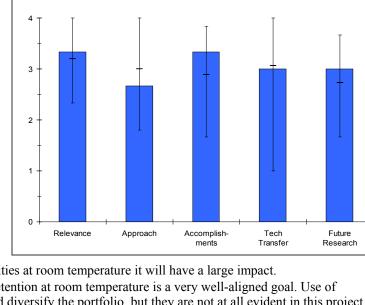
Question 2: Approach to performing the research and development

This project was rated 2.7 on its approach.

- The PIs approach is generally good, if not outstanding, but heavily weighted on much empiricism. While a healthy amount of experimental sorption measurements is refreshing, progress may be accelerated by augmenting the experimental work with more theoretical calculations than have been undertaken at this point in time. In particular, the effects of entatic metal centers on the polarizability and binding energy of dihydrogen deserves further attention as a means of screening potential metal-center candidates and developing trends based upon electronic structure. Such calculations are tenable by various levels of theory and could be applied to exploring open metal sites.
- The team's approach of utilizing open metal sites, interpenetration, and optimal pore size is certainly not new and seems to be following in the footsteps of University of California, Berkeley; University of California, Los Angeles; and several groups in Europe. The actions are suitable, but there is a need to try to plan experiments that will show something new.
- Of the MOF approaches of catenation, mesocavities, and open metal sites, only the open metal sites have the potential to increase hydrogen binding energies, and hence, room temperature adsorption.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated **3.3** based on accomplishments.



Overall Project Score: 3.1 (4 Reviews Received)

- The CoE metal centers appear promising.
- The team made several new linkers and associated MOFs. Many have low capacity but a few are good, *if confirmed*. (7%. These results would be more powerful four years ago when things like the effect of interpenetration and pore volume versus area were hot topics.)
- The 7,200 m²/g specific area by Bruner–Emmett–Teller surface area analysis method (BET) measurements would be a very good accomplishment, but it is called into question by both theory and H₂ capacity.
- Overall accomplishments are outstanding given the time-frame. It would have been helpful, however, to learn more details about PCN-103, which yielded exceptionally large surface area.

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated **3.0** for technology transfer and collaboration.

- There was a partnership with Air Products, but there did not appear to be well connected. They listed several "partners," but there was no evidence that they worked together.
- Collaborative efforts to explore spillover effects might be expanded to other organizations in addition to the University of Michigan.

Question 5: Approach to and relevance of proposed future research

This project was rated **3.0** for proposed future work.

- The project team is seeking H_2 capacity of 7,200 m²/g material and validating the BET.
- The plans seem better than current work, which is good.
- The future plan makes no mention of further characterizing of PCN-103. Given its incredibly large surface area and potential for dihydrogen binding, it would seem this should be a notable priority for the ensuing year.
- Emphasis should be placed on exploring the metal center avenues.

Strengths and weaknesses

Strengths

- The project team seems to have found its special area and should have a chance to make good progress.
- The project has a library of many ligands with which to work.
- The project team is addressing a promising pathway toward achieving significant gains in physisorption binding energies, while addressing gravimetric capacity via exceptionally high surface area.
- The project team is using new innovative MOF approaches to improving hydrogen storage.

<u>Weaknesses</u>

- The project does not at this point make effective-enough use of theoretical predictions, which would otherwise help select the most promising systems for experimental measurements.
- Volumetric hydrogen capacities are on the low side.
- The project team has been catching up to leaders, but seems to have done so.

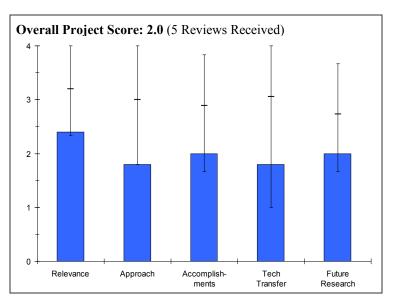
- The project team should test the 7,200 m^2/g material in H₂ as soon as possible; if the result is good, the team should have it reproduced as soon as possible.
- If not already in the scope of work for the ensuing year, further characterization of PCN-103 should be a priority.
- Through additional computations, the project scope could begin to establish trends on the polarizability or binding energy of dihydrogen to entatic metal centers versus the metal type. Such trends could be used to make appropriate selections of the entatic metal for synthesis of the MOF, thus accelerating progress in experimental verification.
- Evaluations of the stability of the MOFs produced would be useful.

Project # ST-24: Hydrogen Storage by Spillover

Anthony J. Lachawiec, Jr., Lifeng Wang, Yuhe Wang, and Ralph T. Yang; University of Michigan

Brief Summary of Project

The objectives of this project are to 1) develop hydrogen storage materials with capacities in excess of 6 wt% (and 45 g/L) at ambient temperature by using the spillover mechanism, 2) develop and optimize new bridge-building techniques for spillover to enhance hydrogen storage in metal organic frameworks (MOFs), 3) develop direct doping techniques for spillover on carbons with ultra-high surface areas (higher than all MOFs) because of the enormous potential of carbon for hydrogen storage by spillover as to be explained, and 4) obtain a mechanistic understanding for hydrogen spillover in nanostructured materials for the purpose of hydrogen storage.



Question 1: Relevance to overall DOE objectives

This project earned a score of 2.4 for its relevance to DOE objectives.

- The project is addressing H₂ storage, which is important for future fuel cell vehicles.
- The project focuses on materials that have recurring problems with reproducibility.
- The concept is relevant to DOE goals and objectives.
- The project team is trying to achieve higher uptake in sorbents at room temperature due to spillover. It is not at all clear whether this technique is really going to produce anything useful in terms of a storage technology.

Question 2: Approach to performing the research and development

This project was rated 1.8 on its approach.

- Systems with high platinum group metals (PGM) loadings being investigated may be of academic interest but are not practical. They will not come close to meeting the cost targets, even if they meet the loading targets. The storage system cost target of \$67/kg · H₂ means less than 2 grams of Pt can be used per kilogram H₂ stored at current prices. For storing H₂ at 5 wt%, the system weight is 20 kg/kg · H₂. This means Pt loading cannot be higher than 2 g/20,000 g or 0.01 wt%. They are investigating systems with 10 wt% Pt loading, 3 orders of magnitude higher Pt loading than would be acceptable than if they reach 5 wt% H₂ storage (which they haven't achieved). They need to focus on non-precious metal dopants for spillover and look at systems with higher initial H₂ storage capacity (MOFs). Spillover in MOFs is likely to be different than spillover on C due to the differences in binding between the metal center and the C or MOF.
- Spillover appears to lead to C-H binding at least judging from the hydrogenation/dehydrogenation rates vs. other sorbents. This coupled with the demonstrated low wt% places spill over in a weaker position vs. the other sorption materials researched.
- The project only uses sorption measurements. This is a very serious weakness, since sorption data alone is not enough to understand the microstructure of the materials and to reach convincing conclusions about the hydrogen adsorption and diffusion mechanisms. Reproducibility of the measurements is suspect in the absence of more information on the properties of the materials used.

- The approach should include objectives toward understanding spillover mechanism in the context of hydrogen storage in order to make research amenable to logical, rational targeting of materials. In its current form, it seems to be more or less a trial-and-error search of materials for which spillover is observed.
- These experimental efforts should be complimentary to analogous computational efforts for cross-validation.
- The spillover approach generated a lot of interest several years ago, but has more recently repeatedly become problematic due to problems of irreproducibility and inconsistent results. Unfortunately, this makes all of the results from a project like this (even the seemingly promising ones) somewhat suspect.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated 2.0 based on accomplishments.

- Work looking at increasing charging rates with co-doping has shown positive results.
- The effect of surface area was determined to be a key factor last year and it still remains a challenge judging from the low surface area spillover systems reported so far on carbon.
- Pt and Pd are known to be perfect for hydrogen dissociation, addition of transition metal halides is not well justified given they reduce the wt% storage unless they are replacing the noble metal catalysts.
- This project has obtained some interesting results on adsorption in the presence of linkers and activation barrier for hydrogen diffusion. However, there is not enough to decide on the validity of the conclusions due to lack of supporting microscopic measurements and microstructural characterization (e.g., TEM, Raman, and NMR).
- In regard to using gas adsorbate molecules as bridges (e.g., co-adsorption of CH₄ and H₂), it is not understood how this will be able to be implemented in practice for fuel cell application. In particular, will not the CH₄ and H₂ simultaneously be desorbed from the sorbent, and if so, this will have serious implications for fuel cell operation. The current SAE J2719 fuel purity standards do not allow greater than 2 ppm (C1 basis) for hydrocarbons. Currently 50 ppm CH₄ is being explored as a bridge which exceeds these limits. In the current form, it is unclear how this research topic is practical.
- While the back-up slides indicate that this research program focuses on exploration of both MOFs and carbons for spillover, the vast majority of the last year's research appears to be devoted only to carbons. Given that MOFs (in particular IRMOF8) remains the project's top performer, it is unclear why this topic has been seemingly abandoned. Previously cited sample "synthesis reproducibility issues" are something that should be easily overcome given that other research groups/companies are capable of producing such materials.
- All results shown are for ~1-1.5 wt% at room temperature and ~100 bar. There were no high capacity results shown and no discussion or mention of volumetric capacities (presumably because they are extremely low).
- The project team found some results that dosing with CH₄ could produce an enhanced spillover effect (within a certain range of CH₄ pressures).
- The project team found enhanced spillover in graphite due to oxidation. Even so, one would need to obtain a very high surface area material to make these results useful, and it is not clear that there is a path towards achieving this.
- The project team catalyzed spillover with metal catalysts and attributed the enhanced rates to a lower binding energy upon metal doping, but the increased rates were in *both* directions (desorption and absorption), and it is difficult to understand how a decreased binding energy could increase the rate of absorption.

<u>Ouestion 4: Technology transfer/collaborations with industry, universities and other laboratories</u>

This project was rated **1.8** for technology transfer and collaboration.

- Collaboration with NREL for testing is visible.
- Beyond the collaborators listing on the overview slide, it was not obvious what the extent and role of these collaborations are in the research program. Although other research projects in the Sorption CoE are actively investigating spillover, both in terms of experimental validation and theoretical investigations, the integration of these important activities into this project was absent. Going forward, it is essential that this project coordinate with the other activities in the CoE devoted to spillover.
- There are seemingly very few collaborations. It appears as though the program is largely isolated, which is unproductive from DOE's standpoint, since one of the main drawbacks of this idea is the lack of consensus, reproducibility, and reliability in the results.
- There seems to be no collaboration with other projects.

Question 5: Approach to and relevance of proposed future research

This project was rated 2.0 for proposed future work.

- Future work should look at realistic loading levels and non-precious metal dopants. The project team plans to look at MOFs and continue work on kinetics of spillover, which is good.
- Illustration of surface area enhancement is strongly recommended
- Measurement of charge/discharge rates for oxidized systems and comparison with other systems are necessary.
- Approach to and relevance of proposed future research was not discussed in the presentation and/or slides. Assuming that the project will continue "as is," it suffers from the lack of characterization measurements.
- The project team should focus on reproducibility of synthesis and measurements within this project as well as validation by other groups (e.g., round robin testing).
- The project team should focus on achieving an experimental understanding of spillover mechanism to avoid continuation of trial-and-error testing of diverse sorbent material. That is, the team should strive to understand why one MOF works better than another (i.e., derive structure-property relationships).
- The project team should continue to actively investigate MOFs since they are the top performers.
- Much of the promise of the graphite oxide depends on the ability to create high surface area samples. However, the plans for how to achieve this are not very convincing.

Strengths and weaknesses

Strengths

- The team has performed studies of kinetics of spillover and attempted to increase rate of H₂ uptake.
- A unique, novel approach has been used and has shown promise.

<u>Weaknesses</u>

- The project team has focused on precious group metals at high loadings.
- Low wt% H₂ combined with the slow charge rates is a weakness.
- The addition of catalysts impact the storage capacity.
- Utilization of expensive noble metal catalysts to allow for the spillover could be an issue.
- The project needs characterization of the materials and probes of hydrogen dynamics (collaborations with other projects could help, if they existed). Measurements in this area often suffer from irreproducibility. Many of the considered materials and catalysts are too expensive.
- There has been a misdirection of efforts (which should be focused on reproducibility of measurements across CoE partners as well as striving for an understanding of the spillover mechanism).
- The project should focus on why only certain materials are amenable to spillover.

Specific recommendations and additions or deletions to the work scope

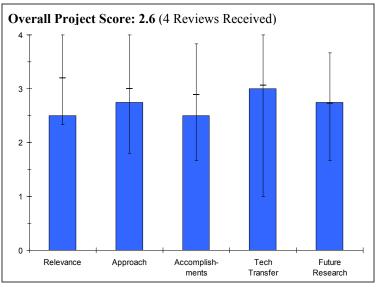
No recommendations were received for this project.

Project # ST-25: Optimization of Nano-Carbon Materials for Hydrogen Sorption

Boris I. Yakobson and Robert H. Hauge; Rice University

Brief Summary of Project

The overall objectives of this project are 1) to model materials structures' interaction with hydrogen, optimize their makeup for storage, and assess the volumetric and gravimetric capacity; and 2) provide recommendations for the synthetic goals (e.g., pore/channel size, metal enhancement routes). The 2008-2009 objectives include to 1) identify the obstacles (thermodynamics and kinetics) for the spillover for suggesting the materials design to overcome them; 2) enhance the binding of hydrogen by introducing charge into the carbon lattice by adding a highly stable superacid anion that also acts as a spacer; 3) explore doping as a anchor to metal/metal cluster, role of bridges and dopants on the threshold of



spillover; 4) synthesize metal-and electronegative-group-(F, BF₃) enhanced VANTA (vertically aligned nanotube arrays, contrast to fibers) for H_2 adsorption; 5) assess the effect of impurities and environment on the spillover; and 6) study the conditioning of graphitic substrates, by adding O, B, and organic molecules.

Question 1: Relevance to overall DOE objectives

This project earned a score of 2.5 for its relevance to DOE objectives.

- The use of theory to reduce mass and volume and increase the capacities of sorption materials is correct, and the method is good. The centerpiece of the group, targeting spillover, is well chosen.
- This project supports the DOE RD&D objectives. The strong emphasis on computational analysis and modeling of porous sorption media, catalytic spillover effects, and metallocarborane-based MOFs supports experimental efforts within the Hydrogen Sorption CoE.
- The project considers materials that can hardly be synthesized (e.g., H₂-filled carbon nanocages) or are thermodynamically unstable at ambient conditions (metallacarborane MOFs).
- Spillover simulations seem to be the most relevant part of this project.

Question 2: Approach to performing the research and development

This project was rated **2.8** on its approach.

- The pairing of theory and experiments is a good approach and the theory platform is suited to doing the work. The use of bookending potentials is also good.
- Experiments seem well chosen.
- The multi-task modeling and computation effort focus on storage properties of nanoporous materials, diffusion barriers, and H-binding energies in presence dopants in catalytic spillover systems and hydrogen sorption energies in metallacarboranes and MOFs. The approach is well formulated and is providing information that helps to guide experimental efforts within the Hydrogen Sorption CoE.
- At this stage in the project, the computational studies on storage capacity in nanoporous foams and the experimental effort on storage in vertically aligned carbon nanotubes appear to be much less likely to overcome the technical barriers for high capacity storage than the work on spillover and metallacarboranes.

• The project team uses a combination of first principles and classical potential approaches to study the thermodynamics of hydrogen physisorption. This is appropriate for studying hydrogen-material interactions theoretically, but not enough to suggest new realistic storage materials.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated 2.5 based on accomplishments.

- The results on spillover, especially computations of binding energies in the key states and evaluation of anchors for metal clusters are particularly noteworthy contributions and support related theory and experimental efforts within the Hydrogen Sorption CoE.
- The project team seems to have found a great surface super acid, but seems to be off when compared to measurements. The validity of the experiments is unclear. Likewise, the Ni work seems in contrast to the results which have never been shown to work.
- The majority of the work on this project focuses on simulations of hydrogen binding energy and storage capacity in nanoporous materials and analysis of spillover mechanisms. Although this information is valuable, at this late stage in the project, experimental validation is needed.
- Metal aggregation remains a serious problem for the spillover process in weakly bound metal-carbon systems. A clear plan for addressing this issue is not readily apparent from this presentation. An estimate of the spillover efficiency with cluster size would be useful. Likewise, a more detailed investigation into the problem of slow hydrogen uptake rates in spillover systems is needed.
- Although from a materials science perspective the carbon foam work (including quantum corrections to the foam capacity) is intriguing, it is not evident why subtle changes in foam pore size distribution can produce significant changes in hydrogen storage capacity. Comparisons with other carbon systems containing micropores (e.g., activated carbon) would be useful.
- The experimental results on the vertically aligned nanotubes appear is less promising. Advantages of vertically aligned nanotube arrays (VANTAs) over simple activated carbon for enhanced storage by addition of electronegative groups are not obvious.
- Numerical results for many cases of hydrogen-material interactions have been obtained. Unfortunately, it is not clear how these results can lead to better understanding of the fundamentals and/or to improved hydrogen storage materials.
- Not as impressive as last year's, which was very good.

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated **3.0** for technology transfer and collaboration.

- The project team is well connected to other teams in the CoE. The team is helping other teams and being helped by them, so there is value. Examples include the teams at University of Michigan, Rice University, NREL, and Air Products.
- Good collaborations between this project and other CoE partners, especially in areas of hydrogen capacity testing (California Institute of Technology [Caltech]) and comparison with experimental results on spillover (University of Michigan) are evident.
- It is not clear that the technical effort on this project is integrated adequately into the overall work within the CoE. There are numerous activities within the CoE on spillover (both computational work and experimental work) and on substituted MOFs. A stronger connection between this project and those efforts would be helpful.
- There is a long list of collaborations; some of them are productive (e.g., with Caltech on aligned nanotube arrays).

Question 5: Approach to and relevance of proposed future research

This project was rated 2.8 for proposed future work.

- Future plans are well oriented to address problems within the CoE.
- Unfortunately, the project team is not solving the discrepancy in experiments.

- The future work builds upon the current technical effort and addresses the important issues that have been identified. A missing aspect seems to be a candid assessment of key technical barriers and how they will be addressed during the remainder of the effort. It is critical to identify those obstacles, determine their severity, and then focus on finding solutions.
- The plans are to continue along the same lines as done previously. There needs to be sharpening of the focus to study phenomena outside of the present scope (e.g., thermodynamic stability of the proposed materials).

Strengths and weaknesses

Strengths

- The project team was able to explain the spillover work.
- The project is well aligned to experimental teams' greatest needs.
- This is a strong research team that is highly qualified to conduct leading-edge work on hydrogen storage in substituted nanophase carbon materials.
- This broad-based computational effort supports experimental work in the Hydrogen Sorption CoE.
- The project has added some understanding to the energetics of the so-called spillover effect.

Weaknesses

- The project team might benefit from association with other theory groups in other CoEs.
- It is not clear that a continued emphasis on porous foams and VANTAs is appropriate. Although the materials have interesting physical properties, high storage capacity for hydrogen appears to less promising than in other materials.
- Several materials being considered are unrealistic (e.g., nanocages) and there are too few comparisons with experimental data; which currently not even on a qualitative level.

Specific recommendations and additions or deletions to the work scope

- It is important for this project to identify and focus sharply on the critical technical barriers that remain.
- Simply continuing work on several on-going tasks will undoubtedly produce some useful results, but could give insufficient emphasis to the key technical obstacles.
- A heart-to-heart on theory with the team at Air Products (especially on the work from last year on spillover limitations where hydrogen was on both sides of the graphene) would still go a long way; however, to have value the CoE lead would need to first elucidate both team's concerns about the other's work in private and then mediate the exchange.
- There needs to be a stronger focus on materials that work in the lab and are well characterized and quantitative comparison to experimental data needs to be added.

Project # ST-26: NREL Research as Part of the Hydrogen Sorption Center of Excellence

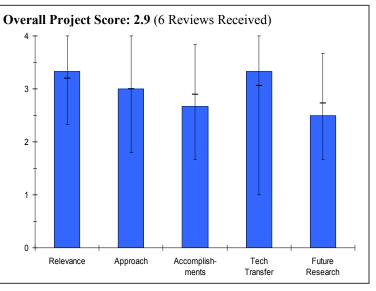
L.J. Simpson, A.C. Dillon, J.L. Blackburn, J. Bult, C.J. Curtis, M. Davis, T. Elko-Hansen, C. Engtrakul, T. Gennett, A. Groves, , A. Herwadkar, K.M. Jones, Y-H. Kim, K.J. O'Neill, P.A. Parilla, J.D. Rocha, E. Whitney, and Y. Zhao; National Renewable Energy Laboratory

M.J. Heben; University of Toledo

S.B. Zhang; Rensselaer Polytechnic Institute

Brief Summary of Project

NREL's research in the Hydrogen Sorption CoE is targeted at addressing key technical barriers in DOE's Hydrogen Storage Program: 1) efficiency - it is clear that the highest efficiency storage system will be achieved with a sorbent material that operates reversibly on board with a hydrogen binding energy in the range of 15 to 20 kJ/mol (room temperature operation); 2) refueling time - the fastest on-board refueling time will be found for a sorption system when the materials are not limited by heat transfer processes; 3) weight and volume - when the sorption material has an optimized binding energy and thermal conductivity, non-sorbing system hardware can be kept to a minimum, capacities of the



system will then be approximated by the capacities of the materials; and 4) cost - closing the gap between the idealized sorption materials that have been predicted and the synthesis of actual materials using low-cost source materials and synthesis processes.

Question 1: Relevance to overall DOE objectives

This project earned a score of **3.3** for its relevance to DOE objectives.

- The project is well aligned with DOE objectives and is providing good leadership for the overall Hydrogen Sorption CoE effort. The overall relevance of the project has been enhanced in 2009 by the greater emphasis on sorption materials capable of higher capacity storage at near-ambient temperature.
- These materials have a chance to meet all goals and exceed compressed gas. The challenges they have targeted (i.e., mass, volume, and cost) are the keys.
- This project covers virtually all aspects of hydrogen storage by sorption methods for on-board fuel cells, including system cost, gravimetric and volumetric H₂ storage targets, reversibility, refueling time, and efficiency.
- This is a centerpiece project within the Hydrogen Sorption CoE.
- Project's focus on enhancing dihydrogen binding energies in novel, high-surface area chemistries and elucidating sorption/spillover mechanisms is clearly essential to the technical goals of the hydrogen program.
- Generally well aligned with DOE goals, with a few projects focusing on more basic energy science concepts rather than applied research.

Question 2: Approach to performing the research and development

This project was rated **3.0** on its approach.

- Near-ambient work is a big enabler and a good thing to research.
- The low temperature work by doping is good.
- Indicate 5 minute fill of 82% capacity with new catalyst.

- This project conducts high-quality research that seeks pathways to increasing the H₂ binding energy, the number density of binding sites, and the number of H₂ molecules per binding site. The project also seeks to achieve near ambient temperature regeneration.
- NREL leads and assures coordination of activities within the Hydrogen Sorption CoE. In this role, NREL evaluates progress across the entire Hydrogen Sorption CoE in terms of demonstrated achievements versus the entire set of DOE hydrogen storage system targets.
- Project effort now places more emphasis on low-cost materials and viability of synthetic routes than in previous years. This approach to materials discovery should continue for both the experimental and theoretical efforts. However, theoretical predictions appear to be outpacing experimental verification, which can be expected. Synthesis and characterization of theoretically promising candidates need to be undertaken expeditiously in collaboration with other groups (including groups outside the center).
- A welcome shift in emphasis in 2009 away from more exotic materials (e.g., OM-fullerenes, Ca-C60 compounds, Co-intercalation) toward more experimentally accessible systems that have a better prospects for hydrogen storage at acceptable temperatures.
- A new approach using chemical vapor deposition (CVD)/templating has provided a pathway for evaluating physisorption, dihydrogen binding, and spillover using a well-controlled process.
- Important focus on materials capable of multiple H₂ storage via Kubas interactions. This is a potentially useful approach to increasing storage capacity. Likewise, work on CA-COFs is a promising new research direction.
- Continuing effort on spillover is directly supporting related efforts in the CoE. Work on improving rate of hydrogen uptake and on understanding lack of reproducibility in spillover results is especially important.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated 2.7 based on accomplishments.

- The project team continued to develop novel, scalable synthetic processes for adequate storing of hydrogen on high surface area materials.
- Calculations show that the modeling formalism can predict what is seen in Si systems with Ti catalyst.
- Boron-doped carbon lattice increases H₂ binding temperature.
- Calculation says COF with Ca would be stable and hold around 5.6% at modest temperature.
- There is possible insight on the batch-to-batch, lab-to-lab problems with spillover.
- The project team demonstrated that B substitution in C increases H₂ capacity and binding energy.
- The project team validated initial, theoretical prediction that single, metal atoms dispersed and stably supported on a matrix are able to reversibly hold more than two H₂.
- The project team identified new inexpensive materials that make use of unique properties of Ca via viable synthetic routes.
- The project team continued to make advances in the understanding and application of spillover, including the development of a new catalyst processing method that improved spillover capacity and charging rates.
- The project team identified potential issues that produce irreversibility and cause irreproducible hydrogen sorption measurements.
- The project team continued to improve the measurement capabilities to provide more accurate determination of H₂ storage characteristics.
- The team continues to produce an impressive amount of work along diverse paths, perhaps too diverse in some instances. It is not clear why the project team is, in some instances, spending effort on the analytical validation of material performance for other groups when that time could be utilized on verifying the hydrogen uptake in novel materials predicted from theory. Analytical validation should be directed to the DOE-designated storage testing laboratory (Southwest Research Institute [SwRI]).
- The improved spillover catalyst processing is showing some promise for enhancing capacity and uptake rate. Results on elucidation of mechanisms that affect hydrogen diffusion during spillover is improving understanding of this potentially important process. However, it is not clear how this information is being used to guide experimental work. Have differences between NREL and University of Michigan results been reconciled? The lack of reproducibility remains a serious issue.
- The new CVD/templating work is providing a well-controlled platform for studies on physisorption, enhanced H-binding, and spillover. Is the CVD templating process scalable?

- The work on high specific surface area (SSA) BC₃ and Ca-COFs (covalent organic frameworks) is especially intriguing. Materials synthesis appears to be comparatively straightforward, and both material systems show considerable potential for high capacity hydrogen storage.
- The accomplishments are not very strong. Much of the highlighted accomplishments either have to do with (1) spillover materials, where the results are not very compelling and clouded by issues of irreproducibility and inconsistency or (2) theoretical or idealized models of sorbent materials. This CoE was largely founded on ideas of the theorists in this field and unfortunately the experimental efforts simply have not been able to verify a large number of these theoretical calculations. So, the number and impact of accomplishments having to do with real, measured materials of high capacity is quite limited.
- The Ca doping prediction is quite suspect, since CaH₂ is such a strongly bound phase. It seems quite likely that this system would simply form the CaH₂ phase upon repeated cycling. The binding energy of CaH₂ is larger than the binding energy quoted for Ca to the COF, thus making this a very real possibility.
- It is disappointing to see that not much progress has been made on the reproducibility or characterization of spillover.

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated **3.3** for technology transfer and collaboration.

- The project team has connected with many other groups, lead other groups well, and provided international leadership in this area for years.
- The project team has collaborated with institutions within the Hydrogen Sorption CoE include Rice University, Air Products, Duke, California Institute of Technology, LLNL, NIST, ORNL, Pennsylvania State University, University of Michigan, University of Missouri, University of North Carolina, Texas A&M, ANL, and University of Chicago.
- NREL has done an admirable job of spearheading and coordinating research throughout the Hydrogen Sorption CoE.
- This project has extensive collaborations both with the Hydrogen Sorption CoE and with external research groups that are facilitating more rapid progress. Impressive publication and presentation record is resulting in efficient dissemination of research results.
- The CoE teams seem to work together reasonably well.

Question 5: Approach to and relevance of proposed future research

This project was rated 2.5 for proposed future work.

- The project team's close-out plan is suitable and wise to have.
- The project team has good plans; the Ca work will be very instructive.
- The team's plans focus on spillover sorption, which is right.
- The down-select on material is good.
- A down-select is recommended on theory approaches to those that can predict, not just tune, results to reproduce data in hand.
- Develop and optimize H₂ storage materials; prepare for program culmination:
 - Optimize templating processes used to synthesize high surface area materials.
 - Create stable coordinated unsaturated metal centers with higher site density that exhibit substantial hydrogen storage using inexpensive materials.
 - Perform experiments to identify surface/material processing strategies that increase spillover capacity and sorption rates; determine H₂ state on receptor; investigate site poisoning.
 - Accelerate theoretical efforts to design viable H₂ storage materials and synthetic routes thereto.
 - Complete down-selection process for all materials and assist CoE with go/no-go decisions based on material/system potentials.
 - Scale up synthesis of most promising materials for round-robin verification of samples.
 - Provide materials/systems recommendations; determine viability of high surface area materials to meet DOE 2010, 2015, and "ultimate" hydrogen storage system targets.

- Future plans/recommendations appear to be overly ambitious given that many of the theoretically promising candidate materials have not yet been synthesized.
- Solid plan for building upon recent results on templating, modifying surface properties to enhance spillover capacity and rates, and testing new materials is in place. However, the presentation provides very little information concerning a candid assessment of specific technical obstacles and barriers and the status of the project with respect to overcoming those barriers. Instead, general statements about how results in each of the areas are providing a "development path to meet DOE goals" are given.
- Without a more compelling assessment of critical problem areas (especially at this stage in the project), it is difficult to adequately evaluate whether the plan effectively meets the program needs.

Strengths and weaknesses

Strengths

- This is a highly qualified, multidisciplinary research team. The NREL team has shown ability to effectively make "midcourse corrections," which enhance technical efforts in areas that are most promising.
- There has been excellent collaboration between theory and experiment. Results are paying off in areas of multiple H₂ binding, enhanced spillover rates, and materials discovery (e.g., high SSA BC₃ and COFs).
- There are mixed strengths on this team.
- The cost target could be met, that is not a trivial thing to do!
- The project team has made a broad attack on the problem (e.g., room temperature, low temperature, theory, experiment, Kubas, spillover).
- The project was well represented and well presented by the PI.
- The project team has made strong collaborations with other Hydrogen Sorption CoE partners are starting to bear fruit.
- Reconsideration of the storage system targets by DOE (to define more realistic values) gives hydrogen sorption a much better chance of meeting the targets in a timely manner.
- Diverse pathways and mechanistic issues are being addressed.

Weaknesses

- This project has no significant weaknesses.
- It is troubling that the predictions are never verified, but the new ones are always assumed to be correct.
- The volume is troubling, but new goals will be more possible.
- Synthesis and characterization of theoretically promising candidates need to be undertaken expeditiously in collaboration with other groups (including groups outside the center). More active collaboration with the DOE-designated storage testing lab (SwRI) to share the burden of verifying theoretical predictions needs to be included.
- The lack of a straightforward assessment of the severity and scope of the remaining technical barriers, as well as a statement concerning the extent to which the R&D in the remainder of the project will be able to effectively deal with those obstacles, are weaknesses.

Specific recommendations and additions or deletions to the work scope

- The project team needs to do everything possible to make the COF with Ca and find out if the theory works predicatively, or only can be tuned, to match known results. It is absolutely essential that they are funded enough to do this.
- It seems essential to obtain a clear elucidation (theoretical and experimental) of the best way to optimize spillover and how much can be gained from its application under conditions that meet all the DOE hydrogen storage targets.
- In the current light of the "revised" DOE storage targets, NREL should put more emphasis on the many storage system targets that hydrogen sorption methods can seemingly meet, particularly in respect to the other two storage options (metal hydrides and chemicals).
- Any activities aimed at validating material performance that is beyond the phase of pure research should be directed to the DOE-designated hydrogen testing laboratory (SwRI).
- A sharply focused effort is recommended on improving rates and storage reproducibility in spillover materials and on synthesis and testing of Ca-COFs.

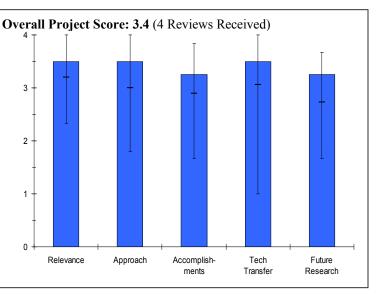
Project # ST-27: Hydrogen Storage through Nanostructured Polymeric Materials

Di-Jia Liu, Shengwen Yuan, Brian Dorney, Scott Kirklin, Suhas Niyogi, Shengqian Ma, Ricky Regalbuto, and Peter Zapol; Argonne National Laboratory

Jiangbin Xia, Zhou Wang, and Luping Yu; University of Chicago

Brief Summary of Project

The objectives of this project are to 1) design, synthesize, and evaluate nanostructured polymeric materials as new hydrogen storage adsorbents for transportation applications and 2) support polymer materials development with modeling/simulation and advanced structural characterizations. Polymer surface properties such as specific surface area (SSA) and porosity can be controlled at the molecular level. Polymer-hydrogen can be enhanced through incorporating different functional groups and atomically dispersed metals. Polymers are generally stable under the temperature and humidity required for hydrogen storage application.



Question 1: Relevance to overall DOE objectives

This project earned a score of **3.5** for its relevance to DOE objectives.

- The project is relevant to the storage goals.
- The design and synthesis of nanostructured polymeric materials as new hydrogen storage adsorbents is critical to Hydrogen Program.
- The present project, which aligns with the hydrogen program objectives, is concerned with developing novel porous organic materials and their use for hydrogen storage applications.
- The most novel area of this work is the formation of metallo-organic porous polymers. There appears to be analogies here with the MOF work, but unlike the MOFs, this is an amorphous system. The approach means that there is a high degree of control of the chemistry and it will be interesting to see what the effect of this is on the hydrogen characteristics. This system therefore has the potential to tailor the chemistry for higher isosteric heats of adsorption.
- It should be mentioned that the reviewer missed the oral presentation due to an injury.

Question 2: Approach to performing the research and development

This project was rated **3.5** on its approach.

- The approach well combined theory calculation, experimental design, H₂ uptake measurement, and fundamental understanding.
- Very interesting approach, any estimate on other objectives (kinetics and prices, for instance)?
- It is not clear from the PI presentation and answers to the questions how the H₂ gravimetric uptake will be increased toward the DOE target at higher temperatures and moderate pressures. In addition, the reported isosteric heats of sorption are low to moderate, far from the needed ~15kJ/mol. The lower heats of sorption suggest that it will be difficult using the present materials which possess narrow pores to access elevated isosteric heats.
- Independent verification should be sought from CoE partners for the hydrogen isotherms, as these have an uncharacteristic shape. If this proves to be true, then the PI should look to investigate with partners who can

investigate the phenomenon (e.g., neutron work to investigate any swelling effect or other potential sorption mechanisms).

- A potential flaw in the metal-loaded polymer strategy is that if the metal centers are not coordinatively unsaturated, then any enhanced interaction of the materials with H₂ is likely to be low. The PI should think about ways to activate the metal centers.
- Further understanding is needed on the porosity and diffusion of H₂ within these materials.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated 3.3 based on accomplishments.

- Given that this is a new area, this project really made excellent progress in a short time frame.
- Interesting that compression does not affect specific surface (in contrast with activated carbons where densification invariably lowers it).
- The present group has synthesized a series of porous organic polymers that can adsorb higher amount of H₂ at 77 K and high pressures.
- They also showed the ability to control the pore size of the obtained porous polymers.
- The group initiated collaboration with the University of North Carolina (UNC) to study H₂ uptake using nuclear magnetic resonance (NMR) at higher pressures. The recently obtained results from this collaboration are encouraging.
- Nevertheless, it is not clear what will be the rational to be pursued to improve the H₂ uptake and isosteric heat adsorption toward better materials that can answer the DOE target at higher temperatures and moderate pressures.
- Significant progress has been made on synthesis and characterization of the polymers. Given that the metalloaded polymers are the most likely candidates to give hydrogen properties closer to the DOE targets, it was disappointing that more had not been undertaken. The PI showed that this would be the focus for the next 12 months, and this reviewer hopes that this remains the case.

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated **3.5** for technology transfer and collaboration.

- Close collaboration not only with the center partners, but also with other parties in the field.
- There seems to be good integration with other teams.
- The new collaboration with the NMR group at UNC is very important to the future success of the proposed research.
- There was a good level of collaboration, but further collaborations to verify uptake measurements and to probe the characteristics of the materials would benefit the project.

Question 5: Approach to and relevance of proposed future research

This project was rated **3.3** for proposed future work.

- Hopefully this very interesting adsorption approach will continue.
- Good plans for coming year and focus on addressing the barriers.
- The polymer synthesis and hydrogen interactions with the samples have been investigated. The focus for the future work is on metal loaded polymers. A clear strategy for the synthesis was given, and the design and selection of metal centers will be developing through the next 12 months.
- The incorporation of new potential sites into the available pores is very critical to the success of the present project and may indeed lead to higher isosteric heats of sorption. It is recommended that such a proposed approach be pursued. It is also recommended that the choice of guest molecules to be incorporated into the voids of the porous polymer be based on the input of the computational team on the project.

Strengths and weaknesses

Strengths

- Relative invariance of specific surface after densification.
- Is it easier to include metal dopants in the structures with respect to AC or other adsorbents?
- It is a novel approach.
- Addresses the material's engineering properties at very early stage.
- The team has access to a large library of porous organic polymers. They also showed that the organic functionalities, as well as pore sizes, can be tuned with ease.
- Such modularity offers the potential to design the desired porous polymers suitable for H₂ storage with the help of the computational component.
- Strengths for this project are the novel materials being investigated. There is a lot of transferable knowledge and expertise from the CoE partners that will benefit the project. The PI has the necessary expertise to undertake a logical and in-depth investigation of these interesting materials.

Weaknesses

- It is not clear how the present project will lead to a material that will answer the DOE target for H₂ storage at higher temperatures and moderate pressures. It is not obvious from the presented data that incorporation of extra sites into the pores will lead to higher uptakes.
- The achieved storage densities are still below MOFs and activated carbons.
- This is not a major weakness, but greater collaboration will strengthen the project and aid refining the direction of the project.

Specific recommendations and additions or deletions to the work scope

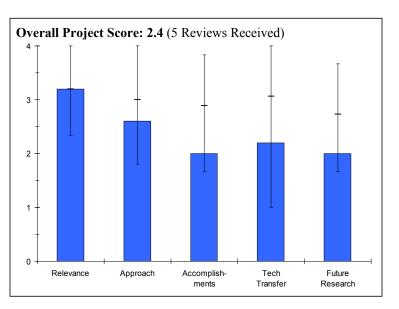
• The specific surfaces obtained so far seem somewhat low compared to MOFs and some activated carbons. Is it possible to increase it, or is there some limit to below 2,000 m²/g? It would be interesting to see if the uptake scales with specific surface area.

Project # ST-28: Discovery of Materials with a Practical Heat of H₂ Adsorption

Alan Cooper, Hansong Cheng, Wade Bailey, Xianwei Sha, Garret Lau, John Zielinski, and Guido Pez; Air Products and Chemicals, Inc.

Brief Summary of Project

The objectives of this project are 1) development and testing of new materials with high hydrogen storage density and appropriate enthalpy of hydrogen adsorption and 2) development of enabling technologies for hydrogen storage materials development. Air Products' goal is the reversible adsorption of hydrogen at nearambient temperatures at densities that will enable meeting the 2010 DOE system-level targets for hydrogen storage. Air Products has leveraged existing materials science and chemistry capabilities in carbon materials and fluorine chemistry to generate new hydrogen storage materials for testing.



Question 1: Relevance to overall DOE objectives

This project earned a score of **3.2** for its relevance to DOE objectives.

- Materials with a practical heat of hydrogen adsorption are critical to the success of Hydrogen Program.
- Good relevance and hopeful signs from theory on the BC₃-related compounds, but disappointing results for graphite intercalation compounds (GIC).
- The project generally supports the objectives of the Hydrogen Storage Program.
- The project team focused on increased binding energy in sorbents and did not seem to address issue of volumetric capacity, which is two one of their main weaknesses.

Question 2: Approach to performing the research and development

This project was rated **2.6** on its approach.

- Use of modeling as a guide for synthetic targets appears to be promising.
- Although the approaches pursued in this project (H-adsorption on F-intercalated graphite and H-spillover in BC₃) are fairly high-risk, they are novel and broaden the overall scope of the Hydrogen Sorption CoE. There is a good mix of computational work (molecular dynamics [MD] simulations and energy path calculations related to spillover on BC₃) and experimental work (H adsorption in F-intercalated graphite).
- The computational techniques employed here are not adequate for the complex systems. Can they be used as a guide?
- Worth trying!
- Good idea, but limited approach.
- The approach appears ad hoc. For example, why was a graphite system chosen when the Center has many high surface area materials? How did F-/BF₄-GIC become a candidate? There are several experimental projects within the Carbon Center that could have used a basis for experimental approach. Was that considered?

Ouestion 3: Technical accomplishments and progress toward project and DOE goals

This project was rated 2.0 based on accomplishments.

- Concluding that fluoride materials are not practical H₂ storage materials is very useful information for other partners.
- Do the results of the first part of the work indicate that the approach was inadequate? What are the implications and critical analysis?
- In view of the conflicting experimental results, what does the spillover work simulation show?
- The GIC compounds exhibit lower adsorption density than traditional materials (AX-21, for instance). There is a definite problem with the specific surface of these materials, however, no measurable beneficial effect of BF₄-intercalants for AX-21.
- At what temperature and pressure is the calculated hydrogen intake for bulk BC₃?
- The isosteric heats of adsorption seem high compared to the achieved storage densities.
- The results obtained in 2009 are not consistent with the funding level for the project. There has been only very limited progress in 2009 on improved hydrogen adsorption in F(-)- and BF₄(-)-intercalated graphite. In 2008 nitrogen-doping of the graphite host was suggested as a strategy to increase the heat of adsorption. However, follow-up work employing this approach was met with only very limited success. Likewise, only minor progress on increasing the overall surface area is evident.
- Although the work on chemisorbed hydrogen on BC₃ sheets is showing more progress, the stability of the hydrogen-BC₃ bond at high loadings is problematic with respect to reversibility and cycling (the investigators have chosen not to pursue this experimentally). The pathway to overcoming this problem is not clear (i.e., is there evidence to support the notion that inclusion of other heteroatoms will modify chemisorption energies?).
- The F work had largely negative results, the B doping work does not look promising because of the very large chemisorptive binding energies and very little has been accomplished yet in terms of actual enhanced sorption measurements.

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated **2.2** for technology transfer and collaboration.

- Good team integration.
- The project does not seem to use or benefit from the considerable amount of work and experience that the Hydrogen Sorption Center of Excellence has been collected over the past few years.
- There are limited collaborations within the Hydrogen Sorption CoE and with external investigators on the two major materials systems being investigated in this project. Although there are numerous partners within the Hydrogen Sorption CoE working on spillover mechanisms, it is not obvious that this project is well-integrated with those efforts.
- Not clear how close the collaborations really are and whether a significant exchange of ideas is occurring.

Question 5: Approach to and relevance of proposed future research

This project was rated **2.0** for proposed future work.

- Although not successful, the team did make a reasonable effort in completing the tasks.
- The proposed work is a straightforward extension of the on-going spillover work on BC₃. However, at this stage of the project, a more definitive statement of future work is needed in some of the project areas (i.e., "develop strategies for increasing surface area of BC_x materials" and "develop a systematic model of B content and H₂ adsorption enthalpy ..." are far too general and vague for a project that is more than 90% complete).
- There is a weak connection between the results and the future plan. A critical analysis of the results would be helpful especially with respect to approach and veracity of the techniques employed.
- The boron-containing compounds are worth exploring, although there has not been an experimental realization offering significant improvement towards DOE storage density targets in using spillover strategies as of yet.
- The B doping work seems to be a dead end given the large binding energies. It's not clear why this is being pursued.

Strengths and weaknesses

Strengths

- Project leverages extensive capabilities at Air Products in materials science and chemistry. The PI and his team are well qualified to conduct this work.
- Interesting approach from a fundamental point of view.
- Use of modeling as a guide for synthetic targets appears to yield promising approaches.

Weaknesses

- The project needs to identify the right types of material to study at the early stage. The down-select criteria for the approach should also be identified.
- The project is nearing completion, but future plans suggest an ongoing effort without a clear delineation of the outstanding technical barriers and obstacles. It seems unlikely that given the very general statements regarding proposed future work and with limited progress achieved in 2009 that a breakthrough on the BC₃/BC_x systems will be forthcoming.
- Overall, given the significant level of funding, the payoff from this project is low.

Specific recommendations and additions or deletions to the work scope

- Based on the approach and the results, it is recommended to rework the work scope and rationalize the first part of the project. The spillover work will also require some reconsideration in view of the question raised.
- With the limited time left for this project, the team should limit their effort in further exploring higher surface area BC_X materials.
- A very focused effort on the most promising aspect of the BC₃ spillover study is recommended. Dilution of the effort through inclusion of subordinate tasks would be counterproductive to the technical effort in the remainder of this project.

Project # ST-29: Optimizing the Binding Energy of Hydrogen on Nanostructured Carbon Materials through Structure Control and Chemical Doping

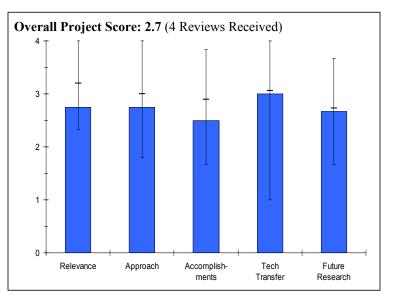
Jie Liu, Anmiao Wang, and Tom McNicholas; Duke University

Brief Summary of Project

The objectives of this project are to 1) design and synthesize carbon-based materials with optimized binding energy to hydrogen molecules that will show storage capacity meeting the DOE 2010 goal in hydrogen storage and 2) design and synthesize microporous carbon-based materials with enhanced binding energy to hydrogen including pore size control, surface area increase, metal doping of microporous carbon materials, and B doping of microporous carbon materials.

<u>Question 1: Relevance to overall DOE</u> <u>objectives</u>

This project earned a score of **2.8** for its relevance to DOE objectives.



- Project attempts to address the need to optimize interactions between physisorption materials and hydrogen to increase binding energy. This is consistent with the DOE objectives.
- Relevant to DOE goals and objectives; however, unclear if this approach will ultimately be capable of achieving the short- or long-term targets.
- The project is investigating a range of microporous carbons (MPC) made from polyether ether ether ketone (PEEK). The rationale behind the project is to make small pores to increase the isosteric heat of adsorption. It is, however, unlikely that this alone will lead to significant room temperature uptake capacities.

Question 2: Approach to performing the research and development

This project was rated 2.8 on its approach.

- While the idea of modifying a high-temperature thermoplastic, such as PEEK, is intriguing from the perspective of future scale-up, the premise of the project plan does not seem to hold much promise. In particular, the essential premise is to make PEEK behave like a highly active, porous carbon through high-temperature treatment. This seems uneconomical since there are already activated carbons that outperform the converted PEEK product.
- Multifaceted approach toward achieving enhanced binding via control of pore size and incorporation of dopants.
- While these are both relevant approaches, it is not clear what the ultimate (ideal) materials characteristics are and why. In particular, pore diameters of <1 nm are targeted for the PEEK materials; however, it is not clear what binding energy is ultimately feasible if this goal is reached and whether the center's 15 to 25 kJ/mol H₂ binding is possible. For the boron substitution, it should be specified what the desired content of boron is and why.
- The group is relying on partners for porosity measurements and >2 bar hydrogen isotherms. The uncertainty about the values for the materials is a significant weakness in the project, which is not the fault of the investigators but sounds to be a problem in the CoE partners being overwhelmed with samples. This is slowing down the project, and the CoE should look into ways that it can service the characterization needs of its members.

Ouestion 3: Technical accomplishments and progress toward project and DOE goals

This project was rated 2.5 based on accomplishments.

- Nuclear magnetic resonance (NMR) analysis appears to be very useful and diagnostic for determination of micro- and macropore content. This capability is being fully utilized for efficient screening and characterization of materials.
- The conclusion that steam heat treatment of PEEK samples is more effective than that for carbon dioxide (stemming from preservation of microporosity) suggests promise and approaches the properties of state-of-theart activated carbon but with potential for improved volumetric capacity. Given this important dependence between heat treatment gas and resulting structure/properties, it makes sense to perform a more systematic investigation of heat treatment gas size/composition and resulting PEEK pore structure.
- Survey of many materials with complete property summary. Nevertheless, materials capacities are still uncompetitive with other sorbents. Thus, it is unclear if this method is ultimately capable of reaching other state-of-the-art sorbents.
- A range of materials were made and higher isosteric heats of adsorption were measured. However, there is currently uncertainty that these very narrow pores can store the hydrogen as efficiently and what the high pressure capacities will be.
- As indicated from the results presented, it is evident that any manipulation of the PEEK processing conditions still only yields surface areas and gravimetric capacities that are comparable to an already commercially available activated carbon (AX-21). The statement that "PEEK-MPCs have significant H₂ storage capabilities compared to other pure carbon materials" is not supported by the data. PEEK-MPC is comparable to AX-21, with each yielding ~3 wt% at 2 bar and 77 K. Given that there are no gains in surface area, it is not likely that Pd-doped MPC will yield any major gains above current spillover materials (such as the Pd- or Pt-doped AX-21).

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated **3.0** for technology transfer and collaboration.

- Collaborations with NREL and University of North Carolina appear established and clear. Although in responses to reviewer's comment, it was pointed out that this work is quite different than that at University of Penn (also looking at boron doping). Nevertheless, at a minimum it is logical and reasonable to coordinate and communicate results between these two projects.
- The PI had little faith in the porosity analysis that its partners supplied. This needs to be addressed to improve the quality of the project. If there is a characterization capacity issue, then the CoE needs to address this (either by expanding capacity or prioritizing resources).

Question 5: Approach to and relevance of proposed future research

This project was rated 2.7 for proposed future work.

- Project needs to include in future work, room temperature sorption measurements on the highest surface-area PEEK-MPCs.
- Broader, systematic investigation of heat treatment gas size/composition and resulting PEEK pore structure.
- Gain an understanding of the theoretical potential for capacity and hydrogen binding energy for this approach.
- Higher pressure measurements to continue to understand comparison of PEEK materials with other carbonbased sorbents.
- Investigating B-doped carbons is a valid line of approach. This reviewer was unconvinced at the suggestion to investigate spillover enhanced hydrogen storage, especially as Ralph Yang predicted a maximum capacity of 2 wt%. Modeling work for B-doped carbons shows much greater likelihood of leading to enhanced uptakes, and the PEEK synthesis gives a versatile route to forming such materials with higher porosities and surface area.

Strengths and weaknesses

Strengths

- Project started with an intriguing idea based upon long-range potential for scale-up.
- Range of microporous carbons made.

Weaknesses

- Project has not devoted enough effort to characterizing PEEK-MPC materials in sufficient detail. What is the resultant state of carbon hybridization (Raman analysis)? What are the phase-change properties of the material (differential scanning calorimetry [DSC] measurements)? What is the room temperature hydrogen uptake? Are there other high-temperature thermoplastics that would give more favorable results?
- The characterization and high pressure H₂ isotherms are needed to assess the usefulness of these materials.

Specific recommendations and additions or deletions to the work scope

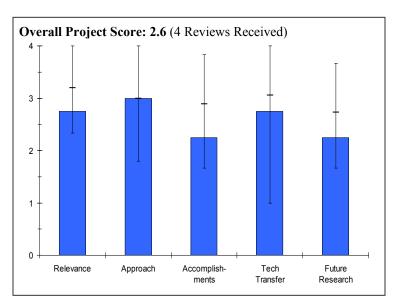
- Recommend abandoning PEEK-MPC materials. However, complete work to measure possible spillover effects.
- Suggest that PI focuses on doped carbons rather than investigating spillover catalysts.

$\label{eq:stars} Project \ \# \ ST-30: \ Nanoengineered \ Graphene \ Scaffolds \ with \ Alternating \ Metal-Carbon \ Layers \ for \ H_2 \ Uptake \ at \ Ambient \ Temperatures$

Carter Kittrell and James Tour; Rice University

Brief Summary of Project

The primary objective is to design and produce carbon-metal media and/or mobile nanoparticle catalyst in a graphene slit-pore scaffold to 1) achieve more than 9 wt% uptake of hydrogen, 2) be capable of exceeding 80 g/L volumetric uptake of dihydrogen at near ambient temperatures, and 3) simultaneously meet all major DOE 2015 targets and other desirable traits. This will be accomplished with fibers spun from a graphene slit-pore nanoengineered scaffold or with mobile catalyst particles to convert graphene to hydrogen-saturated graphane.



<u>**Ouestion 1: Relevance to overall DOE**</u> <u>objectives</u>

This project earned a score of 2.8 for its relevance to DOE objectives.

- This project is well suited to the program's objectives and is one of the few open metal sites on carbon substrate projects with much hope of keeping those sites open over time. As such, this project could truly address mass and volume goals.
- The project is focused on the development of a specific material concept for hydrogen storage and attempts to meet the DOE targets.
- It is not really clear what the overall direction and goals are for this project. The synthesis effort seems good, but is not clearly connected to the DOE goals for storage. There are many statements are made about the H₂ storage properties of these materials, but essentially no data is shown.

Question 2: Approach to performing the research and development

This project was rated **3.0** on its approach.

- The approach is good and logically organized and has a good hope of functional success, if the technical steps can be achieved. It includes both science and engineering steps so the product, if successful, will have a better possibility of scale up. Some of the steps are less likely to be done well (e.g., properly spacing graphite at all points will be much harder than separating nanotubes).
- Enhanced binding of H₂ and utilizing spun graphene instead of single-walled nanotubes (SWNT) is a very good approach.
- Mobile Pd catalyst intercalation as "H₂ capture" might not work as expected since the catalyst would agglomerate and loose its small size and mobility.
- The advantages to using nanotubes for some measurements and for synthesis are not clear. Why study these materials when there is so much room for advancement on the graphene materials?
- The project team uses a unique approach of intercalating alternate layers of metal with graphene.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated 2.3 based on accomplishments.

- The project team made tubes of graphene and expanded them without lithium.
- There are four new data points on uptake chart.
- The concept of dynamic multilayer adsorption was proposed last year, but it is applied using SWNT. It is important to illustrate the synthetic viability and proof-of-concept using the graphene.
- Developed process for making metal intercalated graphene ribbons and measured enhanced H uptake compared to carbon.
- So far, it appears all of the measurements were made at 77 K. Room temperature behavior, that is, enhanced binding properties, have not yet been shown.
- Synthesis accomplishments are noteworthy, but it is not clear how this impacts the DOE storage goals and the CoE.
- The project team made less progress than expected relative to what was listed in last year's poster; in fact, many of the figures are the same.

<u>Ouestion 4: Technology transfer/collaborations with industry, universities and other laboratories</u>

This project was rated 2.8 for technology transfer and collaboration.

- Good collaboration with NREL. There were other partnerships listed, but it was not clear what interactions/collaborations are active or whether they are productive. However, the level of collaboration is probably adequate since the PIs appear to be progressing well.
- The project team certainly talks to others, but there does not seem to be evidence of meaningful exchanges lately or value from the C & C.

Question 5: Approach to and relevance of proposed future research

This project was rated 2.3 for proposed future work.

- The project team seems focused on the right steps to make progress.
- There is not a whole lot of detail, but that is normal at the AMR.
- Few actual tasks are planned, but they will be difficult so that is fine.
- Mobile Pd catalyst intercalation as "H₂ capture" might not be feasible given that the catalyst would agglomerate and loose its small size and mobility.
- Focus on illustrating the graphene functionalization and metal intercalation to illustrate the concept viability.
- There was no discussion of future work.

Strengths and weaknesses

Strengths

- Working to reduce costs of material.
- Very good experience with CNT systems.

Weaknesses

- It was not very clear that there is actual progress toward goals; the capacity is too low and was unchanged over the years. It is the same pictures and concepts each year and not much advancement.
- Graphene metal intercalation and functionalization concepts illustration.

Specific recommendations and additions or deletions to the work scope

- The project team really needs to get a full-pressure pressure-concentration-temperature (PCT) done because the 2-bar capacity (i.e., tank has no usable H₂) may also be the high-pressure capacity given how much above the Chahine rule the 2-bar data is.
- Propose to focus on graphene dynamic multilayer work.

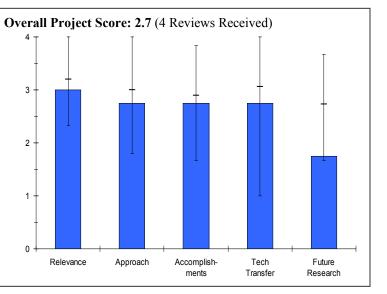
Project # ST-32: A Synergistic Approach to the Development of New Hydrogen Storage Materials, Part I Jean M.J. Fréchet, Martin Head-Gordon, Jeffrey R. Long, Thomas J. Richardson, and Samuel S. Mao; University of

California, Berkeley

Brief Summary of Project

The objectives of this project are the 1) synthesis of porous polymers, 2) synthesis of porous coordination solids, 3) calculations of hydrogen binding energies, 4) synthesis of destabilized hydrides, 5) hydrogen storage characterization instrumentation, 6) metal/metal hydride nanocrystals, 7) synthesis of nanostructured boron nitrides, and 8) theory for boron nitride materials.

<u>Question 1: Relevance to overall DOE</u> <u>objectives</u>



This project earned a score of **3.0** for its relevance to DOE objectives.

- The project is exploring a subset of novel materials and processes with potentially useful hydrogen storage properties. The project contains elements that are unique within the overall DOE Hydrogen Storage Program, and, for the most part, the project is well-aligned with Hydrogen Program goals.
- Relevance to Hydrogen Program goals is adequate. The project investigates a number of interesting nanostructured framework materials (e.g., hypercrosslinked polymers, metal organic frameworks [MOF]) based on a synergistic approach that includes theoretical modeling and materials design aspects.
- Highly relevant project which fully supports DOE research objectives.

Question 2: Approach to performing the research and development

This project was rated 2.8 on its approach.

- The development and testing of hypercrosslinked polymers and other nanoporous polymeric materials as hydrogen storage media is an intriguing and worthwhile approach.
- The approach is well designed, combines modeling and characterization, but needs to focus further on the most interesting and promising systems for the last phase of the project.
- On the basis of the overall program topic listing, the breadth of this project is extensive and spans basic science and applied research.
- A simply stated R&D approach that includes the rationale and criteria that drives the selection of compounds would be helpful. For example, a wide range of materials, from hypercrosslinked polymers to substituted MOFS, to paddlewheel frameworks, and to several other metal-substituted porous coordination solids is being explored. What criteria are driving the selection of those particular compounds?
- While the general approach for this project was not provided and remains unclear, one can infer that it has evolved into a multifaceted strategy toward realizing increased binding energies in sorbents (e.g., polymers, MOFs).
- The additional task related to destabilization of metal hydrides (i.e., partial substitution of MgH₂ with Mn, Fe, etc.) has already been exhaustively studied. It is unclear what is new beyond the dearth of previous work.
- Not clear what the purpose is of the destabilized work on MgH₂. Work on alloying of this hydride has been ongoing for decades, and it is not clear what the present project will do to overcome the obstacles for this material that no one else has been able to overcome.

Ouestion 3: Technical accomplishments and progress toward project and DOE goals

This project was rated 2.8 based on accomplishments.

- Good progress is being made on characterizing the hydrogen sorption properties in hypercrosslinked polymers and other porous coordination solids. These are novel materials for hydrogen storage, and understanding their sorption behavior directly complements the work in other EERE projects (especially efforts in the Hydrogen Sorption CoE).
- The results from calculation of substituent effects are interesting and may provide a predictive capability for compound selection. Have any of those predictions been experimentally validated?
- Very impressive results on high-capacity gravimetric and volumetric storage in MOF-5 at 77 K.
- The destabilization work on the enhanced utilization and improved cycling capacity of MgH₂ in the presence of a MgF₂ additive is an important new contribution.
- A number of promising and original systems have been identified. This includes the Mn-BTT, M3(BTC)₂, and Zn-BTT structures, as well as the addition of MgF₂ in MgH₂ that offers the possibility for enhanced desorption amounts despite added weight. Interesting new knowledge is generated by the project in that respect.
- Hydrogen storage in hypercrosslinked polymers has promise but appears to be relatively slow moving.
- Beryllium analog of MOF-177 is a good synthetic achievement. Based on low-pressure measurements, higher pressure uptake looks promising. However, obvious concerns regarding the potential toxicity of material would have to eventually be considered/addressed.
- Nice library of frameworks possessing open-metal sites. Should be aware of potential overlap with Texas A&M University and University of California, Los Angeles, who both have projects in the same area.
- The concept of using Cr (m) (or other metal) functionalized linkers was presented in the 2008 AMR. What progress is being made in regard to synthesis and experimentation?
- Despite a large amount of data, the overall results are quite disappointing in terms of the actual sorption measurements.

<u>Ouestion 4: Technology transfer/collaborations with industry, universities and other laboratories</u>

This project was rated **2.8** for technology transfer and collaboration.

- Some collaboration is reported, especially with industry.
- A great deal of independent, non-EERE collaborations appears to be established; however, it is not clear that there are ongoing, regular communications between other independent projects and/or the Sorption CoE. Strengthening of such communications is highly recommended.
- Although internal collaborations (within University of California, Berkeley) are occurring, collaborations with other institutions are not readily apparent. Extensive efforts on porous coordination solids and MOFs, as well as on destabilized systems are ongoing in other Office of Energy Efficiency and Renewable Energy (EERE) projects. Collaborations and interactions with those groups (especially the CoEs) would be beneficial.

Question 5: Approach to and relevance of proposed future research

This project was rated 1.8 for proposed future work.

- Future plans are not clearly described. Only limited information concerning future work is provided in a few of the results slides. Likewise, there is very little mention of the remaining technical barriers that must be addressed. A more detailed research plan that focuses on the remaining obstacles is needed.
- Future work suggested interesting elements (e.g., Zn-BTT structures and the addition of MgF₂ in MgH₂), but the investigators need to focus to those that are most promising as the project end approaches fast.
- Beyond a few indirect comments at the bottom of the slides, no clear discussion of future work was given.
- Future plans were not described.

Strengths and weaknesses

Strengths

- Well-qualified team exploring hydrogen-surface interactions in novel porous coordination materials. The project is generating results that will be important in understanding the details of hydrogen adsorption in nanoporous media.
- Very high expertise on the topics studied.
- Interesting innovative ideas on a number of framework materials and metal hydrides.

Weaknesses

- Only limited information concerning the overall approach is provided. Rationale for selection of specific chemical systems and compounds is missing and virtually no information is given about remaining obstacles and future plans for overcoming them.
- There is a lack of focus on promising aspects.

Specific recommendations and additions or deletions to the work scope

- A large number of chemical systems are currently being explored. In the remainder of the project it will be important to focus on the most promising set of materials. The priority should be established by the most critical technical barrier(s) and the investigation of materials that are capable of most effectively meeting those challenges.
- Project finishes soon and the only suggestion would be to focus on the promising aspects of the work.

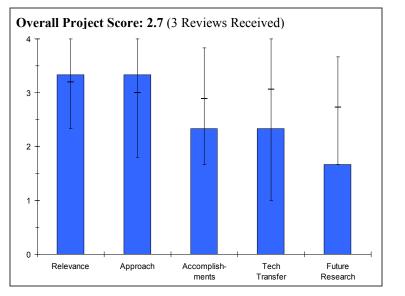
Project # ST-33: Hydrogen Storage in Metal-Organic Frameworks

Chris Doonan and Omar M. Yaghi; University of California, Los Angeles

Brief Summary of Project

The objectives of this project are to 1) research the relationship between metal organic framework (MOF) structure and binding energy (low pressure measurements at various temperatures), 2) conduct high pressure hydrogen adsorption measurement at room temperature (impregnation of polymer and metal complex), 3) move toward the practical use of MOFs (cycling and kinetics of hydrogen charge/discharge), and 4) coordinate with theory (prediction of hydrogen uptake capacity).

<u>**Ouestion 1: Relevance to overall DOE**</u> <u>**objectives**</u>



This project earned a score of **3.3** for its relevance to DOE objectives.

- The project has a high relevance to the DOE R&D objectives. The capabilities and expertise of this project are among the best in the sorbent area, one of the primary classes of hydrogen storage materials.
- This project is well aligned with goals of mass- and volume-efficient storage.

Question 2: Approach to performing the research and development

This project was rated **3.3** on its approach.

- The approach of increasing the hydrogen storage of MOFs at room temperature by improved binding energy demonstrates a correct focus on the key challenge associated with such materials. This project appears to be actively developing and testing numerous strategies (e.g., metal and linker modification and impregnation) in this regard.
- The approach is reasonable.
- Attempting to increase binding energy with new corners and metal sites.
- Replace ligands or atoms on attached groups with active metal, in addition to simply decorating on rings.
- No specific slide on approach was used in this presentation. Coordination with theory was poor, and no apparent feedback to theory was employed.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated 2.3 based on accomplishments.

- The project has not actually realized significant progress in improved binding energy via the numerous outlined approaches, but it is clear that quite a bit of research and testing has been done. Although progress was not demonstrated, the focus and development on the most challenging area for this class of materials is technically significant.
- Every sample that was made showed performance that was worse than already published data. If the PI had presented some rationale, it would have been of some value. Instead, the investigators have put all of their effort into metal additions that do not have a likely chance of producing a material of technological value.

- Slide 5 shows volumetric data, but this is for a theoretical single crystal of material. Are the investigators proposing that this is what will be employed? If they want to discuss volumetric density, they need to indicate a real material packing density as a function of the theoretical crystal density.
- Made many new systems, but headway was minimal. Still, the techniques are good (leaving aside use of Pd and Sc as major mass components of material).
- Even though all this work was done with DOE funding, it seemed to overlap with much outside work that has been presented elsewhere.
- I doubt that the fourth route, making structures with very large pores, is likely to meet the volumetric requirements, even with metal groups. The PI should show how that would work first.

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated **2.3** for technology transfer and collaboration.

- The presentation did not highlight the role of the partners within this project. The collaboration with BASF is beneficial for an industry-scale perspective.
- While one might infer that showing computational results from collaborators suggests that collaboration is taking place, it has never been clear that theoretical structures with high delta H can be synthesized. There has not been an example of a material that has been modeled and synthesized that is of relevance to this program.
- Largely independent work, perhaps because the PI is seen as a leader. Still, leaders can help the whole portfolio by collaborating with other teams.
- They have partners, but only Goddard group seemed to be relevant to the DOE work.

Question 5: Approach to and relevance of proposed future research

This project was rated 1.7 for proposed future work.

- The future work information was limited and could be expanded to provide confidence in the progress and plans for the next steps.
- Plans were scant and vague. They have done interesting work in the past though, so one hopes this will continue.
- No "Future Work" slide was included.

Strengths and weaknesses

Strengths

- This group makes a lot of material.
- World leading team.
- Capable of making the measurements and exotic compounds well.

Weaknesses

- This group makes a lot of material, but appears to do so as an end in itself.
- Somewhat unfocused.
- Not clear that DOE gets full value, much of this work is presented in other forums also and seems to sell the same work to several funders.

Specific recommendations and additions or deletions to the work scope

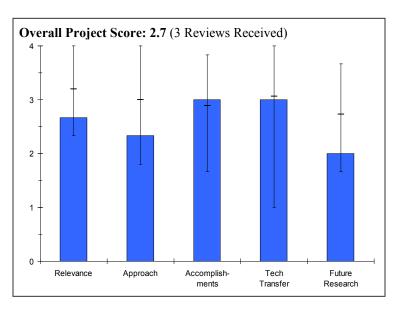
• More closely monitor what work is being done for DOE and discuss future plans to verify that plans are suitable.

Project # ST-34: Compact (L)H₂ Storage with Extended Dormancy in Cryogenic Pressure Vessels

Gene Berry, Salvador Aceves, Francisco Espinosa, Tim Ross, Vernon Switzer, Ray Smith, and Andrew Weisberg; Lawrence Livermore National Laboratory

Brief Summary of Project

Cryogenic pressure vessels offer technical potential to exceed 2010 hydrogen storage goals and approach the 2015 goals. The project objectives are to build systems exceeding 2010 volume/weight targets in collaboration with industrial partners and to understand the fundamental potential of both system and H₂ behavior. Approaches include to 1) fabricate third generation cryotank storing >45 kg H_2/m^3 system, 2) achieve more than 1 week of dormancy, 3) understand dormancy impacts of para-ortho conversion, 4) investigate composite vessel impacts on vacuum quality, 5) demonstrate adequate cycle life (cryogenic shock, high pressure), 6) perform cryogenic vessel development and burst testing, and 7) explore superliquid H₂.



Question 1: Relevance to overall DOE objectives

This project earned a score of 2.7 for its relevance to DOE objectives.

- Adequate and convenient on-board hydrogen storage is one of the key challenges to fuel cell vehicle commercialization. This project is developing one option to meeting DOE targets.
- Vessel design is a required research activity for meeting the DOE objectives. The optimal pressure and temperature operating regime must be investigated with the effects of sub-ambient temperature systems in concert with pressure fully understood.
- The project supports enhancing the gravimetric and volumetric capacity, however, the storage temperatures are still very low.

Question 2: Approach to performing the research and development

This project was rated **2.3** on its approach.

- The project is building on past experience to achieve extended dormancy, verify cycle life, and continue cryogenic vessel development.
- Biggest issue is the excessive size of the tank. The density can be made to look artificially good since bigger systems tend to have better densities. A 2251 tank is 2 to 3 times larger than the tank required for the FreedomCAR targets. Unfortunately, the storage density of this tank system will decrease significantly as the tank size decreases. This type of system is best suited for large commercial and transport vehicles that have high fuel requirements and relatively low dormancy events.
- The utilization of high-pressure tanks with cryogenic H₂ practicality could be an issue (i.e., liquefaction cost, unknown tank component integrity).

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated 3.0 based on accomplishments.

- PI continues to refine and understand the limits of the technology.
- They have refined vessel and structural designs to reduce weight, reduce heat in-leakage, and improve vacuum jacket reliability.
- They are working closely with an automobile original equipment manufacturer (OEM) (but outside of this project) to address some real-world issues.
- The third generation showed improvement over the previous generation.

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated **3.0** for technology transfer and collaboration.

- Choosing BMW as an automotive partner will help the PI to understand vehicle requirements and costs.
- They are working with an automotive OEM and a composite tank manufacturer.
- New collaborations started, however, recommend strong collaboration with ANL and TIAX to conduct well-towheel analysis.

Question 5: Approach to and relevance of proposed future research

This project was rated 2.0 for proposed future work.

- This project needs to address the infrastructure and fueling interface issues.
- The energy required for fueling is prohibitive.
- The interface is complicated/undefined, and not likely applicable for the whole fleet.
- This technology needs to find a compromise on temperature and pressure to make it more compatible with standard pressurized fills (5,000 psi).
- PI should investigate the use of storage materials in the system that either increase dormancy or reduce the fill cooling energy requirements (endothermic materials) to make the system feasible on an energy basis.
- The planned future work is described in rather generic terms and lacks specificity. It is difficult to evaluate the merits of the planned work.

Strengths and weaknesses

Strengths

- This system is achieving real world results.
- This project has been an evolutionary one, where each improvement builds on previous developments.
- They are validating concepts and designs with in-vehicle installation and testing.
- Engineering system capabilities.

Weaknesses

- Choosing BMW as an automotive partner will help the PI to understand vehicle requirements and costs. However, BMW's business case tends to favor high-end (expensive), large, and powerful cars. This model could favor larger tanks, but may not align with the entire range of the U.S. fleet mix that the FreedomCAR targets wish to address. One must question the viability of a technology that requires a completely different filling infrastructure from other methods if it is only applicable for quarter of the U.S. fleet.
- The PI has not provided sufficient information (as in past) regarding the charging interface and energy requirements for tank fill. There are many fill scenarios that could make this system more or less applicable to the targets. They need to narrow in on the optimal fill protocols and temperature/pressure specifications.
- There were no weaknesses identified.
- Focus on gravimetric and volumetric capacity and oversight of liquefaction costs.
- There needs to be a well-to-wheel cost analysis.

Specific recommendations and additions or deletions to the work scope

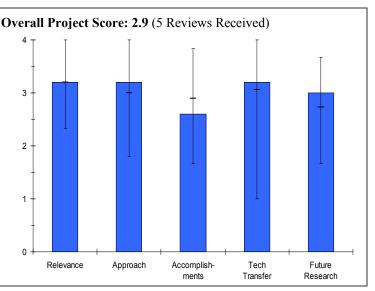
• The project should identify and address institutional issues such as 1) public perception and acceptance of liquefied hydrogen as an automotive fuel and 2) the evolution of safety standards and relaxation of U.S. Department of Transportation (DOT)-type constraints.

Project # STP-01: Lifecycle Verification of Polymeric Storage Liners

Barton Smith and Lawrence Anovitz; Oak Ridge National Laboratory

Brief Summary of Project

The overall objective of the project is to verify durability of polymer liners in highpressure storage tanks. The approach will include 1) subject polymer specimens to extreme temperature cycling while pressurized with hydrogen, 2) measure hydrogen permeation at prescribed intervals to assess the ability of the liner materials to maintain the required hydrogen barrier capability, and 3) test protocol derived from SAE J2579, Technical Information Report for Fuel Cell and Other Hydrogen Vehicles (January 2008).



<u>Question 1: Relevance to overall DOE</u> <u>objectives</u>

This project earned a score of **3.2** for its relevance to DOE objectives.

- It is important to verify the lifetime of tank liner materials, and it is especially important to determine lifetime under cycling conditions.
- The durability of hydrogen storage tank liners is almost as important as the durability of fuel cell systems.
- It is important to understand the failure modes of tank liners and the influence of ambient and operational parameters on the failure mechanisms for the liner materials.
- Definitely pertinent and relevant given that polymeric liners are now being used.
- The work is relevant to the hydrogen program goals and objectives.
- The overall objectives of the project, and how it fits into the gaseous and liquid storage effort, was not discussed or illustrated. This should be communicated in the future.

Question 2: Approach to performing the research and development

This project was rated **3.2** on its approach.

- The size of the liner test specimens is too small to be representative of total liner area. Larger specimen sizes should be considered.
- They are exposing 1-cm-diameter samples of tank liner polymers and subjecting them to extreme temperature (-40 to +125°C) and pressure (6,250 to 12,500 psia) cycles. The specimens are then tested for hydrogen permeation.
- They are using standardized test protocols as recommended in SAE reports.
- Additional details on how permeation measurements will be carried out should have been discussed (i.e., what is actually contained in SAE J2579).
- Even though project has NOT delivered results yet (based on experimental difficulties around seals), the approach is truly innovative and "out-of-the-box" in working at constant pressure while executing thermal cycles. Normal recommendations: pressure cycle at different temperatures.
- Project is also limited in scope, but the presenter was truly excellent.
- Project leverages previous work.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated 2.6 based on accomplishments.

- They have built and put into service an automated pressure and temperature cycling system, and they have begun testing polymer samples with it.
- They have successfully addressed issues of leak-tight specimen mounting at low temperatures and high pressures.
- This project is a new start and, hence, little or no data has been generated thus far. However, good progress on set-up of experimental apparatus.
- Project has shown great understanding of the issues.
- My contention is that we should move to aromatic polymers (e.g., aromatic amides or imides) because they are better materials than high density polyethylene (HPDE) in barrier properties.
- Progress appears to be slow, and the project is behind schedule. After almost a year, the May 2009 milestone is only 50% complete.
- I only rated it fair because of stage of progress: no definitive results because of experimental difficulties in sealing.

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated 3.2 for technology transfer and collaboration.

- Collaborations are with tank suppliers and are appropriate.
- They are collaborating with industrial developers of hydrogen storage tanks and polymer liner materials.
- The project team is working with the key players in the industry.
- The project team is partnering with leading organizations in application space.

Question 5: Approach to and relevance of proposed future research

This project was rated **3.0** for proposed future work.

- The project team will conduct hydrogen permeation tests at 1,500 and 5,500 cycles at 6,250 psia and then begin testing at 12,500 psia.
- If the project is continued into the next year, they will test alternative tank liner materials.
- The approach is clear and to the point.
- The project needs to be accelerated. Tank liner durability needs to be verified as soon as possible.

Strengths and weaknesses

Strengths

- Good laboratory facilities, personnel, and external collaborators.
- This project addresses the pressing need to acquire cyclic permeation data on candidate barrier materials for hydrogen storage systems.
- Innovative approach of thermal cycling at constant pressure versus pressure cycling at constant temperature.

Weaknesses

- No weaknesses identified.
- No weakness noted.
- Test specimen size needs to be increased.
- Progress needs to be accelerated.
- Experimental problems in analysis of permeation properties.

Specific recommendations and additions or deletions to the work scope

- Execute the test plan and future work as proposed.
- Include more discussion on the experimental details of standard test methods employed so that an assessment can be made about their relevance to polymeric materials.
- Continue to correct sealing problem so that experiments can be ran.
- Move to aromatic polymers because of their improved barrier properties.

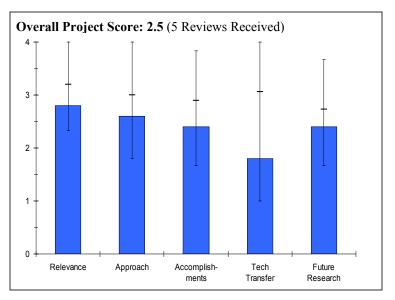
FY 2009 Merit Review and Peer Evaluation Report

Project # STP-02: Electron-Charged Hydrogen Storage Materials

Chinbay Q. Fan; Gas Technology Institute

Brief Summary of Project

The overall objective of the project is to develop a hydrogen storage material and device for hydrogen quick charge and discharge, high wt% and vol% storage capacities, good durability over many cycles, and safe handling and transport. Objectives for 2008 were to 1) combine internal electron-charge (doping) and external charge to increase hydrogen storage capacities and 2) investigate performance optimization and prototype container systems. Objectives for 2009 are to 1) reselect the best hydrogen storage materials for charge modifications and 2) explore carbon-based materials, such as AX-21 and other high surface carbon using polymer as a precursor, metal-modified carbon, and ammonia-borane.



Question 1: Relevance to overall DOE objectives

This project earned a score of 2.8 for its relevance to DOE objectives.

- The project addresses the hydrogen storage targets related to cost, storage capacity, refueling rate, and durability.
- This project offers a unique approach that needs to be fully explored for its potential to assist on-board hydrogen storage.
- Shows promise for higher capacities.
- Fits the objective of kinetics, but capacity and operating temperature are probably more important focus in sorption.
- In the big picture, this is relatively low impact.
- This project is researching the usefulness of external and internal (doping) electron-charges to increase hydrogen storage capacity and hydrogen desorption kinetics. It was initiated in 2005. Results to date are not at all promising in terms of having the major positive impact on hydrogen storage materials required to meet the DOE targets. The cost of this approach would seem to be quite high. It does not appear to be a very useful project to the DOE Hydrogen Program.

Question 2: Approach to performing the research and development

This project was rated **2.6** on its approach.

- The project has taken the approach of modifying the electron charge distribution structure to increase the hydrogen uptake and sorption kinetics.
- Good exploration of effect of electric fields, both internal and external, on the adsorption of carbons and hydrogen release and reabsorption in ammonia-borane.
- Interesting approach. Should get independent confirmation of results and have a clearer theoretical explanation of the results. It would be useful to know what metals were used for materials modification; the metals cost may make the system too expensive.
- The project is stated to be only 55% complete, but is 80% of the way through its time schedule (began in 2005 and ends in 2010).

- There are well-planned milestones and go/no-go decisions, yet it is not at all clear that the September 2008 milestones were met.
- Task 6, due to be completed by July, 30 2009, calls for scale-up to an 11-liter tank for fueling. The project seems nowhere ready for this and has not demonstrated significantly improved useful performance of a storage system based on the project's approach.
- The project is primarily focused on increasing wt% hydrogen adsorbed, with some work also being done on adsorption/desorption kinetics. There is no attention being paid to the DOE volumetric target for the system or target cost considerations.
- The project has recently shifted its focus from increasing the wt% of carbons to trying to increase the rate of desorption of aminoborane. Aminoborane is being studied by the Chemical Hydride CoE. It is not clear why this project is looking at it or how electrostatic charging would increase its rate of desorption, though it appears to be having that effect to some degree.
- The approach is fine, but also appears pretty Edisonian. There is not much understanding of the mechanism or what is happening at the surface.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated 2.4 based on accomplishments.

- The effect was demonstrated and is interesting, however the design appears difficult to scale. There is no assessment of what the data mean in terms of impact to a system design, operating conditions, and so on.
- The technique has shown some encouraging results for AX-21 at room temperature, but the improvement is small at cryogenic temperatures needed for adequate storage capacities. The project has now shifted focus to boron nitride material.
- Significant increases in capacity at low pressures. Analysis is needed to find the "sweet spot" for optimum storage.
- There has been some good science and experiments done. There has been some positive impacts of electrostatic charging on carbons and aminoborane in terms of improving hydrogen wt% stored and increasing the desorption rates respectively. However, the results are very modest and fall far short of DOE targets.
- Interesting effects of electric polarization; however, capacities are low in most cases. Understanding and overcoming capacity limitations will be vital going forward. Some characterization efforts were delayed by slow sample turnaround by others.

<u>Ouestion 4: Technology transfer/collaborations with industry, universities and other laboratories</u>

This project was rated **1.8** for technology transfer and collaboration.

- The project is collaborating with State University of New York (SUNY)-Syracuse. The arrangements with a Japanese manufacturer and University of Houston were also mentioned.
- Work with SUNY is good, but need to get independent confirmation of results and analysis of ultimate system capacity and cost. Should work with OEM or tank manufacturer to understand how system might be manufactured and implemented.
- There is no evidence of collaboration except for obtaining some storage material candidates from SUNY. Collaboration with the Japanese charge control agent (CCA) manufacturer; ATMI, Inc.; and the University of Houston is mentioned but it is not clear what this "collaboration" entailed. There is no collaboration with any of the DOE CoEs or the many other universities and organizations in the hydrogen storage arena.
- Some collaboration indicated with SUNY-Syracuse, ATMI, University of Houston, and a Japanese manufacturer.
- This appears to be an independent effort.

<u>Ouestion 5: Approach to and relevance of proposed future research</u>

This project was rated 2.4 for proposed future work.

• The project proposes to continue the boron nitride work and scaling up to an 11-liter tank.

- The 11-liter prototype is good step; however, before it is built, investigators should get independent confirmation of results and analysis of ultimate system capacity and cost.
- The future work plan is reasonable, but the lack of significant progress of this approach to hydrogen storage makes one question the value of this effort.
- It was unclear if this would continue. In terms of overall impact to the sorption cause, this appears lower priority with respect to other activities within the Hydrogen Program.
- It would be interesting to address the following question: What happens if the material, say metal modified AX-21, starts filling in the absence of an electric field, and then the field is increased in situ (i.e., referring to Slide 9) to 2,000 KPa in the absence of field, and then slowly increase the field to +100 V)? How does the hydrogen capacity respond?

Strengths and weaknesses

Strengths

- Knowledgeable and experienced PI.
- Adequate facilities.
- Some initial success with capacity improvement of metal-modified AX-21 at room temperature and enhanced desorption kinetics of boron nitride material.
- Novel approach.
- Demonstration that applied electric fields and/or polarized materials appear to influence hydrogen storage characteristics, in particular kinetics, of adsorption materials and ammonia-borane. Unique approach to augmenting hydrogen storage. Partial re-hydrogenation of ammonia-borane.

Weaknesses

- Lack of theory.
- Initial results are not very positive.
- Need to know if increases in H_2 capacity seen so far are really enough to make a difference in a final system. There is no clear vision of whether the increases in capacity are enough to enable materials.
- This project is researching the usefulness of external and internal (doping) electron-charges to increase hydrogen storage capacity and hydrogen desorption kinetics. It was initiated in 2005. Results to date are not at all promising in terms of having the major positive impact on hydrogen storage materials required to meet the DOE targets. The cost of this approach would seem to be quite high. It does not appear to be a very useful project to the DOE Hydrogen Program.
- It is not at all clear that the milestones that were due in September 2008 have been met.
- The project is primarily focused on increasing wt% hydrogen adsorbed, with some work also being done on adsorption/desorption kinetics. There is no attention being paid to the DOE volumetric target for the system or target cost considerations.
- There is no evidence of collaboration except for obtaining some storage material candidates from SUNY. Collaboration with Japanese CCA Manufacturer, ATMI, and the University of Houston is mentioned, but it is not clear what this "collaboration" entailed. There is no collaboration with any of the DOE CoEs or the many other universities and organizations in the hydrogen storage arena.
- Not clear whether high capacities can be achieved or maintained with this approach. System cost will be increased by additional hardware, however this might be mitigated by augmented control available through applied fields (i.e., another real-time knob to turn in controlling system behavior). Some lack of familiarity with the hydrogen storage literature.

Specific recommendations and additions or deletions to the work scope

- This project is still in an exploratory stage. It appears premature to initiate the proposed scale-up effort.
- Techno-economic system analysis. Cost estimates for material and tank.
- This project should be terminated.

Project # STP-03: Polymer-Based Activated Carbon Nanostructures for H₂ Storage

Dr. Israel Cabasso; State University of New York

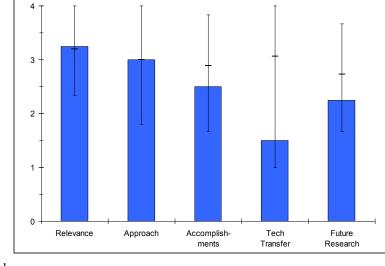
Brief Summary of Project

The overall objective of the project is to develop and demonstrate reversible nanostructured activated carbon hydrogen storage materials with materials-based volumetric capacity of 50 g \cdot H₂/L, with the potential to meet DOE 2010 system-level targets.

Question 1: Relevance to overall DOE objectives

This project earned a score of **3.3** for its relevance to DOE objectives.

• Increasing surface area and getting into an appropriate pore structure is really driving the entire adsorption area at the moment. This is consistent with that goal.



Overall Project Score: 2.6 (4 Reviews Received)

- Overall the concept is well within the Carbon Center activities even though this is an independent project.
- Project aligns generally well with DOE hydrogen research objectives.

Question 2: Approach to performing the research and development

This project was rated **3.0** on its approach.

- Approach is clear and comprehensive, containing all necessary elements for a productive research program (i.e., synthesis, processing, and testing capabilities). It was good to see focus shifting toward strategies which could increase binding energy (for ambient temperature storage).
- The reviewer understands the approach but does not seem to have a clear understanding of the data. If there is in fact a substantial increase in the temperature at which these materials operate, then there should be a substantial change in the heat of adsorption. This was not demonstrated in the poster. Although significant capacity was claimed at -25°C, the data was not shown. Why? This is the most important result.
- The approach is well within the norm.
- There does appear to be potential overlap with Duke concerning polyether ether ketone (PEEK) materials, which both research groups are actively investigating.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated 2.5 based on accomplishments.

- It is evident that a large number of materials have been prepared and tested. Moreover, the corresponding property correlations that have been insightful for establishing trends in behavior.
- A good number of samples were tested, but the results need to be independently validated. This data will be highly controversial until another laboratory can validate the claims.
- It is imperative to have the higher adsorption temperature samples tested independently (for example, at Southwest Research Institute [SwRI]).
- While the goals of this effort make sense, a lot of data is presented in tabular form, for 77 K H₂ uptake. These numbers do not make much sense. I have never seen data from carbons that exceeded ~5.5 wt% but some of the carbons reported on page 12 have values above 6.5 wt%. At least part of the problem is that the investigators have not made a distinction between mass and wt%. The isotherms on page 14 do not appear to be characteristic

312 FY 2009 Merit Review and Peer Evaluation Report of a predominantly microporous carbon. I would have expected isotherms to appear more "Langmuir" with a maximum between 20 and 40 bar. At 60 bar, the H_2 adsorption data continues to rise. Because there is no discussion of how the data were obtained, it is impossible to judge the accuracy of what is presented. The data on page 19 indicating 8 wt% H_2 release at dry ice temperatures is incorrect. Given that this is a solvated carbon, and given no mass spec data, other organic groups being released. The adsorption enthalpies for these materials make an 8 wt% release impossible.

- The PIs have been able to make high surface area substrate with impregnating compounds to increase the adsorption energy. Some results indicate a possible effect on adsorption/desorption temperature. While the implications are significant and noteworthy, the results are not clear.
- The PIs state that some samples could adsorb at ~ −50°C but no data is shown. The highest TPD data is at ~ −120°C.
- The table of materials is very informative and is a testament to the breadth of work. When reporting volumetric densities in this table, it is helpful to provide what material density form this is in respect to. That is, are these based on single crystal, loose powder, or tableted densities?
- The performance of the Melem-Carbon blends appear promising, however, it is interesting that with only a 14 kJ/mol·H₂ binding energy room temperature uptake is possible. This seems at odds with thermodynamics given the temperature and pressure ranges.
- For the "solvated"-carbon alloy work, what is the identity of the "solvent"? And, is the solvent volatile under the measurement conditions? That is, has it been ensured that only hydrogen is being released?

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated 1.5 for technology transfer and collaboration.

- It the response to reviewer's comments section, the collaborations are mentioned. However, it would be helpful in the future to integrate these efforts into the presentation because, in the current form, it is not clear the extent or value of these interactions.
- This appears to be an independent effort. Collaboration is needed to validate results.
- All the hydrogen measurements appear to be done by one company, Gas Technology Institute (GTI). There seem to be errors in the way that data is measured or processed, resulting in the work that been rendered virtually valueless.
- Further collaboration with other team(s), especially the SwRI measurement group or Carbon Centers, could be very valuable to the project. It is important for PIs to do their best and utmost to share samples and further validate their results.
- Communication with between the State University of New York (SUNY) and Duke University is recommended in the area of PEEK materials which both groups are actively working on.

Question 5: Approach to and relevance of proposed future research

This project was rated 2.3 for proposed future work.

- This project was ending. Validation would be worthwhile.
- This work needs to be done in collaboration with someone who can report the uptake data accurately, otherwise the correlation between synthesis and uptake properties have no meaning.
- See comments in Recommendations.
- The focus on exploring methods to increase hydrogen binding energies is appropriate and valuable. More detailed analysis of the preliminary compositions (i.e., Melem or solvated carbons) which could involve residual gas analyzer (RGA) would also be beneficial.

Strengths and weaknesses

Strengths

• Philosophically, the correct approach in designing sorbents.

Weaknesses

- Inaccurate uptake measurements.
- Need better measurement techniques through utilization of existing project and collaboration with appropriate teams within the program.

Specific recommendations and additions or deletions to the work scope

• It is important to independently test and verify the veracity of the high-temperature adsorption materials stated by the PIs. Further support for this project should be contingent upon verifications of the aforementioned claims.

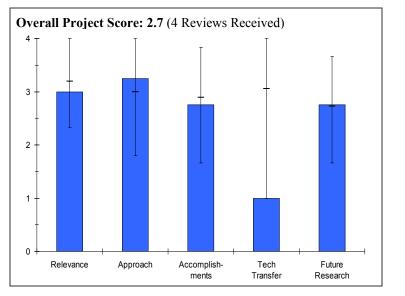
Project # STP-04: Low-Cost High-Efficiency High-Pressure H₂ Storage

Carter Liu; Quantum Fuel Systems Technologies Worldwide Inc.

Brief Summary of Project

The overall objective of this project is to improve the cost and weight efficiency of Type IV compressed H₂ storage vessels to approach the 2010 DOE targets by reducing raw material costs through material development and design and manufacturing parameter modifications. The project is split into the following tasks: 1) plastic liner development, 2) metal fitting development, and 3) optimization of carbon fiber composite usage.

<u>Question 1: Relevance to overall DOE</u> <u>objectives</u>



This project earned a score of **3.0** for its relevance to DOE objectives.

- Development of low-cost, high-efficiency tanks for compressed hydrogen storage is directly relevant to DOE Hydrogen Program objectives.
- High-pressure tanks are the only viable option for storage of hydrogen on board vehicles at the present time. Even though tanks cannot meet the DOE ultimate targets for weight and volume, they have the potential to meet the 2010 targets and are in virtually every fuel cell vehicle on the road today.
- Cost-effective tank development is a crucial piece towards achieving the DOE objectives. However, this project looks to be an engineering exercise instead of a high-risk research project that could result in a disruptive technology to current Type IV tanks construction methods.
- PI was not present; review is based on read of presentation only.

Question 2: Approach to performing the research and development

This project was rated **3.3** on its approach.

- PIs and Quantum have considerable experience in designing and manufacturing carbon fiber composite tanks for high pressure gas storage.
- Good approach to address cost and weight by focusing on liner development, metal fitting, and optimization of carbon fiber composite.
- Quantum is investigating various options to reduce the weight and cost of 700 bar tanks to meet the DOE targets.
- PI is proposing incremental improvements to an existing technology that will not meet the DOE objectives.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated 2.8 based on accomplishments.

- Considering that this is a new project (Start Date: July 2008), good progress has been made.
- There does not appear to be a great deal of progress in the project to date. Most of the presentation concerns future work.
- PI did not demonstrate any results from the blow molding trials. This process is not new INERGY in collaboration with Lincoln composites have already evaluated several different materials with blow molding processes.

315 FY 2009 Merit Review and Peer Evaluation Report

<u>Ouestion 4: Technology transfer/collaborations with industry, universities and other laboratories</u>

This project was rated **1.0** for technology transfer and collaboration.

- They should be partnering with fitting companies (e.g., Parker, Swagelok) for boss development and plastic blow molding experts for their liner work. No partners have been indicated.
- No external collaboration or partners as yet.
- There are no partners associated with the Quantum effort.

Question 5: Approach to and relevance of proposed future research

This project was rated 2.8 for proposed future work.

- Proposed future work is well planned to reduce material cost by more than 50% and weight by about 15%.
- The 50/50 cost share is appropriate for an engineering exercise.
- Almost all of the presentation related to future work. The approach is good, but there are limited results.
- Future work will lead to incremental gains and will not result in the significant improvements in cost, weight, etc. required to meet the DOE goals.

Strengths and weaknesses

Strengths

• Significant experience in designing high-pressure tanks for hydrogen gas storage.

Weaknesses

• Lack of external collaborations.

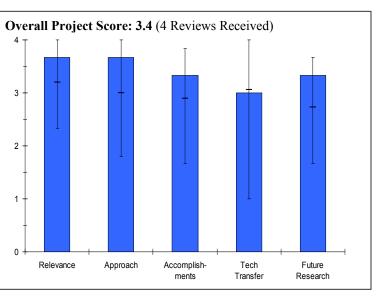
Specific recommendations and additions or deletions to the work scope

• No specific recommendations were given.

Project # STP-17: Solutions for Chemical Hydrogen Storage: Hydrogenation/Dehydrogenation of B-N Bonds Karen Goldberg, Mike Heinekey, Tony St. John, Brandon Dietrich, Travis Hebden, and Steve Matthews; University of Washington

Brief Summary of Project

The Center-wide objective of this project is directed toward the use of amine borane (BN) materials as on-board vehicular hydrogen storage materials. The University of Washington objectives are to 1) develop cost-effective metal catalysts for the dehydrogenation of BN hydrogen storage materials, 2) optimize catalysts to meet the DOE target goals of hydrogen discharging rates from BN materials, and 3) identify and develop new BN materials to address challenges for automotive hydrogen storage materials.



<u>Question 1: Relevance to overall DOE</u> <u>objectives</u>

This project earned a score of 3.7 for its relevance to DOE objectives.

- This research team is developing new catalyst materials for the ammonia borane desorption reaction. The catalysts being developed are Ru-based and Co-based. The team established the performance level of the costly Ru-based metallorganic catalyst and is working on lower-cost Co-based metallorganic catalysts. In their earlier work, they have stabilized the highly exothermic ammonia borane desorption reaction by mixing with an endothermic hydride. This is a very nice strategy.
- This project is of great importance for the Chemical Hydrogen Storage CoE's work on B-N materials and how to improve H-discharge rates by exploring catalysts, as well as screening for new materials.
- Project objectives primarily centered on catalyst design for ammonia borane (AB)-based dehydrogenation. Effective strategies for demonstrating improved kinetics in hydride-based storage reactions (e.g., via catalyst identification) remains a key area of focus toward reaching the DOE goals.

Question 2: Approach to performing the research and development

This project was rated 3.7 on its approach.

- The major technical barrier being addressed is to improve the desorption kinetics in ammonia borane through catalysis.
- The team is combining theory/computational work with experimental work in catalyst design. This is always a very effective platform in new materials development.
- The project is well designed, but it wasn't clear if there was a systematic search for new materials and catalysts? This procedure could have been better clarified.
- Efforts surrounding investigation of organometallic catalysts for AB dehydrogenation add value to Chemical Hydrogen Storage CoE. This approach provides for catalyst optimization (activity and stability) by exploring various metal-ligand combinations.
- The large scope of catalyst metal-ligand candidates should attempt to be narrowed by understanding the identity and role of intermediate AB species. In doing so, the catalyst structure could be more rationally designed to favorably interact with intermediates. This year's work appears to begin to focus on this task (i.e., using electrospray ionization mass spectrometry [ESI-MS]).
- Tasks related to exploring endothermic (and potentially on-board reversible) C-B-N compounds are interesting and leverages theory to guide experiments.

Ouestion 3: Technical accomplishments and progress toward project and DOE goals

This project was rated 3.3 based on accomplishments.

- The group has used experience with the performance of Ru-based catalysts to move on to Co-based catalysts (a less expensive and more readily available starting material).
- Within the Co-based catalysts, the team has tested an assortment of at least four different organic functional groups attached to Co. The outcome of those tests is a potential catalyst, which the team will pursue for future studies.
- The team did not directly address go/no-go decisions in their project planning matrix. However, it was clear from their presentation and planned future direction that performance measures for the Co-based catalysts were considered. Additionally, the development of catalysts for the ammonia borane system is at such an early stage (for all researchers in this field), that a clear measure during development is that some catalysts simply do not work. With that said, it would still be a useful activity if the authors were to "spell out" performance measures for acceptable catalysts.
- It was not clear what other catalysts, or how many catalysts, had been tried.
- Progress toward the identification of products/intermediates via ESI-MS techniques is clear and should prove very valuable for catalyst design. However, it was unclear how the identification of these product oligomers is linking to subsequent selections of catalyst metal/ligand combinations (i.e., still appears to be trial-and-error based)? Many of the catalysts shown here seem the same as last year (e.g., with Co).
- Work on C-B-N heterocycles also appears relatively slow moving. No data on these compounds, which were proposed last year, were provided. What is the desorption/decomposition profile for these molecules?

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated **3.0** for technology transfer and collaboration.

- The University of Washington team is working collaboratively with the University of Oregon, University of Alabama, PNNL, and LANL. This represents a good mixture of universities and national laboratories contributing to the effort. Each group has a well defined project goal: the University of Oregon is working on catalyst development, the University of Alabama is working on thermodynamic predictions, PNNL on gas phase chromatography, and LANL building comparable catalysts with differences in the organic functional groups (relative to the University of Washington's catalysts).
- The poster did not highlight contributions/comparisons/collaborative work with the LANL catalysts. Only after discussing the project did the PI mention the role of LANL in alternative catalyst development. Perhaps the collaboration with LANL is not developing as firmly as with the other collaborative efforts.
- The team has appropriate collaborations, but it perhaps needed to get help from another institute on the synthesis of catalysts to increase the outcome.
- Clear collaboration with University of Alabama for computational data on C-B-N compounds, as well as University of Oregon for synthesis and testing, is apparent.
- Further coordination of research and data with PNNL in the area of determining AB intermediates is encouraged and should be helpful for rationale design of catalysts.

Question 5: Approach to and relevance of proposed future research

This project was rated **3.3** for proposed future work.

- The proposed future work is building on their past experience and steady progress is expected on the identified tasks in support for the Chemical Hydrogen Storage CoE and towards meeting the DOE technical barriers.
- Proposed work is logical extension of current work. More focus on HOW ligand and metal selections for future catalysts will be made (on what basis?) is important for determining ultimate efficiency of this project (e.g., trial-and-error vs. rationale design).

• The team did not directly address go/no-go decisions in their project planning matrix. However, it was clear from their presentation and planned future direction that performance measures for the Co-based catalysts were considered.

Strengths and weaknesses

Strengths

- This project represents a very good mixture of synthesis, experimental testing, characterization, and computation-guided work relevant to metal organic catalyst development for a promising hydrogen storage material system.
- Focuses on crucial issues for improving materials that has potential to meet the DOE targets.

Weaknesses

- The collaborative with LANL seems to be lagging behind the development of collaborative efforts with PNNL, the University of Oregon, and the University of Alabama.
- The team did not directly address go/no-go decisions in their project planning matrix. The team should develop performance targets and assess catalysts according to those performance targets.

Specific recommendations and additions or deletions to the work scope

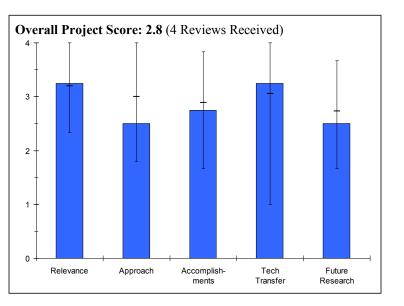
- The idea of adding an endothermic hydride to stabilize the ammonia borane (exothermic system), and to remove some of the excess heat associated with H₂ desorption from ammonia borane, is an excellent one.
- The researchers may also consider other endothermic hydrides, such as borohydrides or other complex metal hydrides.
- A more quantitative assessment of the heat released (per gram of ammonia borane) and heat taken in (per gram of endothermic hydride) would be a good addition to this work.

Project # STP-18: Chemical Hydrogen Storage Using Ultra-High Surface Area Main Group Materials & The Development of Efficient Amine-Borane Regeneration Cycles

Philip P. Power and Susan M. Kauzlarich; University of California, Davis

Brief Summary of Project

The objectives of this project are to 1) provide new materials, compounds, and support for chemical regeneration of amineboranes or borane amides from B-X (X =halide or oxide) compounds, 2) develop a method of regenerating amine-boranes from spent fuel with use of a metal formate/hydride cyclable system, 3) develop light element hydride regeneration such as ammonia borane (AB) regeneration, and 4) enhance the hydrogen release for chemical hydrides such as AB with light element hydride nanoparticles.



<u>Ouestion 1: Relevance to overall DOE</u> <u>objectives</u>

This project earned a score of 3.3 for its relevance to DOE objectives.

- Efficient regeneration of spent ammonia borane is a primary area of focus in the Chemical Hydrogen Storage CoE and aligns with the DOE RD&D objectives.
- This is an interesting project.
- Chemical hydrogen materials are one of the primary routes to meeting the hydrogen storage challenge. And, regeneration of candidate materials is considered to be one of the major issues facing the identification of viable chemical hydrogen materials.
- Project is relevant to one of the regeneration schemes of ammonia borane, as being investigated by the Chemical Hydrogen Storage CoE.
- The work on regeneration of AB, assuming formic acid and metal hydrides are available commercially, does not constitute a closed-cycle regeneration pathway.

Question 2: Approach to performing the research and development

This project was rated **2.5** on its approach.

- The approach is reasonable, systematic, and appropriate.
- The light element hydride nanoparticles work is interesting.
- Tasks related to augmenting hydrogen release properties of AB are relevant. However, the effort here (involving addition of nanoparticles) appears somewhat redundant and at the expense of focusing on the primary regeneration project.
- Approach on AB regeneration by the formate system with the use of formic acid will not likely lead to a viable scheme.
- Creation of a simple, efficient chemical regeneration cycle for ammonia borane remains a critical area of research in the Chemical Hydrogen Storage CoE. The approach of this project (involving main group formates) is complimentary to the larger regeneration effort in the CoE.
- Good progress. Rigorous plan with go/no-go decisions; good turn around.

Ouestion 3: Technical accomplishments and progress toward project and DOE goals

This project was rated **2.8** based on accomplishments.

- Progress to date is reasonable. The down-select of candidate systems is an important step in the overall chemical hydrogen process. This project has effectively eliminated systems that are not viable and has moved on to the more viable approaches.
- Light element hydride nanomaterials eliminate foam problem associated with H₂ release.
- Effects of nanoparticles on kinetics and elimination of foam are not well understood.
- No results on impurities (i.e., borazine NH₃, diborane), a very important issue.
- What is the ratio of nano-BN to AB? The ratio directly affects the H₂ material capacity
- For the task related to addition of nano-BN to AB, the amounts of BN being explored seem much more than typically employed (e.g., 4:1 BN:AB) if the intent is to use BN as "catalytic" product seeds. This large amount of "dead weight" BN also suggests a drastic decrease in capacity. What is the effect of adding much smaller amounts (e.g., 1 to 5 wt%) of BN?
- Limited meaningful progress on regeneration of AB.
- In the area of AB regeneration, progress is apparent with respect to synthesis, testing, and down-selection of appropriate tin formates. Additionally, "down-selected" reactions are beginning to be optimized by substituting undesirable reactants/products (e.g., NaCl).

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated **3.3** for technology transfer and collaboration.

- Extensive collaborations with other partners in the Chemical Hydrogen Storage CoE have greatly benefitted this project.
- Good collaboration with CoE partners.
- Need better coordination with the CoE regarding approach of work, such as those involving formic acid in regeneration pathways.
- Coordination for the regeneration efforts (e.g., with PNNL and LANL) appear to be in place. Additional collaborations are encouraged to routinely estimate regen efficiency, which can aid in the direction of current and future regen reactions/pathways.
- Given the numerous other strategies that are currently being pursued in the Chemical Hydrogen Storage CoE for augmenting hydrogen release from AB, this relatively narrow scope of adding nano-BN might fit better at PNNL where the testing is already occurring.

Question 5: Approach to and relevance of proposed future research

This project was rated 2.5 for proposed future work.

- Future plans for this project are sound and reasonable and will support joint CoE efforts.
- Proposed work on preparation of meso-BN to optimize hydrogen release is sound.
- While kinetics is very important, the issue of impurities can be problematic. Need to quantify the release of impurities.
- Future work on AB regeneration that does not involve formic acid is in the right direction.
- The proposed future work suggests that the metal formate regeneration approach will be abandoned, being replaced with hydrogenolysis. Is there a reason for terminating the formate-based route?
- If BN nanoparticle work is to be continued, suggest significant reductions in the amount of additive (e.g., to catalytic levels). It is recommended that this work be completed as a lower priority to that for regeneration.

Strengths and weaknesses

Strengths

- Rigorous plan with go/no-go decisions, good turn around.
- Strong technical approach.
- Collaborations with other CoE partners.
- Significant experience in experimental work on synthesizing nanomaterials.

Weaknesses

- More detailed discussion of efficiency and scale-up would be nice.
- Absence of data on the release of impurities from AB with nanoparticle additives.
- Pursuit of formic acid route toward regeneration of AB is fruitless.

Specific recommendations and additions or deletions to the work scope

• Work on formate route with formic acid should be discontinued because it is no longer considered an acceptable approach for regeneration of AB spent fuel.

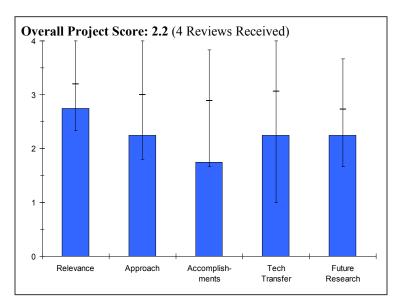
Project # STP-19: Electrochemical Hydrogen Storage Systems

Dr. Digby Macdonald, Justin Tokash, Jason McLafferty, Dr. Amr Saleh, and Dr. Rezwana Sharna; Pennsylvania State University

Dr. George Engelhardt; OLI Systems

Brief Summary of Project

The objectives of the project are to 1) demonstrate an electrochemical route to the conversion of spent ammonia borane (AB) (lower hydride) back to AB fuel (higher hydride) to meet DOE 2010 regeneration process goals, 2) explore the feasibility of electrochemical regeneration of organotin hydrides for use as a reagent in the regeneration of AB, and 3) develop a general model of electrochemical impedance spectroscopy to study coupled reaction mechanisms and utilize the model to extract kinetic parameters from experimental data.



Question 1: Relevance to overall DOE objectives

This project earned a score of 2.8 for its relevance to DOE objectives.

- Looking at a major roadblock for ammonia-borane systems AB regeneration.
- Electrochemical regeneration of spent fuels being investigated in this project differs markedly from the chemical regeneration approaches in the Chemical Hydrogen Storage CoE. This generally broadens the scope of the spent fuel conversion effort. Since the development of an efficient method for regenerating spent fuels is a linchpin issue for chemical hydride technologies, this project is a useful and potentially valuable complement to the more conventional methods.
- Project is supportive of regeneration efforts for ammonia borane.

Question 2: Approach to performing the research and development

This project was rated 2.3 on its approach.

- The use of EIS for analysis of reaction mechanisms is an important component of the overall approach. The electrochemical reactions investigated here are complex and strongly coupled. The use of EIS for elucidating mechanisms and key reaction steps will be vital to developing an understanding of the reaction sequences.
- Addresses regenerating spent ammonia borane, the major roadblock for ammonia-borane systems.
- Electrochemical reduction has some potential advantages.
- Utility of electrochemical impedance spectroscopy (EIS) model has not been demonstrated.
- The fundamental basis for pursuing this approach has not been stated in a compelling way.
- Although the electrochemical regeneration approach is novel and potentially useful, a more detailed description of predicted energy balance(s) and efficiency, as well as a comparison of those predictions with results from more conventional methods, would greatly help to motivate the present approach.
- The project has made a significant effort to reconfigure itself, given the fact that the electrochemical approach for the direct regeneration of ammonia borane was unsuccessful.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated 1.8 based on accomplishments.

- Interesting results have been obtained on hydrogenation using the Devanathan cell.
- Experiments with Devanathan-Stachurski cell showed low conversion of simple test material (styrene to ethylbenzene 17% in 6 days). Tests not yet performed with material of interest.
- Metal hydride electrodes for R₃SnH regeneration have not been successful.
- EIS model development is completed, and validation with ferrocyanide is underway. Model has not yet been able to provide impact on systems of interest.
- Progress has been slow and results limited for a project that started in 2005. Electrochemistry of these systems may be more complicated and not provide simpler routes to regeneration than chemical methods.
- Only limited experimental results are provided on electrochemical regeneration of ammonia borane and on solution-based generation of inorganic hydrides using the new Davanathan-Stachurski cell. At this stage of the project (>70% complete), it is expected that a stronger proof of feasibility and a more extensive base of supporting data would be available. Likewise, the EIS model has only been validated using a comparatively straightforward (single-electron) reaction in ferricyanide. Although the extension to the more complex reactions involved in AB regeneration is non-trivial, it should be viewed as a crucial part of the project.
- No information is provided concerning the important issue of overall efficiency. Without experimental data (or at least predictions from modeling studies) it is impossible to assess the efficacy and utility of the electrochemical regeneration work.
- It is not clear how the developed model will help develop practical AB regeneration strategies.

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated **2.3** for technology transfer and collaboration.

- Good collaboration in attempting to find a role for the electrochemistry approach in the regeneration of ammonia borane.
- Collaborations with other CoE members are present, but they do not seem to be productive.
- Although there are collaborations with PNNL and LANL (the two lead organizations in the Chemical Hydrogen Storage CoE) are listed, it is not readily apparent what roles those organizations are playing or what specific contributions they are making to this project. The project would benefit greatly from a closer collaboration with those organizations, especially in the area of benchmarking the electrochemical regeneration results with results obtained from other methods in the Center. Likewise, beyond a purely advisory function, it is not clear what role Rohm and Haas is playing in the project.

Question 5: Approach to and relevance of proposed future research

This project was rated 2.3 for proposed future work.

- The proposed future work is reasonable, given the fact that the project is in its final stages.
- Plans for R₃SnH regeneration appear to focus on developing analytical techniques to characterize products. This should not be the focus.
- Plans to demonstrate electrochemical transformation of ammonia borane are vague.
- The most important remaining technical obstacles are not clearly identified. A clear and detailed statement of technical barriers is needed to provide a proper context by which to assess the future work.
- The future work statement is very general; it does not inspire a great deal of confidence in the ability to understand and test the electrochemical regeneration concept described here.

Strengths and weaknesses

Strengths

- Good collaboration with other center members.
- Development of an understanding of the reaction chemistry.

- The EIS analysis capability is an especially valuable component of this project. The use of this tool can hopefully guide the experimental work by providing a better understanding of the complex reaction steps involved in the electrochemical processes being explored here.
- Excellent electrochemistry expertise.

Weaknesses

- Too much work on model systems (i.e., styrene-ethyl benzene and ferrocyanide) versus work with systems of interest (e.g., ammonia borane, R₃SnH).
- An identification of the critical technical barriers and a sharply focused effort that addresses those barriers is needed. The project is nearly complete; without a focused effort, it is unlikely that a meaningful conclusion concerning the utility of the electrochemical approach will result from this work.
- The electrochemistry approach does not present that much utility for ammonia borane regeneration.

Specific recommendations and additions or deletions to the work scope

Rapid validation of the EIS model for complex reaction systems is needed. A parallel, very focused effort on AB regeneration is critical. Recommend less effort on the organotin system.

Project # STP-20: Chemical Hydrogen Storage Using Aluminum Ammonia-Borane Complexes

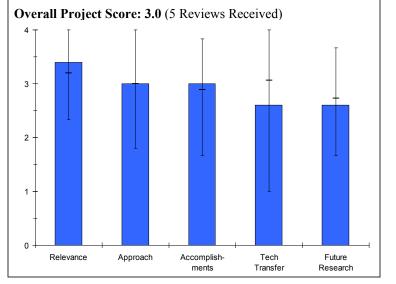
Satish S. Jalisatgi, Jianguo Wu, and M. Frederick Hawthorne; University of Missouri - Columbia

Brief Summary of Project

The objectives of this project are to 1) evaluate aluminum amidoborane derivatives as hydrogen storage candidates that can achieve DOE targets; 2) in collaboration with CoE partners, develop efficient thermal dehydrogenation methods for hydrogen release from aluminum amidoborane derivatives; and 3) in collaboration with CoE partners, determine a suitable route for the regeneration of the spent material.

<u>Question 1: Relevance to overall DOE</u> <u>objectives</u>

This project earned a score of **3.4** for its relevance to DOE objectives.



- The project is quite relevant to the DOE Hydrogen Program objectives. Aluminum aminoborane complexes and their derivatives have high hydrogen capacity that can meet the DOE targets.
- This project is making important contributions to the total effort of the Chemical Hydrogen Storage CoE by studying viable candidate materials.
- Project goals and targets are aligned with H₂ Storage Sub-program targets.
- Al(NH₂BH₃)₃ and other systems being investigated have a high enough material storage capacity that they may be able to meet targets. They are looking to influence reaction rates and improve hydrogenation with Al addition.
- The issues/barriers addressed by this project include the following:
 - Hydrogen storage system gravimetric and volumetric targets.
 - o Flow rate.
 - Overall energy efficiency.
 - System cost.
 - Regeneration process.

Question 2: Approach to performing the research and development

This project was rated **3.0** on its approach.

- The approach is technically sound and logical. It is consistent with the joint directions of the Chemical Hydrogen Storage CoE.
- The approach to look at Al-(ammonia borane [AB)] compounds to try to influence rates of hydrogen release and uptake has merit. The Al should alter chemistry some, but not drastically from B. Previous work showing regeneration of AlH₃ suggests that this approach may lead to easier or direct regeneration. They have addressed hydrogen release issues, but need to increase focus/work looking at regeneration, which is still the major barrier for this class of materials. They have not addressed the effect of Al on regeneration.
- Evaluate aluminum amidoborane derivatives as hydrogen storage candidates that can achieve DOE targets.
- In collaboration with CoE partners, develop efficient dehydrogenation methods for hydrogen release from aluminum amidoborane derivatives.
- In collaboration with CoE partners, determine a suitable route for the regeneration of the spent material.
- The approach centers on the basis that Al-AB complexes will have lower enthalpy on dehydrogenation than AB. The poster does not present evidence that this is indeed true.

Ouestion 3: Technical accomplishments and progress toward project and DOE goals

This project was rated **3.0** based on accomplishments.

- Good progress continues to be made in this project. Project milestones have been accomplished on the established project schedule.
- Have made Al(AB)₃ and LiAl(AB)₄ and have demonstrated reduced H₂ release temperature for Al(AB)₃.
- Synthesized Al(AB)₃, LiAl(AB)₄ complexes, and their ammonia adducts in good yields.
- Preliminary dehydrogenation studies indicate Al-AB complexes release hydrogen at 60°C, lower than AB alone. They currently release 8+ wt% H₂ at <190°C.
- Thermogravimetric analysis-mass spectrometer (TGA-MS) studies show that the ammonia adduct forms of Al-AB complexes tend to release ammonia. (These forms need to be avoided.)
- Two key milestones were met.
- Several Al-AB complexes have been synthesized and characterized. Al-(AB)₃ starts to release hydrogen at around 60°C, lower than AB alone. Li Al(AB)₃ starts to release hydrogen at around 175°C. NH₃ Al-(AB)₃ releases ammonia when heated. Preliminary differential scanning calorimetry (DSC) analysis indicates that the hydrogen release is exothermic.

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated **2.6** for technology transfer and collaboration.

- Extensive collaborations have occurred during the course of this research with other partners in the CoE.
- Collaboration appears to be good across the CoE. Direct collaboration with LANL and PNNL is evidence.
- DOE Chemical Hydrogen Storage CoE (LANL, PNNL).
- Should University of Missouri, Columbia (UMC) have broader collaborations in the Chemical Hydrogen Storage CoE?
- Collaboration not evident in this project. Not clear what collaborators provided to this project. Collaborators listed as working on regeneration efforts, but no regeneration efforts were discussed.

<u>Ouestion 5: Approach to and relevance of proposed future research</u>

This project was rated **2.6** for proposed future work.

- Plans for future work in this project are logical and complete and will ensure the timely completion of the proposed research program.
- Continue the analysis of hydrogen release from new materials.
- Determine long-term stability of new materials.
- Establish hydrogen release kinetics for new materials.
- Determine solid state structures.
- The proposed future work continues and builds upon the success of the current work. There ought to be some emphasis on understanding how clean the release is. Stability of the material needs to be established. In what form is the spent fuel?
- Future work plans do not focus on the major issue for these materials, which is regeneration. Future work needs to look at regeneration and the effect of Al on regeneration of amino-borane type materials.

Strengths and weaknesses

Strengths

- Strong technical research activities.
- A systematic approach is being taken to address the research objectives of the project that is consistent with the overall objectives of the Chemical Hydrogen Storage CoE.
- The primary mentor of the group at University of Missouri, Columbia (Professor Fred Hawthorne) has worldclass experience in the synthesis chemistry required for success in meeting program objectives.

- The resources at LANL and PNNL help this project move forward in an orderly fashion.
- Directly related to the CoE objectives.

Weaknesses

- The project team needs more work in the regeneration area.
- The proposed future work was very generally stated. It needs more specificity (approach details) and more depth (e.g., which new materials and why).
- It seems that UMC does the synthesis work while LANL and PNNL do much of the characterization work. It's not clear how much work is being done for \$350K/year.
- It is not clear how involved Professor Hawthorne is in the detailed planning and execution of the project.
- Not much time left in the CoE lifetime to establish this work, if the material is viable and can be regenerated.

Specific recommendations and additions or deletions to the work scope

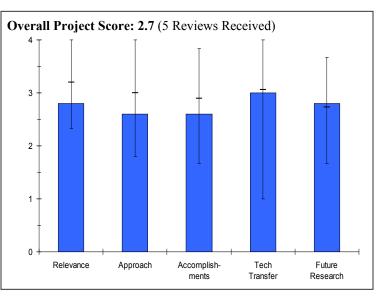
• The Chemical Hydrogen Storage CoE needs to evaluate whether the general types of materials under study at UMC have a chance of providing a leading candidate for on-board storage compared to the other promising material types under study in the CoE. Aluminum seems too heavy an element to be a viable hydrogen storage material when one takes account of the fact that, for any aluminum amidoborane, one cannot remove all of the hydrogen and expect to be able to perform a cost-effective regeneration. So, the question is "Can aluminum amidoboranes achieve upwards of 11 wt% H₂ (a likely material gravimetric target that permits meeting system targets) and also pass the acceptable regeneration litmus test?"

Project # STP-21: Novel Metal Perhydrides for Hydrogen Storage

Jiann-Yang Hwang, Shangzhao Shi, Steve Hackney, Douglas Swenson, and Yunhang Hu; Michigan Technological University

Brief Summary of Project

The overall focus of this project is to 1) develop new kinds of materials that are able to bind hydrogen molecules into clusters, and 2) enhance hydrogen adsorption/desorption by means of hydrogen cluster formation/decomposition so that the capacity of materials for hydrogen storage and the kinetics for hydrogen release have the potential to meet the DOE 2010 and 2015 targets. The objectives over the past year were to 1) study the H₂ adsorption behavior of material systems having charged species in the material structure, 2) design and develop material systems capable of auto-charging under H_2 pressure, 3) study the H_2 adsorption behavior of materials systems



capable of auto-charging under H_2 pressure, 4) design and develop devices for directly measuring H_2 sorption in an electric field, and 5) study the H_2 adsorption behavior of materials systems charged by applied electric potentials.

Question 1: Relevance to overall DOE objectives

This project earned a score of 2.8 for its relevance to DOE objectives.

- Project aligns with the Hydrogen Program and DOE RD&D objectives.
- This project is the original attempt to solving this problem.
- The project addresses appropriate barriers for hydrogen storage.
- This project includes trying to improve room temperature hydrogen storage capacities.
- I did not receive a clear understanding that the work, if successful, would lead to progress against the Hydrogen Program goals and objectives.

Question 2: Approach to performing the research and development

This project was rated **2.6** on its approach.

- The approach is effective, but has some room for improvement.
- The research is focused towards the program goals.
- The approach appears to be solid.
- Systems with applied potentials of 2 kV to generate charged species are impractical, and at these potentials, it is unclear if any increase in adsorption observed is not due to non-reversible reactions. What would be the cost to apply this large potential across the storage media, and what effect would this have on system efficiency? Also, Pt doping will likely increase the cost of the storage material beyond the allowable cost. Need to check reversibility of H₂ adsorption and determine that gas desorbing is all H₂ (i.e., not H₂O, a hydrocarbon, or other species). Integration/collaboration with other CoE should allow for adsorption/desorption measurements to be made on these materials.
- The basic physics behind the approaches being pursued for introducing extra hydrogen into materials is not clear.

Ouestion 3: Technical accomplishments and progress toward project and DOE goals

This project was rated 2.6 based on accomplishments.

- There are too many unknowns.
- The existence of (H+)x clusters remains to be proven.
- Mechanism of hydrogen absorption is still poorly understood.
- Good progress (experimental), interesting results, good indication that the phenomena enhances adsorption.
- Materials with the required H₂ adsorption capacity have not been identified. Small improvements are noted for "charged" materials over the baseline materials used. It seems that for any appreciable amount of adsorption, the increases in adsorption seen for materials with charge generating materials (CGM) are relatively small (~ 10% increase from carbon without CGM). Could this be due to sample-to-sample variation or small changes in surface area upon adding CGM? In NiO, CGM enhancement is a larger percentage, but overall adsorption is much smaller (<0.2%, more than an order of magnitude less). Similarly for Pt/C with an applied potential, it is more difficult to measure these small amounts accurately. Depending on level of doping or potential, other changes are likely to be occurring which can affect adsorption, including just the presence of a metal atom on the surface (spillover effect vs. a charge effect).
- The claimed "charge enhancement" for vermiculite may not be related to charge at all, but just to increasing the free volume by removing water with increased temperature. While the Bruner–Emmett–Teller surface area analysis method (BET) area did not increase with increasing treatment temperature, it is clear that water molecules take up space and are most likely interacting with some of the interior surfaces. Removing these should free more surface sites where H₂ could adsorb.
- Only marginal increases in absolute room temperature hydrogen storage capacities were obtained, but there were significant relative increases.
- Progress appears to be made, but again, it is hard to understand from the materials available how this will lead to significant progress against the program goals and objectives.

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated **3.0** for technology transfer and collaboration.

- There has been adequate collaboration.
- The specific role of the partners could be more explicitly highlighted in the presentation.
- Collaborations with other universities, companies, and a national laboratory are in place. Collaborations on measurements (reversible adsorption/desorption) would be beneficial.
- Collaborative activities appear limited.
- A diverse team has been established.

Question 5: Approach to and relevance of proposed future research

This project was rated 2.8 for proposed future work.

- Plans to look at materials with higher intrinsic storage capacity are appropriate. Plans to utilize the ORNL neutron facility to try to look at materials and the uptake mechanism should move the work towards improved understanding.
- The future work makes sense, but is not quite clear how it will be accomplished.
- Why does the effect vanish as a function of pressure?
- Temperature dependence studies could help determine heat of adsorption?
- Reversibility?
- This should really be "Not Applicable," since this project is essentially over.

Strengths and weaknesses

Strengths

- Good collaboration.
- Clear understanding of challenges
- Some indications that the approach works at low pressure.
- None.

Weaknesses

- Conclusions are not always supported by facts.
- Adsorption measurements methodology should be discussed.
- Measurements have not shown reversible adsorption/desorption. Charge effects observed have been fairly small.
- Approaches adopted are vague in their scientific justification.

Specific recommendations and additions or deletions to the work scope

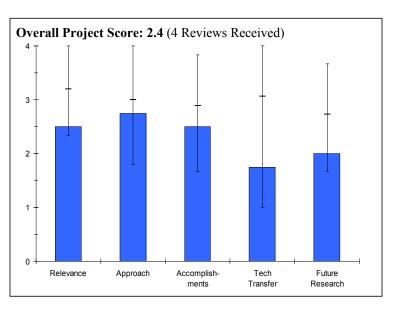
- Continue the project. Make go/no-go decision at the next AMR meeting.
- None.

Project # STP-22: Purdue Hydrogen Systems Laboratory

J. Gore, A.P. Gagare, S. Basu, A. Brockman, M. Diwan, A. Al-Kukhun, H.T. Hwang, Y. Zheng, P.V. Ramachandran, and A. Varma; Purdue University

Brief Summary of Project

The objectives of the project are to 1) improve the extent, rate, and control of hydrogen release from ammonia borane (AB) by hydrolysis reactions; 2) discover practical uppermost hydrogen storage density of the AB hydrolysis approach; 3) understand engineering properties of the AB hydrolysis approach; 4) characterize the dehydrogenation products and develop new methods for AB regeneration; 5) investigate the reaction mechanism and effect of process parameters on yield of hydrogen generation by novel noncatalytic AB hydrothermolysis; 6) determine parameters that maximize anaerobic biological hydrogen production; and 7) understand energy balance for a local modular energy system using biological/solar technology.



Question 1: Relevance to overall DOE objectives

This project earned a score of 2.5 for its relevance to DOE objectives.

- AB recycling is well aligned with program goals in that it supports use of one of the few materials that can meet goals. Slurry work is interesting in that it may allow for liquid filling which will be easily accepted by the public, but the claimed density is not especially at the system around 4%. Additionally, it is not suitable to cold weather use as it becomes very viscous below 0°C and freezes around 0°F. The hydrolysis work is poorly aligned because, energetically, it is unreasonable to recycle efficiently.
- Project goals align with DOE R&D objectives.
- This project is focused on the development of ammonia borane as a hydrogen storage material.
- The project addresses hydrogen storage system gravimetric and volumetric targets.
- It also addresses the development of by-product/spent material removal and regeneration processes.
- The project is well aligned with the RD&D objectives, but it appears that there is overlap with efforts in the Chemical Hydrogen Storage CoE.

Question 2: Approach to performing the research and development

This project was rated **2.8** on its approach.

- AB approach is good in that it is new and may work. The energy pathway seems less optimal, but it is not bad.
- The slurry at the level of water contemplated seems unlikely to be fluid at low temperature as a reactant, and will be a solid in the product state. The use of the water to make H₂ will leave a solid. There will almost certainly be a need for more water in real systems, which will reduce the capacity to perhaps 2% or so.
- The approach to hydrolysis is well conceived and has the advantage of working at fuel cell exit temperature so heat is "free."
- Rheological measurements are useful for systems design.
- Calculations suggest regeneration of borates or B(OH)₃ is too energy intensive due to the stability of the B-O bonds. The authors try to get around this using triflate ligands. It is not clear what happens to the Me₃SiOTf in this recycle scheme. It appears the project will have an even larger problem with forming a Si-O bond than with

the B-O bond. The project must reduce the Si-O bond now or Et_3SiH becomes a consumable reagent driving up cycle costs. Most likely, having to reduce this stable Si-O bond will drive down energy efficiency for the cycle when its recycle or manufacture of Et_3SiH from starting materials is included.

- Approach to AB recycling:
 - Spent fuel, ammonium borate converted to boron tris(triflate) or boron tris(trifluoroacetate), which provides molecules with weaker B-O bond.
 - Further reduction of boron tris(triflate) or boron tris (trifluoroacetate) in the presence of triethyl amine, followed by the displacement of the amine -using ammonia, leading to efficient ammonia borane regeneration.
- Approach to dehydrogenation of AB Slurry:
 - Enhance the AB powder, water, and catalyst mixing process using ultrasonic mixing and high shear mixing to obtain high hydrogen yields near stoichiometric.
 - Characterize transportability of AB slurries and associated hydrolysis by-products by viscoelastic property measurements.
 - Use a reactor module to provide engineering studies of AB and other materials that have potentials for off-board recyclable chemical hydrogen storage.
- Approach to non-catalytic AB hydrothermolysis:
 - Perform isotopic experiments to understand reaction mechanism of H₂ release from aqueous AB solutions/slurries.
 - Investigate solubility of AB in water at temperatures in the range 25–70°C.
 - Study H_2 yield over a wide concentration range (5–50 wt% AB).
- Approach to characterization of reaction by-products:
 - o Initiate development of a continuous-flow reactor for hydrogen release.
- The approach has potential when it comes to addressing technical barriers, but could be improved to make the Purdue approach more distinguished from other on-going efforts. Clarifications needed for how to improve the performance of the AB slurry.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated 2.5 based on accomplishments.

- The program ends soon. It would have been nice to have seen more progress on the recycle chemistry at this point, but they may still finish on time. The utilization has made suitable progress in glassware and a bomb-like device, It would have been nice to have seen a larger scale demonstration in metal that showed the expected mass transport devices. Still, they are showing, at least in idealized conditions, what might be done and making good use of design to be more efficient.
- Have proposed an AB recycling scheme for hydrolysis of AB going through B(OH)₃ and demonstrated reduction of boron tris(triflate) to BH₃.
- It is not clear what happens to Me₃Si(OTf) in this recycle scheme.
- Non-catalytic hydrothermolysis is interesting, but it is not clear what is happening. It appears to increase H₂ released/mol AB, especially at low AB concentrations; however, it is not clear that it increases the H₂ storage density on a wt% basis. UPenn obtained 7.2 wt% at 50% AB in IL at 120°C while this project obtained about the same for 50 wt% AB at 135°C. At 50% AB, is this project just doing thermolysis in water, in place of the ionic liquid? The potential for water soluble products in this system is attractive. If it need to be pressurized much, it is probably not practical.
- AB recycling:
 - o Achieved reduction of B-OTf bond in dibutyl boron triflate followed by hydroboration of 1-octene.
 - The reduction of boron tris (triflalte) was achieved using diethyl silane.
- Dehydrogenation of AB slurries:
 - A 92% hydrogen yield in a (1:2) AB/water slurry hydrolysis test using ultrasonic mixing was observed; it provided a material based hydrogen storage capacity of 8.2 wt%.
- Investigation of non-catalytic AB hydrothermolysis:
 - \circ AB solubility is ~ 50 wt% at 70°C; at >70°C, hydrogen generation is observed.
 - While varying AB concentration from 5 to 50 wt% (\sim 135°C, 200 psia), the total hydrogen yield (H₂+HD) remained at around 2.5-2.75 equivalent per mole of AB.

- Hydrogen yield varied linearly with AB concentration (for <50 wt% AB), with a maximum hydrogen yield of ~8 wt% as reported in slides. But at poster session, they reported >11 wt% recovery at 85°C. In addition to hydrogen, some NH3 formation is also observed.
- OK.

<u>Ouestion 4: Technology transfer/collaborations with industry, universities and other laboratories</u>

This project was rated **1.8** for technology transfer and collaboration.

- While they show General Motors (GM) as a partner, it turns out they are not a partner in this work. GM may have given some vehicle requirements, but that may have also done that in previous programs and not this one. They do not seem to be working with the Chemical Hydrogen Storage CoE very much at all even though there is a natural synergy.
- Collaboration with General Atomics and General Motors.
- Collaborators are General Motors (lab infrastructure) and General Atomics (AB synthesis)
- Seemingly, no direct collaboration with the Chemical Hydrogen Storage CoE or its member institutions.
- Seems like most work is done by Purdue University. There is a need for interacting with the Chemical Hydrogen Storage CoE to learn fundamental aspects of ammonia borane chemistry and to avoid overlap. The presentation did not indicate any ongoing communications with the CoE and the experts on ammonia borane.

Question 5: Approach to and relevance of proposed future research

This project was rated **2.0** for proposed future work.

- The program is a little diffuse, trying to cover all aspects at a low level of intensity rather than making a major step in one area; that is OK, but perhaps less efficient use of DOE money. That said, each component seems well planned, with the recycle using surrogate systems to demonstrate the process and then refining reactants and conditions. The bomb reactor tests are also well designed, making good use of heat streams. A little hazier in the glass bomb demo, that seems to have ignored the fate of the products (i.e., how they will be moved from the reactor in solid form). They did nice mechanical tests, but did not have a convincing plan for dealing with the products.
- Include all parts of cycle in regeneration scheme (i.e., recycle of Me₃SiH or other reducing agents).
- Future work on AB recycling:
 - Calculation of bond energies for the proposed AB recycling is underway.
 - The conversion of ammonium borate or boric acid to boron tris(triflate) will be examined.
 - Optimization of the reduction of tris-acylborate to borane-ammonia.
- Future work on dehydrogenation of AB slurry:
 - Conduct AB slurry hydrolysis using a high shear mixing reactor.
 - Conduct catalytic AB hydrothermolysis below 85°C (joint effort).
 - Conduct AB ionic liquid slurry thermolysis tests.
 - Design, construct, and test an AB slurry dehydrogenation reactor module.
- Future work on non-catalytic AB hydrothermolysis:
 - Determine reaction mechanisms and yield of hydrogen generation from AB hydrothermolysis in aqueous solutions and slurries.
- Future work on quantification of reaction by-products:
 - Develop, test, and analyze continuous flow reactor setup.
- Seems to be potential for improvements, but the future plans need to be more specific regarding how to meet the DOE targets. What about trying other AB recycling paths?

Strengths and weaknesses

Strengths

- Strong team intellectually and good support from the university the assistant dean helped present the work!
- High capacity material.
- Simple concept to execute (except for the recycle, which is complex).
- Potential for soluble products or well-behaved, pumpable slurries for reactants and spent products.

Weaknesses

- Huge energy efficiency barrier in recycle of borate.
- Moving solids is difficult in rectors; liquids would be better, but that option would destroy the mass efficiency.
- Not taking advantage of knowledge in the DOE system.
- Overcoming potential energy sink of borates formed from the hydrolysis.
- The project does not appear to be well connected to the Chemical Hydrogen Storage CoE.
- Hydrolysis of AB is not generally considered to be a promising route to hydrogen evolution from AB in terms of meeting DOE hydrogen storage system performance targets.
- No apparent teaming with other ongoing efforts on ammonia borane.

Specific recommendations and additions or deletions to the work scope

- Nearly complete; really too late for meaningful change.
- The extent to which this project is covering ground already plowed by the Chemical Hydrogen Storage CoE needs to be evaluated. Their results/accomplishments should be confirmed by another institution (e.g., the Chemical Hydrogen Storage CoE). The approach needs to be clarified to make sure that this project is distinguished from other ongoing efforts.

Project # STP-23: Hydrogen Storage Research

Lee Stefanakos and Sesha Srinivasan; University of South Florida

Brief Summary of Project

The overall objectives for this project are to 1) synthesize and characterize materials with high hydrogen storage potential; 2) discover new materials and processes; 3) perform catalytic doping, destabilization, and substitution strategies to improve the kinetics and reversibility of hydrides at low temperature; and 4) employ ab initio calculations to validate the experimental observations.

<u>Question 1: Relevance to overall DOE</u> <u>objectives</u>

This project earned a score of **2.8** for its relevance to DOE objectives.

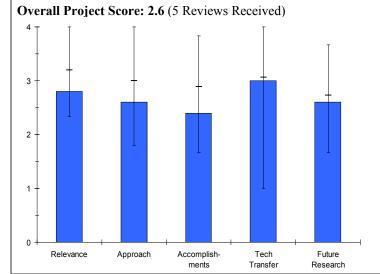


- Project contains both theory and experimental components that are generally well aligned with Hydrogen Program objectives. Although there is significant overlap between this independent project and individual projects within the DOE Centers of Excellence (especially in area of complex hydrides), there is sufficient new work here to justify continuing support.
- Very good results and progress towards DOE goals.
- Overall, they are not moving the ball much; thought area is reasonably aimed. If the polymer work proves valid, this would need to be changed to "good."
- This project addresses the following hydrogen storage system technical targets:
 - Volumetric H_2 density, >45g H_2/L .
 - Gravimetric H_2 density, >6.0 wt.%.
 - Operating temperature, -30/50°C.
 - Delivery temperature of H_2 , -40/80°C.
 - Cycle life, 1,000 cycles.
- Fast absorption/desorption rates.

Question 2: Approach to performing the research and development

This project was rated **2.6** on its approach.

- The project integrates synthesis, analysis, characterization, and computational studies of selected complex hydrides and polyaniline nanostructures. The PI and his colleagues have done a good job of making mid-course corrections during the project to focus on the most promising materials.
- The approach is effective but could be further improved.
- Sharp focus; promising results.
- The approach is alright. Not so well integrated with itself or others, but adequate. The work is in some regards a rehash of existing work with only small variation. For example, particle size is the repeat of the UOP work. This could have been good except that there was no control for other effects that might have gone along with particle size such as temperature reached in preparation, addition of unintended catalytic metal, and the other usual problems. The polymer work was again not sufficiently well planned for the experimenter to understand what they saw.
- Synthesis, characterization, and performance testing of (1) ternary and higher order borohydrides and (2) polyanaline nanostructures.



- Stabilization, nanocrystalllization, and nanomaterial doping are among the issues explored using crystal structure methods and thermodynamic stability calculations.
- A fairly detailed experimental process was used to arrive at the specific component concentrations and physical morphologies for the LiBH₄/LiNH₂/MgH₂ system. However, the conclusion that use of nanoscale MgH₂ results in dramatic improvements in hydrogen storage compared to earlier results obtained by investigators at Ford Motor Co. in a similar complex hydride system is questionable based upon the experimental data that were presented.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated 2.4 based on accomplishments.

- A lot of interesting and very useful results, both basic and applied.
- Synthesized multinary complex hydrides involving LiNH₂, LiBH₄, and MgH₂ using solid-state mechanochemical process; prepared Li-Mg-B-N-H complexes showing efficient/reversible hydrogen storage capacity (>6 wt.% at 150-175°C). Independent validation of (pressure concentration temperature) PCT characteristics by Southwest Research Institute (SwRI) closely matched USF results and showed no evolution of ammonia or diborane.
- Synthesized complex borohydrides, e.g., LiMn(BH₄)₃, by mechanical milling of LiBH₄ and MnCl₂. Accomplished reversibility of hydrogen sorption cycles in LiMn(BH₄)₃ by self catalyzing effect using Xmol% MgH₂.
- Studied the effect of nanomaterial doping and co-doping on the hydrogenation and dehydrogenation behavior of Li-Mg-B-N-H and Li-Mn-B-H.
- Established the structure of Mn(BH₄)₂ and calculated the thermodynamic stability by Density Functional Theory.
- Synthesized polyanaline nanostructures using chemical and electrospinning processes. Accomplished reversible hydrogen storage capacity of 3-10 wt.% from room temperature to 100°C.
- The results on the LiNH₂/LiBH₄/MgH₂ are intriguing. Previous work on this system (Ford Motor Co.) showed only modest gravimetric capacity (~3% at 200°C). The improved sorption behavior measured in the present work is attributed to the method of preparation and the suggested importance of nanoscale MgH₂. However, particle agglomeration/sintering upon repeated cycling occurs, and it's therefore difficult to understand how these results can be rationalized by invoking nanoscale effects. A very thorough examination of possible experimental artifacts in the PCT measurements is needed before conclusions can be drawn concerning significantly enhanced storage capacity at reduced temperatures in this multinary complex hydride.
- They have produced many results, and credit should be given for that accomplishment; however, the understanding is not good. For example, the assignment of delta particle size is simply a result of the fact they saw a rough correlation in five data points. With all the other variables in play it is hardly wise to assign a band of optimal size difference, especially with no theory as to why. Likewise, there was no indication of understanding of why the polyaniline (PANI) had higher reversible capacity at higher temperature, in contradiction to all other studies. Most difficult to accept was that in a series of runs, they saw a continuing loss of mass in pressure-composition isotherm (PCI) tests; however, when weighed, the sample had not lost mass. Clearly, this is a big problem and makes it impossible to accept an otherwise exciting result: room temperature and even high temperature storage of 8%.
- The stated sorption results on the nanophase PANI materials are extraordinary (6% gravimetric capacity at 125°C, multiple cycles). If correct, this is a breakthrough result. However, very unusual sorption behavior is evident, and the sorption data strongly suggest that experimental artifacts could be important (e.g., no threshold is observed in the H-uptake vs. pressure data). It is imperative that the PCT system is carefully calibrated using well-known standards to ensure that the PANI measurements are valid. Likewise, great care must be taken in the analysis of the PANI data to rule out any possible effects due to chemical reactions during testing. Finally, given the extraordinary nature of these results, it is crucial for the measurements to be validated by other laboratories.
- The reaction enthalpy (~78 kJ/mol) from the Van 't Hoff plot is totally inconsistent with the measured temperatures for hydrogen uptake and release (i.e., enthalpy much too high).
- The overall benefit of the computational work (density functional theory [DFT] calculations) seems to be limited. Although the calculations have some utility in establishing thermodynamic characteristics of selected

reactions (e.g., reactions involving $Mn(BH_4)_2$), it is not clear how those calculations are being used to guide the experimental work in this project.

- Validation of ab initio calculations? This is the weakest area.
- Both chemisorption and physisorption mechanisms are proposed to explain the PANI sorption data. However, a compelling argument concerning the mechanistic details and the relative contributions of these two processes to the overall sorption behavior has not been provided.

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated **3.0** for technology transfer and collaboration.

- Good degree of interactions between participants; nice slide on the structure of the collaboration.
- They use both industrial and lab partners to good advantage in getting catalysts and also in obtaining spectra that may illuminate the meaning in the data.
- Collaborations with:
 - o QuantumSphere, Inc.
 - o NIST
 - SWRI®
 - o Nano-RAM Technologies, India
 - o University of Hawaii
 - 0 NNRC
- Seemingly, no direct collaboration or interaction with the Chemical Hydrogen Storage CoE.
- Many collaborations are listed (slide 42). These efforts are assisting the materials discovery and characterization in the overall University of South Florida program.

<u>Question 5: Approach to and relevance of proposed future research</u>

This project was rated **2.6** for proposed future work.

- Plans build on past progress and are designed to address existing challenges and barriers. There is some chance for discovering new materials.
- They have plans, and they are aligned with the goals. Again, they do not seem aimed at understanding the problems in the current work. For example there seemed to be no attempt to work out the odd mass conservation difficulty in the PANI work or any systematic approach to really understand if the particle size conclusion was supportable.
- Future work is clearly stated and represents a logical extension of the current effort. However, since the project is more than 85% complete, the plans seem to be unrealistic. It would have been helpful to establish some kind of priority for the future work based upon the most noteworthy remaining barriers (i.e., what are the most critical specific technical problems and what plans are in place to solve them?).
- Proposed future work includes:
 - o Investigate hydrogen performance of nanoscale, dopant-enhanced complex multinary hydrides.
 - Investigate activation energy and mechanism of hydrogen release from nanoscale doped complex hydrides using Kissinger method.
 - Perform gas evolution analysis in-situ during cyclic hydrogen sorption measurements.
 - Establish the structure of LiMn(BH₄)₃ and calculate the thermodynamic stability by DFT.
 - \circ Investigate the effects of nanomaterial additive on the dehydrogenation and reversible rehydrogenation characteristics of LiMn(BH₄)₃ by determining the cohesive energies and bond strength information.
 - Employ a mechanistic approach to enhance the hydrogen storage characteristics of polyaniline nanostructures by incorporating various materials (e.g., carbon nanotubes [CNT], fullerenes, SnO₂, and Ti) during chemical and electrospinning processes.
- Demonstrate and correlate the analysis results of DFT calculations with the experimental investigations carried out in previous tasks.

Strengths and weaknesses

Strengths

- A comprehensive project conducted by a well-qualified R&D team. Recent results on multinary complex hydrides and substituted PANI nanostructures are especially intriguing. Extensive collaborations are facilitating progress in the project.
- A very comprehensive research effort.
- Interesting results reported for synthesized polyaniline nanostructures.
- Earnestly want to advance the science.
- Well funded.

Weaknesses

- A straightforward assessment of technical obstacles and barriers and a careful validation of the experimental results are needed. Contributions from experimental artifacts appear to be important in the PCT data. These *must* be ruled out before meaningful conclusions can be drawn.
- The group can afford to narrow their focus.
- More validation of theory would be beneficial.
- The project seems more aimed at generation of data than understanding.
- The PI is insufficiently concerned with inconsistencies.
- It's not likely that a material with a significant amount of manganese in it will store upwards of 11 wt% H₂ and thereby meet the gravimetric "system" storage target for 2015.
- The poster is overloaded with details and secondary information. It is difficult to navigate through it without the presenter's assistance.
- •

Specific recommendations and additions or deletions to the work scope

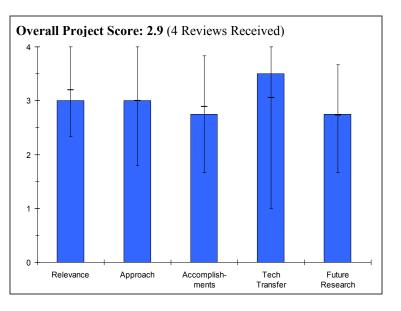
- This group would benefit from direct management (DOE may not accept that data, it clearly does not make sense) rather than just suggestion. They have data that is clearly flawed, and the programs are not as well planned as they would be if working with a more established group.
- Results obtained with the nanostructured polyanaline are interesting, but are also somewhat counter-intuitive. They need independent corroboration and/or vetting by the Chemical Hydrogen Storage CoE.
- Rather remarkable results for sorption behavior in the LiBH₄/LiNH₂/MgH₂ complex hydride and in the nanoporous PANI system have been presented. However, there are serious questions concerning the accuracy and reliability of the PCT measurements. It is imperative to investigate and eliminate any experimental artifacts, and it is strongly recommended that the results be validated by testing at other laboratories. This should be the principal focus in the remainder of this work.

Project # STP-25: Carbon Aerogels for Hydrogen Storage

T.F. Baumann, M.A. Worsley, and J.H. Satcher, Jr.; Lawrence Livermore National Laboratory

Brief Summary of Project

The objective of this project is the design of novel carbon aerogel (CA) materials that meet the DOE system targets (6 wt%, 45 g/L) for on-board vehicle hydrogen storage. The focus is in two areas: 1) engineering of CA-based spillover materials and 2) design of new CA materials as porous scaffolds for metal hydride materials. The specific objectives are 1) to optimize structure for enhanced hydrogen uptake and improved kinetics, 2) storage at reasonable operating temperatures, and 3) the potential to improve kinetic and thermodynamic performance of metal hydrides.



Question 1: Relevance to overall DOE objectives

This project earned a score of **3.0** for its relevance to DOE objectives.

- The study of tailored aerogel materials for hydrogen storage is well aligned with the DOE HFCIT Program objectives and is directly relevant to the ongoing work of the Hydrogen Sorption CoE. There is good project focus on issues of weight, volume, temperature, and cost/scalability.
- Research on scaffolding materials to reduce enthalpy and thermodynamics of the storage materials is critical.
- Very high surface materials. Use as scaffolds has potential for high capacity.
- Use of CA to achieve 6 wt.% and 45 g/L targets. The latter will likely be the more difficult of the two, and so should have been paid more attention (project is almost complete). However, there doesn't appear to be compelling evidence that these scaffolds will actually improve hydrogen storage properties, so the relevance of this project is questionable.

Question 2: Approach to performing the research and development

This project was rated **3.0**_on its approach.

- Interesting use of nanotubes in order to improve the thermal conductivity of the material and facilitate H₂ transport.
- The high surface area, the ability to tailor surface properties, and ease of synthesis make aerogels useful reaction platforms and active media for hydrogen storage. The major elements of the approach in 2009 include engineering of carbon aerogel-metal systems for enhancing spillover and development of porous scaffolds used as nanoscale hosts for simple and complex metal hydrides. The approaches are well formulated, and they address important thermodynamic and kinetic issues that are directly relevant to ongoing work in both the Hydrogen Sorption CoE and the Metal Hydrides CoE.
- Good efforts. Adding Pt may drive cost too high. Scaffolding for metal hydride particles is interesting combination. Some concern about aerogels with low thermal conductivity. May be difficult to heat hydrides for desorption and to remove heat on refueling.
- Cr₂O₃ and ZnO are of potential interest, but surface areas are low.
- Functionalized silica aerogels have potential, but are likely to be expensive.
- Trying to produce tailored CA for sorption. Not clear, even theoretically, how this can allow 6 wt.% and 45 g/L.
- Using aerogels as scaffolds for metal and complex hydrides.

Ouestion 3: Technical accomplishments and progress toward project and DOE goals

This project was rated 2.8 based on accomplishments.

- Progress seems to have slowed somewhat compared to previous years. Would like to see more results on the nanotube scaffolds interesting approach. PI should keep cost of scaffolds in mind with this approach though.
- Solid progress is evident in several areas including synthesis of oxygen-containing aerogels serving as supports and (possibly) catalysts for enhanced spillover, hosts for organometallic complexes that can reversibly bind hydrogen, new sorbent materials (e.g., alpha-Cr₂O₃ aerogels), and improved nanostructured frameworks for metal-hydride reactants.
- The effort in 2009 was focused primarily on materials synthesis and processing.
- Although some preliminary results on hydrogen sorption behavior are available for the encapsulated metal hydride system (collaboration with Metal Hydride CoE) and on the chromia H₂ sorption media, hydrogen capacity data in most of the technical areas are not yet available.
- Although it is recognized that those results are being gathered by other collaborators, the fact that the project is nearly 90% complete underscores the need to obtain the results in a timely way.
- The work on spillover is thorough, and numerous approaches have been explored for improving spillover efficiency. However, rates of hydrogen uptake are prohibitively slow. Likewise, even though there has been some preliminary work on chromia aerogels as sorbent materials, the gravimetric capacity is limited. The most promising direction for this project seems to be the collaboration with the Metal Hydride CoE.
- The investigators used carbon aerogels as scaffold hosts for complex hydride reactants.
- Good work on tailoring pore space. Interesting initial results on LiBH₄ scaffolding. Investigators are moving away from unproductive approach of aerogels alone; this shows good stewardship and project management.
- Some success in fabricating novel scaffold materials. However, the hydrogen sorption data is mostly lacking. There does not appear to be much evidence that these scaffolds will actually improve hydrogen storage properties. Also, the spillover results are unclear in regard to their reproducibility for storage properties.

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated **3.5** for technology transfer and collaboration.

- The PI is working with all the relevant partners.
- Extensive and fruitful collaborations, mainly with several investigators within the Hydrogen Sorption CoE and researchers in the Metal Hydride CoE. These collaborators have accelerated progress and have provided a valuable expansion in the scope of this project.
- Good partners to complement LLNL capabilities.

Question 5: Approach to and relevance of proposed future research

This project was rated 2.8 for proposed future work.

- Please concentrate and continue efforts on nanotube (NT) scaffolds despite the initial setback. The intent is correct to improve heat conductivity and H₂ transport. The motivation is more important than the nanotube material itself. Not enough PIs are concentrating on this critical material property. Please continue this approach with other materials in case NTs do not work out.
- Proposed future work is clearly stated and addresses important technical barriers. However, the future work could be viewed as an entire research project in its own right. Given the fact that the project is 90% complete, a discriminating look at future plans must be made to select the areas that will provide the most impact in the remainder of the project. It is especially important to focus on acquiring hydrogen capacity data at elevated temperatures in the tailored materials already synthesized.
- Still pursuing many approaches. Need to move toward down-selection of most promising systems. Need to begin looking at possible engineering barriers to this approach, such as heat transfer mentioned above.
- A very large amount of future work is proposed, given that the project is essentially over.
- The budget for this project looks strange. Although it is a 5-year project, it appears as though 80% of the funding was obtained in the final two years of the project. Was that planned?

Strengths and weaknesses

Strengths

- PI is working on two important fields for metal hydrides, scaffolding for reducing thermodynamics and also facilitating heat and H₂ transfer within the material. These become big issues as large amounts of materials are packed into a system.
- The PI is an expert at synthesis and properties of nanostructured aerogel systems, and he is an important resource for the overall Hydrogen Storage Sub-Program. Robust collaborations are enhancing the relevance of the project within the Hydrogen Sorption CoE and Metal Hydride CoE.
- Good science. Well executed.

Weaknesses

- Too many approaches. PI should consider narrowing down or down-selecting approaches since the project is near completion.
- Storage at temperatures >77 K remains a serious challenge for these materials.

Specific recommendations and additions or deletions to the work scope

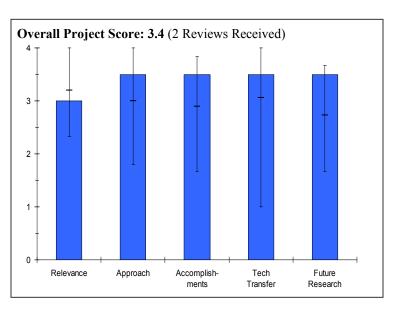
- The work on spillover seems to be open-ended at this point (especially with respect to the issue of slow uptake kinetics). No matter what results are obtained on the preliminary capacity measurements, there will be a large number of questions that cannot be addressed in the short time remaining in the project.
- Recommend that more attention be focused on the use of aerogels as nanoscale hosts for complex hydrides.
- Begin working with Engineering CoE to explore system configuration and possible issues.

Project # STP-26: Single-Walled Carbon Nanohorns for Hydrogen Storage and Catalyst Supports

David B. Geohegan, Alex Puretzky, Mina Yoon, Chris Rouleau, Norbert Thonnaard, Matthew Garrett, Gerd Duscher, and Karren More; Oak Ridge National Laboratory

Brief Summary of Project

The overall objective of this project is to exploit the turnable porosity and excellent metal supportability of single-walled carbon nanohorns to optimize hydrogen uptake and binding energy. The 2008 objectives are to 1) improve surface area to 2,200 m²/g for >3.0 wt% at 77 K, 2) adjust pore size controllably to <1 nm, 3) quantify effects of pore size, 4) theoretically investigate origin of binding energy increase, 5) search for alternative metals to enhance binding energy, and 6) develop new synthesis/decoration approached for these materials.



<u>Ouestion 1: Relevance to overall DOE</u> <u>objectives</u>

This project earned a score of 3.0 for its relevance to DOE objectives.

• Coating carbon nanohorns with Ca is innovative, and it is valuable to see that any carbon can be uniformly coated by any metal without extensive clustering. Less clear whether sufficient capacity can be obtained, although somewhat idealized theory suggests that 8-10 wt% might be possible at 77 K.

Question 2: Approach to performing the research and development

This project was rated **3.5** on its approach.

• Processing is relatively simple, scalable to large quantities, and capable of placing Ca on the surface of carbon materials. Pelletization of materials has been demonstrated, which improves real world material handling.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated 3.5 based on accomplishments.

- Methods developed to produce carbon nanohorns in quantity and to open interiors for sorption.
- Demonstration of deposition of a metal layer on carbon without clustering is an important advance.

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated **3.5** for technology transfer and collaboration.

• Strong collaboration with NIST, NREL, and University of North Carolina is indicated.

<u>Question 5: Approach to and relevance of proposed future research</u>

This project was rated **3.5** for proposed future work.

• Proposed work on charged nanostructures is encouraged.

Strengths and weaknesses

Strengths

• Ability to synthesize Ca layers on carbon materials. Potentially easy to produce in large quantities. Some indications of stronger (i.e., higher temperature) binding, perhaps moving adsorption into the 150 K range.

Weaknesses

• Limited hydrogen capacities so far, even at 77 K; ultimate capacity may be limited. Unclear how to adjust binding energy. (Early results suggest that Ca may improve the binding energy, but opportunity to tune or further improve binding may not be there.)

Specific recommendations and additions or deletions to the work scope

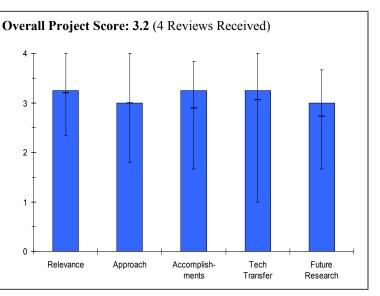
• None.

Project # STP-27: Enhanced Hydrogen Dipole Physisorption: Constant Isosteric Heats and Hydrogen Diffusion in Physisorbents

Channing Ahn, Justin Purewal, and Nick Stadie; California Institute of Technology

Brief Summary of Project

The objectives of this project are the 1) synthesis of framework structures via normal solvo-thermal routes; 2) evaluation of aerogel properties in collaboration with LLNL; 3) evaluation of microporous activated carbon properties; 4) adsorption/desorption evaluation with volumetric Sieverts apparatus capable of measurements of samples at 77, 87, 195, and 298 K temperatures; 5) thermodynamic evaluation of sorption enthalpies via Henry's Law region of isotherm and/or isosteric enthalpy of adsorption; and 6) neutron scattering (diffraction and inelastic) of promising systems in collaboration with the NIST.



Question 1: Relevance to overall DOE objectives

This project earned a score of **3.3** for its relevance to DOE objectives.

- The project is part of the Carbon Center and well aligned with the overall program objectives.
- The project, looking at critical issues of hydrogen sorption processes, is focused on hydrogen program goals and addresses key targets of RD&D objectives.
- The project is initially well focused on engineering or manipulating storage materials that evince binding energies adequate for room temperature storage. Project further explores systems that also yield nearly constant isosteric enthalpies with the view of improving the performance of engineered storage systems. These details are consistent with the Hydrogen Program objectives.
- Project adequately supports the Hydrogen Program goals. It tries to obtain enhanced dipole physisorption of hydrogen while also supporting other partners (e.g., by synthesizing metal-organic framework (MOF)-177 samples for neutron scattering studies).

Question 2: Approach to performing the research and development

This project was rated **3.0** on its approach.

- Good, systematic approach in identifying and evaluating relevant materials properties. It covers framework structures, aerogels, and microporous activated carbons; it also engages both theory and experiment
- The project's approach has become somewhat fragmented in focus. Materials of very different chemistries are being evaluated, from activated carbon to doped aerogels. This approach lacks focus from the central theme. Given the importance of the slit-pore studies for KC₂₄ and CsC₂₄ in intercalated graphites, focusing theoretical and experimental investigation on such systems would be prudent.
- The approach is in general effective and serves the project aims. There is some integration with other efforts (like the neutron scattering studies with NIST and the AX-21 fluorination with Rice University).

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated 3.3 based on accomplishments.

- Significant progress has been accomplished in line with the project objectives. The main achievement is the synthesis of layered enhanced physisorption structures with uniform high Δ H for adsorption and ability to retain 50% of 77 K capacity at 195 K and modest pressures. This also confirms the merit of high Δ H as a materials discovery goal for sorbent research. It was also demonstrated that diffusion kinetics of hydrogen in these systems are influenced by the extent of hydrogen loading with high loadings resulting in slower diffusion.
- Project accomplishments are excellent. In particular, the detailed, quasi-elastic neutron scattering studies on slit pores in intercalated graphite provide valuable insights into the diffusion and barrier properties of these materials. However, the MOF-177 effort seems to duplicate ongoing efforts within the CoE and from outside groups.
- The progress over the last year is fair. The work on alkali (K, Cs) intercalated carbons seems quite interesting. This is also valid for the fluorination efforts on AX-21, although only the first steps have been taken so far. Given that the project end is approaching, more focus on the really interesting parts of the work plan is needed to ensure fulfillment of major objectives.
- Finding materials with constant isosteric heats is desired (although not that important from an engineering viewpoint because these heats are rather small in physisorption). Connecting pore sizes with heat of adsorption could be better served if commercially available carbon molecular sieves with narrow pore sizes were used. It is suggested that the partners try that approach.
- It would have been more effective if high-temperature adsorption or desorption data were provided. Even a temperature programmed desorption (TPD) test would have been helpful.

<u>Ouestion 4: Technology transfer/collaborations with industry, universities and other laboratories</u>

This project was rated **3.3** for technology transfer and collaboration.

- This project is well integrated within the sub-area of the research and appears to be in adequate interaction with the rest of the team. The only suggestion is for the project to make use of the full capabilities of the CoE and other projects to verify the claim on higher adsorption temperature materials.
- Substantial networking and collaborations with a good blend of expertise and access to facilities.
- There exists a sufficient degree of collaboration with other partners. Sample and data exchanges are in place to a certain extent (MOF-177 for NIST, fluorination of AX-21 for Rice University).

Question 5: Approach to and relevance of proposed future research

This project was rated **3.0** for proposed future work.

- Proposed work is sufficiently planned, builds upon present experience and expands current studies.
- Further work on chromia-doped aerogels and MOF or Material Institute Lavoisier (MIL) materials is inconsistent with the theme of the work already initiated on intercalated graphites. Perhaps the focus of the project should remain on the latter since other groups are already addressing the surface area and enthalpic properties of MOF and MIL materials.
- The proposed plans build on past progress, but they could be presented in a more detailed manner. It is important to focus on the more interesting aspects of the work as the project comes to its end.
- It is critical to test the samples and verify the claims.

Strengths and weaknesses

Strengths

- Lengthy experience and competence in the field. Good collaboration record; also, strong interactions within the CoE.
- Project addresses an exceedingly important aspect of materials engineering for physisorption uptake of hydrogen; namely, enhanced binding enthalpy, surface area, and constant enthalpy versus coverage.
- Very good expertise on physisorption.
- Work on intercalated carbons is very interesting. Also, fluorination work may prove useful.

Weaknesses

- No obvious weaknesses, but the field does remain challenging, taking into consideration the set hydrogen storage targets at mild conditions.
- The approach and materials base is fragmented and needs to be focused on the theme that is providing new information, such as the pore-slit intercalated graphites.
- Lack of focus on certain work plan aspects.

Specific recommendations and additions or deletions to the work scope

- A TPD or some other simple test would have been very useful for a quick test of the adsorbents.
- Place extra focus on getting a better understanding of the thermodynamic properties of these materials and on shedding light in the interrelations of pore size/distribution, enthalpies, temperature and pressure effects, and their influence on hydrogen uptake and release.
- Recommend concentrating effort on pore-slit studies based on graphitic structures in collaboration with Rice University.
- Work on AX-21 fluorination should proceed at a faster pace, given that the project end is approaching.

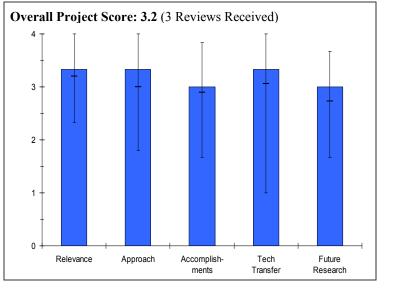
Project # STP-28: Characterization of Hydrogen Adsorption by NMR

Alfred Kleinhammes, B.J. Anderson, Qiang Chen, and Yue Wu; University of North Carolina

Brief Summary of Project

The overall objective of this project is to provide nuclear magnetic resonance (NMR) support to the DOE Hydrogen Sorption CoE team members in developing reversible adsorbent materials with the potential to meet DOE 2010 system-level targets. The 2008 objective is to use NMR porosymetry analysis to obtain detailed information on the micropore structures. This approach is based on the information of local magnetic field inside micro- and meso-pores probed directly by hydrogen.

<u>**Ouestion 1: Relevance to overall DOE**</u> <u>**objectives**</u>



This project earned a score of **3.3** for its relevance to DOE objectives.

- This NMR tool will greatly support the DOE CoE team members in developing reversible H₂ storage materials.
- Relevance to DOE goals is sufficient. Project supports essentially other CoE members on a range of materials, providing useful input to several partners.
- This project is mainly a "support" for the activities of the Hydrogen Sorption CoE. So, the project itself will not focus on storage properties, but will support the other researchers in the CoE to ultimately achieve better storage properties.

Question 2: Approach to performing the research and development

This project was rated **3.3** on its approach.

- The approach of combining commercial NMR and a specialized setup allowing in-situ measurements of hydrogen loading in pressures from 0.001 to 100 atm and temperatures between 77 K and room temperature is one of the best.
- The project is particularly integrated with other efforts within the CoE. A range of materials (e.g., MOFs, carbon nanohorns, poly ether ether ketones [PEEK]) are included. However, as the project approaches its end, more focus on promising (or less understood, like spillover) systems should be exercised.
- The approach is quite straightforward: This project provides NMR support for the Hydrogen Sorption CoE.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated **3.0** based on accomplishments.

- Good progress toward the objectives.
- Good progress has been demonstrated. Enhanced understanding on sorption mechanisms in systems like MOFs and nanohorns has been provided this year. The NMR technique has proven useful, as it may distinguish between different chemical environments for hydrogen and provide interesting information on bonding, diffusion, and other aspects. Issues that need further attention include the validation of the determined (porosymetry??) by NMR pore size distributions and the active investigation of spillover samples.
- Variety of different projects involving MOFs, carbon nanohorns, PEEK, and porous polymers. Some interesting new results regarding interpenetration and H₂ storage in MOFs.

<u>Ouestion 4: Technology transfer/collaborations with industry, universities and other laboratories</u>

This project was rated **3.3** for technology transfer and collaboration.

- The close coordination with partners in other institutions is among the best within the CoE.
- I find the existing collaboration very appropriate. There seems to be extensive exchange of samples and data for a variety of materials and sorption aspects. Several members of the CoE profit from the project results.
- Good connection with many other groups. Due to the nature of a project like this, their ability to collaborate with other groups is essential. Good response to previous year's reviewer comments.

Question 5: Approach to and relevance of proposed future research

This project was rated **3.0** for proposed future work.

- The PI seems to have a good plan in carrying out the future based on past progress and learning.
- The future plans provided are clear and build on past progress. There are two issues that need to be taken in account:
 - 1. The NMR porosymetry should be further validated. It is mentioned that there will be, in the current year, correlation with results from CO_2 isotherms. This is appropriate and should be realized.
 - 2. More efforts should be made to include spillover samples in the investigations. This is mentioned in the "Collaborations," but not specifically addressed in the future plans. NMR may provide useful input to this poorly understood mechanism.
- Mainly a continuation of current activities, which seems appropriate for a project in its final year.

Strengths and weaknesses

Strengths

- The NMR tool developed in this project is a unique approach. It can really help the scientists to better understand the fundamental material properties and their relationship with the H₂ uptake.
- Good support to several CoE members on a range of materials.

Weaknesses

- The work is only limited within the CoE. The knowledge gained in this project can help other CoEs if there is a cross-center collaboration.
- NMR porosymetry needs further validation.
- Focus on promising and/or less understood systems, like spillover, should be applied.

Specific recommendations and additions or deletions to the work scope

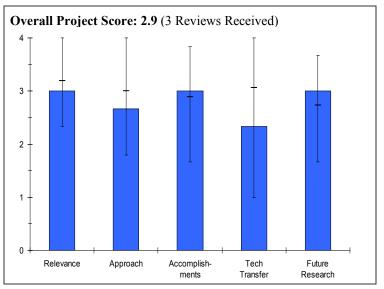
• Spillover studies should be added.

Project # STP-29: Advanced Boron and Metal Loaded High Porosity Carbons

T. C. Mike Chung, Vince Crespi, Peter Eklund, and Hank Foley; Pennsylvania State University

Brief Summary of Project

The primary objective of this project is to achieve the 6 wt% hydrogen storage goal by increasing binding energy (10-30 kJ/mol) and specific surface area (SSA) (>2,000 m^{2}/g). Boron (B) substitution in carbon (C) structures has the following advantages: lightness of B, enhancement of hydrogen interaction, no serious structural distortions, catalyzing carbonization, and stabilizing atomic metal. Activities for FY 2008 include 1) synthesizing the desirable B/Cand metal (M)/B/C materials with B content of >10 mol%, M content of >3 mol%, and SSA of $>2,000 \text{ m}^2/\text{g}$) and 2) studying the structure-property relationship. Activities for FY 2009 include 1) preparing BC_X materials with a combination of high B



content (>15%), acidity, exposure, and surface area (SSA >2,000 m²/g); 2) developing a well-defined B-framework with strong B acidity and high H₂ binding energy (>20 kJ/mol); and 3) studying the storage mechanism for spillover in M/C, M/BC_X materials M (e.g., Pt, Pd).

Question 1: Relevance to overall DOE objectives

This project earned a score of 3.0 for its relevance to DOE objectives.

- BC₃ and B-doped carbons have great potential to meet, or make a major step towards meeting, the DOE targets.
- This work is directly focused on developing an adsorption-based storage material with enhanced binding energy.
- Even with a 10-fold increase in surface area, it is hard to see how these materials will achieve high capacities.

Question 2: Approach to performing the research and development

This project was rated 2.7 on its approach.

- Good approach of using three different methods to make high surface area, B-doped carbon materials.
- This work has also investigated the use of dissociation catalysts and a number of nanosized metal clusters have been successfully deposited on the materials.
- Theoretical work from other groups has shown that BC₃ is expected to have a stronger interaction with dihydrogen. This group has successfully prepared a series of B-doped carbons with differing levels of B doping and surface areas. Higher isosteric heats of adsorption have been measured, but the storage capacities are modest because of low specific surface areas.
- Need to reassess the possibility that the current approach will lead to high capacities.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated **3.0** based on accomplishments.

- Good progress achieved at well-dispersed metal particles on B-doped C surfaces and promising results shown for spillover effect on these materials.
- The project team has achieved very high B content in carbon structures.

- The project team has demonstrated increased hydrogen capacity in B-doped materials over pure carbon for equivalent surface area.
- The project team has measured increased heat of adsorption by B doping in carbon.
- Modeling results indicate promising result that metals are stabilized on B-doped C.
- The project has produced a range of novel BC_x materials. Characterization of their properties is ongoing, but significantly, the isosteric heat of adsorption has been shown to be enhanced. The challenges that remain, are to enhance the isosteric heat of adsorption further (>10 kJ mol-1) which might be achieved through higher B contents and/or the use of a dissociation catalyst. Unfortunately, the investigators have found that high B-content materials have low surface areas, which needs to be addressed (an area highlighted by the investigators).

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated **2.3** for technology transfer and collaboration.

- There appears to be good collaboration within the group combining theoretical work and experimental. There seems to be less collaboration outside of this project. Given the number of groups investigating B-doped carbons, it would appear to be beneficial that all these groups coordinate their efforts to ensure they are not duplicating work elsewhere.
- Collaborations not specifically described in presentation.

Question 5: Approach to and relevance of proposed future research

This project was rated **3.0** for proposed future work.

• The group has identified the main barriers: improving heat of adsorption and increasing surface area, which is the focus for the next 12 months.

Strengths and weaknesses

Strengths

- Excellent progress in forming BC_x and examining the properties of these materials, not only for H surface adsorption, but also in terms of spillover and the effects of topological frustration.
- Appear to be a productive group and have led to greater understanding of the BC_X materials.

Weaknesses

• No major weaknesses, but greater collaboration within CoE will help with the exchange of ideas and reduce the likelihood of duplicating efforts.

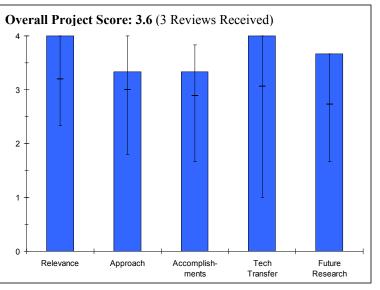
Specific recommendations and additions or deletions to the work scope

• The investigators have clear plans for future work, which is supported.

Project # STP-30: Best Practices for Characterizing Hydrogen Storage Properties of Materials *Karl Gross; H2 Technology Consulting LLC*

Brief Summary of Project

The objective of this project is to prepare a reference document detailing the best practices and limitations in measuring hydrogen storage properties of materials. The document will be reviewed by experts in the field and will be made available to researchers at all levels in the DOE Hydrogen Storage Program. This project is being conducted to 1) reduce errors in measurements, 2) improve reporting and publication of results, 3) improve efficiency in measurements, 4) reduce the expenditure of efforts based on incorrect results, 5) reduce the need for extensive validation, and 5) increase the number of United States experts in this field.



Question 1: Relevance to overall DOE objectives

This project earned a score of 4.0 for its relevance to DOE objectives.

- This project is essential to the objectives of the HFCIT Program, and its final product will be an invaluable resource or reference guide that could be inducted into the standards organizations (i.e., ASTM International, International Organization for Standardization) as the basis for standards development in hydrogen storage measurements.
- The compiling of the "Best Practices Document" is a highly valuable effort. It is most important to have guidelines for researchers when performing reproducible experiments and this document aims at providing a reference on measuring comparable and accurate hydrogen storage properties.
- This project will be a huge benefit to the field. Kudos to DOE and to the PI for taking it on.

Question 2: Approach to performing the research and development

This project was rated **3.3** on its approach.

- This document aims at including all relevant properties, definitions, as well as role model experiments for performing accurate measurements of hydrogen storage properties. It is necessary for the document to engage both beginners and experienced researchers, which is the approach that the PI is taking.
- The project is aimed at developing recommended practices for the characterization of hydrogen storage materials for a broad audience. Presently, the approach comprises individual tasks that address topics on kinetics, capacity, thermodynamics, and cycle-life. A task devoted to instrumentation for each of the measurement techniques (e.g., volumetric, gravimetric, temperature-programmed desorption [TPD]) and other laboratory requirements, such as gas-source purity, should be included as a separate chapter of the final document.
- Considering that materials preparation plays such a key role in hydrogen storage experiments, there may be some logic in including a section focusing on (at least) ball milling and "activation" techniques.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated 3.3 based on accomplishments.

- The project's technical accomplishments are progressing on schedule.
- During FY 2009, a new revision was compiled with requested chapters added, and the document is progressing well towards completion.

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated **4.0** for technology transfer and collaboration.

- The PI is well connected with the hydrogen storage community, both within and outside the United States. New collaborations were initiated as needed to expand the document to cover more materials.
- It is nice to see many different experts involved in the effort.

Question 5: Approach to and relevance of proposed future research

This project was rated 3.7 for proposed future work.

- It is good to see that the interpretation and definition of "capacity" is being addressed individually for physisorption and chemisorption.
- There is no information on borohydrides, a group of materials currently of great interest for high-capacity, lightweight applications. These materials are fairly reversible, and thus challenging, for performing reproducible and accurate measurements. There needs to be a chapter included addressing these issues.

Strengths and weaknesses

Strengths

- The development of a long-needed general guide on hydrogen storage measurements for broad distribution. Contributors to this effort are known experts in the field.
- The "Best Practices" handbook is necessary for making sure that the hydrogen storage community is accurately measuring hydrogen storage properties in the same way in order to be able to compare them with the DOE targets, and thus show progress. It is also providing a reference for experimentalists with different levels of experiences, as well as theorists. Many recognized experts are involved in this project and providing feedback.

Weaknesses

• There were no weaknesses listed.

Specific recommendations and additions or deletions to the work scope

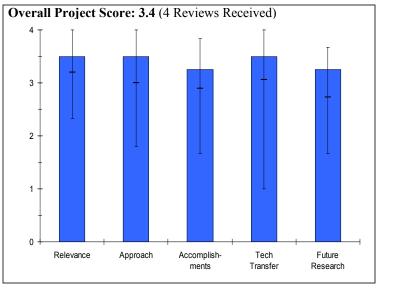
- A task devoted to instrumentation for each of the measurement techniques (e.g., volumetric, gravimetric, TPD) and other laboratory requirements, such as gas-source purity, should be included as a separate chapter of the final document.
- Add a chapter on borohydrides, and also expand the discussion of amide materials.

Project # STP-36: Reversible Hydrogen Storage Materials: Structure, Chemistry, and Electronic Structure *Ian Robertson and Duane Johnson; University of Illinois, Urbana-Champaign*

Brief Summary of Project

The main objectives of the University of Illinois, Urbana-Champaign within the Metal Hydride CoE are to 1) advance the understanding of the microstructural and modeling characteristics of complex hydrides; 2) provide feedback and knowledge to partners within the Metal Hydrides CoE framework; 3) provide more reliable theoretical methods to assess hydrogen storage materials, including key issues affecting materials under study; and 4) help achievement of specific targets and milestones.

<u>Question 1: Relevance to overall DOE</u> <u>objectives</u>



This project earned a score of **3.5** for its relevance to DOE objectives.

- The tools and plans for effectively using these tools are relevant to the DOE objectives in developing catalysts for metal hydride systems.
- This work examines various catalysts for the Metal Hydrides CoE using new characterization tools and computational approaches.
- Transmission electron microscopy (TEM) with holography, density functional theory (DFT), and scanning tunneling microscopy (STM) for in-situ hydriding are used.
- Data presented in the poster directly relate to three projects.
- Important microstructural support activity for the Metal Hydrides CoE.

Question 2: Approach to performing the research and development

This project was rated **3.5** on its approach.

- Three key and relevant technological challenges were worked on this year:
 - MOFs for catalysis
 - \circ Ca(BH₄)₂ computational efforts to elucidate the structure of CaB₁₂H₁₂
 - TiCl₃-catalyzed AlH₃ structure and chemistry
- The investigators have used a combination of experimental and theoretical work to examine and model various materials with the aim of understanding the role of catalyst particles and morphology. The materials studied range from alane, to borohydrides, to MOFs, showing that their approach to the study of the hydrogen storage problem is quite general and likely to have an impact on progress toward satisfying the DOE objectives.
- Approach of combining the experiments and the theoretical finding is very good.
- Provides sophisticated microstructural analysis support to help answer selected key questions associated with advanced metal hydride development activities.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated **3.3** based on accomplishments.

- The project has demonstrated the usefulness of their approach on quantifying the efficacy of ball milling and mixing for the dispersion of catalysts. The use of tomography in the analysis of catalysts is a very good approach. They have advanced the knowledge of the Ca-B-H system as to its reversibility and intermediate phases associated with dehydrogenation. Analysis of surface interactions with hydrogen has begun.
- Good progress.
- A significant amount of high-quality characterization work has been performed to support a number of programmatic issues.
- The research addressed understanding catalysis of metal hydrides and reversibility in borohydrides. In both cases, advances were made which point to fruitful directions for future work. However, there are some concerns about the interpretation of TiCl₃-catalyzed AlH₃ using TEM highlighted below.
 - In the case of understanding catalysts:
 - The research team used TEM to elucidate the location of TiCl₃ in AlH₃ (after addition by chemical means). The samples were provided by BNL. The outcome of that work is the discovery that the Ti was located everywhere in the sample (and not clustered as a titanium aluminide). From TEM (in which the beam transmits through the sample), it is still unclear whether the Ti is within the bulk or at the surface, however, the researchers defined the future direction for this work as an examination of surface layers of Ti over Al (then, hydride the system) in-situ within the STM. This future direction presumes surface distribution of Ti. This reviewer thinks that the future direction will yield fruitful results, but the researchers should also develop strategies for examining subsurface and bulk Ti.
 - Very nice work was presented showing that Ag could be inserted into the Angstrom-sized pores of the metal organic framework. The electron holography 3D images were impressive. The results of that study will provide collaborators an opportunity to use MOFs as regions for nanoconfinement and catalysis. These samples were provided by SNL to the researchers at the University of Illinois.
 - In the case of understanding reversibility:
 - The researchers used DFT to elucidate possible structures for CaB₁₂H₁₂, a nonreversible product phase occurring upon desorption from Ca(BH₄)₂. This is timely and useful work performed with collaborators at SNL.

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated **3.5** for technology transfer and collaboration.

- It is very good that this project includes collaborative research with other Metal Hydrides CoE and other critical DOE programs.
- The researchers are collaborating effectively with SNL (2 separate groups) and with BNL.
- This reviewer gives a "good" rather than "outstanding" rating to this performance category because there was no collaboration with other universities in the consortium. This reviewer urges the researchers to develop collaborations among universities. The tools used at the University of Illinois are advanced, and the project planning is superb. The educational benefits to working with the University of Illinois group are apparent, and this reviewer urges the team to seek out university partners.
- Visible collaboration with several members in the CoE.
- Collaborations both inside and outside the Metal Hydrides CoE.

Question 5: Approach to and relevance of proposed future research

This project was rated **3.3** for proposed future work.

- Each direction presented has a logical future direction associated with it.
- Again, this reviewer suggests examination of sub-surface and bulk Ti (because TEM is a transmission measurement and uniform distribution of Ti observed by this technique is not necessarily an indicator of uniform surface distribution of Ti).
- Good progress has been made, and much future work is planned. All of the areas planned are relevant to the DOE program and important directions to pursue. It seems, however, that some of the focus is on continuing rather than completing various areas of work.
- Project is 80% complete. Reasonable work plan for the remainder of the project.

Strengths and weaknesses

Strengths

- The collaboration between the University of Illinois and two national laboratories will provide tremendous opportunities to students working on this project to interact with researchers at national laboratories.
- The project combines computational and experimental work. Both aspects are very strong. However, these two modes of research were not used synergistically (i.e., TEM plus DFT to address a particular problem).
- The approach used is good and the materials relevant. Many good results are forthcoming.
- Characterization techniques/modeling combination.
- Excellent advanced microstructural characterization expertise and facilities.
- This project represents a number of strengths.

Weaknesses

- There appears to be a lack of collaboration with other universities.
- More of the tasks and future work should be specified so that completed milestones are apparent, rather than
 just continuing working on a material system. Also, one of the areas of future work is listed as "May explore...,"
 and this seems to show that the direction of future work is not entirely clear to the researchers.
- None.

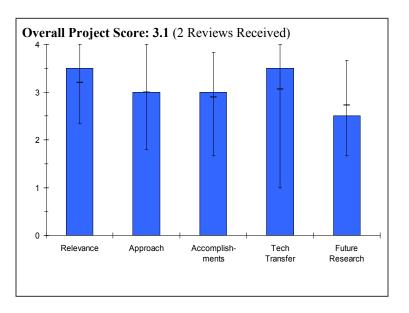
Specific recommendations and additions or deletions to the work scope

- In-situ STM examination of sub-surface and bulk Ti in AlH₃.
- Develop collaborations with other universities to balance out the team.
- Develop a program of student exchange so that University of Illinois students benefit from time at the national laboratory.
- Be more specific about tasks and accomplishments. Publish more of the completed work.
- Prioritization and focusing on compounds with high potential at the CoE is highly recommended

Project # STP-37: Metal Borohydrides, Ammines, and Aluminum Hydrides as Hydrogen Storage Materials *Gilbert M. Brown, Joachim H. Schneibel, Douglas A. Knight, Frederick V. Sloop, Jr., and Claudia Rawn; Oak Ridge National Laboratory*

Brief Summary of Project

The overall objective for this project is to develop the chemistry for a reversible hydrogen storage system based on borohydrides, amides/imides, alane, or the light alanates. Target materials and processes are 1) complex anionic materials (Metal Hydride CoE Project B); 2) amide/imide (M-N-H) systems (Metal Hydride CoE Project C); and 3) regeneration of alane (Metal Hydride CoE Project D). The ORNL goal is to employ solvent-based procedures appropriate for scale-up to production and practical application with a focus on high hydrogen content materials (>10 wt% hydrogen).



<u>Question 1: Relevance to overall DOE</u> objectives

This project earned a score of 3.3 for its relevance to DOE objectives.

- Project is targeting reversible high-hydrogen-capacity materials.
- Very broad area of research and not a realistic target for hydrogen storage.

Question 2: Approach to performing the research and development

This project was rated **3.0** on its approach.

- At this point in time, the project would benefit by focusing on the most promising avenue of its approach.
- The approach used in this project was not well thought out.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated **3.0** based on accomplishments.

- The ammine aluminum borohydride results are very interesting. However, the reversibility of this system may not be possible.
- This work was not well focused.

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated **3.3** for technology transfer and collaboration.

- Good collaboration.
- Collaborations with the Metal Hydride CoE are good.

Question 5: Approach to and relevance of proposed future research

This project was rated **2.0** for proposed future work.

- Concentrate on the most promising avenue.
- The proposed future work was unclear.

Strengths and weaknesses

Strengths

- Good knowledge for hydrogen storage.
- Excellent expertise and capabilities for working with reactive materials.

Weaknesses

- Diversified attempts.
- Project would benefit from more focus.

Specific recommendations and additions or deletions to the work scope

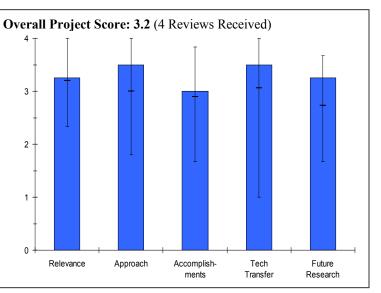
• None.

Project # STP-38: Development and Evaluation of Advanced Hydride Systems for Reversible Hydrogen Storage

Joseph W. Reiter, Jason A. Zan, and Robert C. Bowman; Jet Propulsion Laboratory Son-Jong Hwang; Caltech

Brief Summary of Project

The overall objective of this project is to develop and demonstrate light-metal hydride systems that meet or exceed the 2010/2015 DOE goals for on-board hydrogen storage. The first Jet Propulsion Laboratory (JPL) objective is to validate storage properties and reversibility in light element hydrides including a) nanophase, destabilized hydrides based upon LiH, MgH₂, and LiBH₄; b) complex hydrides (e.g., amides/imides, borohydrides, and AlH₃-based hydrides); and c) samples provided by numerous Metal Hydride CoE partners; and 2) support developing lighter weight and thermally efficient hydride storage vessels.



Question 1: Relevance to overall DOE objectives

This project earned a score of 3.3 for its relevance to DOE objectives.

- The development of advanced hydride systems for reversible on-board application is very critical to the overall Hydrogen Program.
- The project is very well aligned to the overall DOE objectives, addressing a number of key targets working under the umbrella of the Metal Hydride CoE.
- Nuclear magnetic resonance (NMR) provides a valuable tool for investigating reaction pathways and products. In some cases it can identify the presence of compounds in a sample that are not detectable by other characterization techniques such as X-ray diffraction and infrared spectroscopy. Identification of $[B_{12}H_{12}]^{2-}$ and similar species in borohydride decomposition products is particularly noteworthy.
- Project serves a key supporting role to the entire Metal Hydride CoE community by way of analysis and characterization. Such projects are key enablers toward gaining fundamental understanding of complex hydrogen storage reactions and thus are vital for CoE progress and meeting DOE R&D objectives.

Question 2: Approach to performing the research and development

This project was rated **3.5** on its approach.

- The multidisciplinary analysis and characterization combined with theoretical prediction is a good approach.
- Well founded, systematic approach, exploring possibilities within the Metal Hydride CoE and particularly getting the most out of the JPL team's high level expertise in the NMR field.
- Applies characterization tools, especially expertise in NMR, to establish reaction pathways and products. Understanding the reaction mechanisms is critical to finding ways to improve metal hydride storage materials.
- The diverse set of analysis and characterization capabilities is virtually unmatched in the Metal Hydride CoE. It is evident that these resources are being made available across the CoE for determination of reaction pathways (particularly for identification of reaction intermediates).
- State-of-the-art magic angle spinning (MAS)-NMR analyses are particularly invaluable for identification of non-crystalline product/intermediate phases which are very common in complex and chemical hydride systems.

<u>Ouestion 3: Technical accomplishments and progress toward project and DOE goals</u></u>

This project was rated **3.0** based on accomplishments.

- A satisfactory list of accomplishments. NMR once more proves to be a powerful tool for phase, type of bonding, and reaction pathways identification.
- Studies of the reaction mechanism in Ca(BH₄)₂ are valuable. M(B₁₂H₁₂)_n characterization and reactivity studies are useful to understanding formation of these intermediates during borohydride decomposition.
- The MAS-NMR work has proven to be very diagnostic in the experimental identification of the B₁₂H₁₂ intermediates. Given the recent computational work on reaction enthalpies for these species, it would be useful to experimentally corroborate these delta-H values.
- With regard to the prescience of water in the Li₂B₁₂H₁₂ experiments, it unclear what the origin of the water is and if it is possible to be mitigated. This water, that is observed for all MB₁₂H₁₂ systems, is likely prohibitive to facilitating low-temperature hydrogen release.
- Overall, the collaborative synthesis and in-depth characterization of various MB₁₂H₁₂ compositions is significant, high-profile work that is important for future development of complex anionic materials.
- The team made some progress in the past year. However, the progress is not proportional to the funding level compared to other team within the CoE.

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated **3.5** for technology transfer and collaboration.

- Strong collaboration within the Metal Hydride CoE, with other CoE's, and with outside collaborators. This is the "go-to" group for NMR within the CoE and one of the leading NMR groups in the field.
- This project relies on productive collaborations with CoE partners. It is clear that extensive coordination within the Metal Hydride CoE is in place, and PIs have been effectively leveraging JPL's/California Institute of Technology's capabilities.
- The team is fairly well coordinated with other partners within the CoE.
- Substantial, appropriate, and well-coordinated networking and collaborations with other institutions.
- Given that reactions based on chemical hydrides also commonly involve amorphous products, it would be a natural extension to examine these systems (e.g., ammonia borane [AB]) via collaboration.

<u>Ouestion 5: Approach to and relevance of proposed future research</u>

This project was rated **3.3** for proposed future work.

- The future work is well planned. The team should shift more weight to the investigation of destabilization routes.
- Sound and targeted future planning which builds on recent progress and moving a step forward. Of particular interest is the work on the destabilization routes in the MB₁₂H₁₂ system and the use of NMR for investigating the N-enriched amide/imide systems.
- Builds on studies of intermediates to try to identify ways to mitigate or prevent formation of these intermediates, which interfere with reversibility. Studies of complex anionic materials and amide/imide systems will help elucidate reaction pathways in these systems as well.
- The proposed activity involving the collaborative examination of destabilized hydride systems embedded in scaffolds should be productive. Hopefully, an objective will be to gain an understanding of the interaction between the scaffold and metal hydride and impacts on kinetics (or thermodynamics).
- Continuation of work on the MB₁₂H₁₂ phases and M-B-N-H systems is also worthwhile.

Strengths and weaknesses

Strengths

- The tool developed in this project allows CoE partners to verify the reaction pathways predicted by the theory.
- Exploring NMR: a powerful tool and the PI and his co-workers have high caliber expertise in the field.

- NMR is a unique characterization tool which adds considerably to the study of reaction paths in hydrides, especially in cases where other characterization tools such as X-ray diffraction and infrared spectroscopy may be unrevealing.
- Highly valuable expertise in analysis and characterization that is being utilized.

Weaknesses

- No apparent weaknesses.
- Difficult to obtain $M(B_{12}H_{12})_n$ samples in pure form without hydration, in order to characterize pristine material.
- Lack of communication with other CoEs, especially with the ones that have similar knowledge in NMR tool.

Specific recommendations and additions or deletions to the work scope

• Be ready to re-schedule resources and access to facilities in view of down-selections to account for possible new promising materials that may come up.

Project # STP-39: Effect of Trace Elements on Long-Term Cycling/Aging Properties and Thermodynamic Studies of Complex Hydrides for Hydrogen Storage

Dhanesh Chandra, Josh Lamb, Wen-Ming Chien, and Ivan Gantan; University of Nevada, Reno

Brief Summary of Project

The primary objective of the project is to determine the effects of gaseous trace impurities (e.g., O_2 , CO, H_2O , CH₄) in hydrogen on long-term behavior of the complex hydrides/precursors by pressure cycling and/or thermal aging with impure hydrogen. Secondary related objectives are 1) vaporization behavior of hydrides and 2) crystal structure studies.

<u>Question 1: Relevance to overall DOE</u> <u>objectives</u>

This project earned a score of **4.0** for its relevance to DOE objectives.

- The project aligns with the Hydrogen Program and DOE RD&D objectives.
- Project nicely supports DOE objectives in practical engineering areas not covered very well by other projects.

Question 2: Approach to performing the research and development

This project was rated **3.5** on its approach.

- Solid theoretical background and effective experimental approach.
- Project focuses on capacity (weight), cyclic durability (impurities) and kinetics (reaction pathways).
- The work is highly focused toward practical properties.
- The effort has focused mainly on the Li-N-H (Li nitride-imide-amide) system. This system is a logical choice for the time being, but does not necessarily have long-range, practical potential.

Question 3: Technical accomplishments and progress toward project and DOE goals

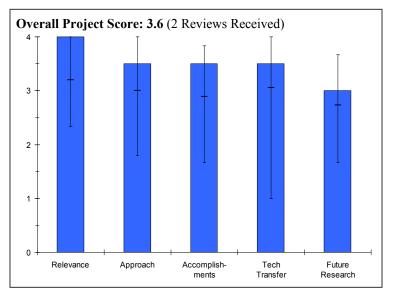
This project was rated 3.5 based on accomplishments.

- The results are simultaneously excellent from both scientific and engineering points of view.
- Large amounts of practical data have been generated.
- PI has derived an excellent picture of the nitride-imide-amide reaction pathways via detailed Li-N-H ternary phase diagram determinations. An important new intermediate phase has been found.
- A more direct, quantitative tying of the results to the DOE goals might have been possible.
- A lot of interesting data. At the same time, some the key assumptions (e.g., Li₄N-H) need additional confirmation.

<u>Ouestion 4: Technology transfer/collaborations with industry, universities and other laboratories</u>

This project was rated **3.5** for technology transfer and collaboration.

- Good industrial collaboration, but there is no direct industrial involvement in the project.
- There are many excellent national and international collaborations in place.
- This PI is an important contributor to the Metal Hydride CoE.



Question 5: Approach to and relevance of proposed future research

This project was rated **3.0** for proposed future work.

- Plans are reasonable, address major issues, and include necessary measures to overcome existing barriers.
- Future plans are good, but it is important to put more emphasis on new materials (i.e., beyond the Li-N-H system).

Strengths and weaknesses

Strengths

- Very good phase analysis results.
- Impressive international collaboration.
- A good, practical approach to hydrides from a material science point of view.

Weaknesses

• There should be more industrial involvement and collaboration.

Specific recommendations and additions or deletions to the work scope

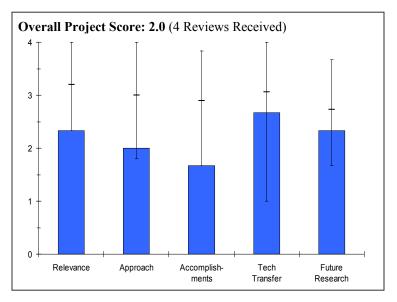
- Extend the project into related areas including materials chemistry (i.e., solid-state chemical transformations in ammonia-lithium-lithium hydride nitrogen system[s]).
- Conduct more gaseous impurity cyclic studies on new candidate hydrides.

Project # STP-40: Amide and Combined Amide/Borohydride Investigations

J. Gray, L. Dinh, M. Bharaty, H. zur Loye and D. Anton; Savannah River National Laboratory

Brief Summary of Project

The objectives of this project are to 1) Collaborate with University of Utah group to perform complementary experiments to analyze the LiMgN system, 2) verify reversibility conditions of TiCl₃-doped LiMgN, 3) explore the effect of catalyst loading on both charge and discharge reaction pathways and kinetics, and 4) outline discharge and charge kinetics under various temperature and pressure conditions to prepare for hydrogen storage system design. The project will perform isothermal kinetic studies under well-defined. controlled reaction conditions to obtain the experimental data required to determine isothermal kinetics and characterize the proposed reaction for hydrogenation and dehydrogenation of LiMgN.



Question 1: Relevance to overall DOE objectives

This project earned a score of 2.3 for its relevance to DOE objectives.

• The research directions followed in this project are generally aligned with the program's objectives, support the DOE R&D plans, and target a number of barriers.

<u>Ouestion 2: Approach to performing the research and development</u>

This project was rated **2.0** on its approach.

- Sensible, straightforward, targeted approach. The Li-Mg-N system study appears to be very well organized and followed up with engineering targets always in mind.
- Ball milling will not result in a high volume manufacturing process suitable for the automotive industry. Ball milling techniques with low yields and long milling times are only suitable for lab purposes. The PI should abandon this approach unless a clear alternative and commercially scalable synthesis process is identified.

Ouestion 3: Technical accomplishments and progress toward project and DOE goals

This project was rated 1.7 based on accomplishments.

- Sound progress and satisfactory degree of achievement with respect to objectives and original planning.
- For what has been achieved over previous years, the charge and discharge temperatures are still far too high. The reversible storage capacity has not been improved significantly.

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated 2.7 for technology transfer and collaboration.

- PI is working with the appropriate partners.
- Not clear whether technology transfer and collaborations are more extended than with the few partners mentioned in the poster/presentation.

Question 5: Approach to and relevance of proposed future research

This project was rated 2.3 for proposed future work.

- The future plans are appropriate and justified by the results produced so far.
- All the proposed work has been conducted countless times (milling time vs. kinetics); the results are predictable. These materials have been heavily studied already. PI should investigate alternate, cost-effective and scalable synthesis techniques for these materials. Without this there is little commercial or research interest at this stage.

Strengths and weaknesses

Strengths

• Investigating the potential of a practical storage material.

Weaknesses

- It was not clear how the data obtained will affect the engineering tank design.
- It was not clear how the minimization of NH₃ by-products is tackled.

Specific recommendations and additions or deletions to the work scope

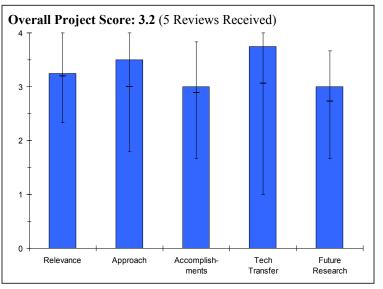
• The project team should stay well tuned to the progress within the Metal Hydride CoE, but also well linked to the Engineering CoE (e.g., for the issue of NH₃, breakthrough in trapping technologies or determination of maximum allowable levels).

Project # STP-41: Synthesis of Nanophase Materials for Thermodynamically Tuned Reversible Hydrogen Storage

Channing Ahn, Sonjong Hwang, and David Abrecht; California Institute of Technology

Brief Summary of Project

The objectives of this project are to 1) understand if thermodynamically tractable reactions based on hydride destabilization, that should be reversible but appear not to be, are kinetically limited; 2) enable short hydrogenation times associated with refueling, which will require short solidstate and gas-solid diffusion path lengths; 3) address the problems associated with large, light-metal-hydride enthalpies (hydrogen fueling/refueling temperatures) and develop strategies to address thermodynamic issues surrounding the use of these materials through hydride destabilization; 4) understand issues related to grain growth and surface/interface energies, which are vital in order to understand the kinetics of



hydrogenation/dehydrogenation reactions; and 5) follow up on previously studied reactions with phase identification via X-ray diffraction, nuclear magnetic resonance (NMR), and transmission electron microscopy (TEM).

Question 1: Relevance to overall DOE objectives

This project earned a score of **3.3** for its relevance to DOE objectives.

- Systems with high overall hydrogen content have been considered.
- DOE goals in the areas of weight, refill kinetics, and reaction pathway understandings are adequately addressed.
- Relevance to HFCIT Program goals is adequate. The project investigates a number of nanophase materials while also offering support to other CoE partners (e.g., microstructural analysis of MgH₂ incorporated in aerogels).
- Destabilized systems offer one of the best routes to meeting the needs for high capacity and low cycling temperatures.
- Identification of phases and compounds formation based on the theoretical estimation results of promising systems is relevant to DOEs objectives.
- Some of the systems are too expensive to be commercialized (e.g., ScH₂).

Question 2: Approach to performing the research and development

This project was rated **3.5** on its approach.

- The work is well aligned with attempting to meet the DOE targets. A significant amount of support is also provided in characterizing materials from other labs, providing essential understanding of materials across a range of projects.
- Utilization of several characterization techniques is a very good approach. Also, looking at potential systems judging from density functional theory (DFT) calculations is reasonable.
- The California Institute of Technology group seems to have a range of skills (especially NMR) that is clearly helpful to the overall CoE.
- The overall approach contributes fairly well to the evaluation and enhanced understanding of the systems investigated. A better integration with other efforts in the CoE could have been attained though.
- The approach seems to be largely of a service and support nature to various partners and projects within the Metal Hydride CoE. This is fine, but makes it a bit difficult to judge the overall impact of this group.

Ouestion 3: Technical accomplishments and progress toward project and DOE goals

This project was rated 3.0 based on accomplishments.

- Quite a lot of interesting results have been obtained during the last year. Some are positive and some are negative, but all are important to developing necessary understandings.
- A number of accomplishments that offer useful data and input have been presented (e.g., on MgB₁₂H₁₂, Li-Sc-B-H, and Li-Ca-B-H systems). The TiH₂ + LiBH₄ system that was investigated (due to its interesting ΔH value) gave the results that might have been expected from the beginning.
- The data provided to other partners regarding the MgH₂ incorporation in aerogels are also useful.
- The systems investigated meet the DOE goals for capacity and in theory have cycling temperatures closer to the target range. Kinetics at these low temperatures is still an issue, but nanostructuring may help with this.
- The results are presented in a rather scientifically objective manner. There should have been clearer connections to practical implications for overcoming the DOE barriers.
- The alane: lithium borohydride system was not reported this year, is it no longer being pursued?
- Much remains unknown about the actual mechanisms of reactions under consideration.

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated **3.8** for technology transfer and collaboration.

- Visible collaboration with several CoE members.
- This effort has good collaborations within the CoE. It is a good example of a collaborative "service" partner within a CoE.
- Collaborating extensively across a range of projects, this is to be commended.
- A sufficient degree of collaboration with other CoE partners exists, although further improvements could be made in that respect.

Question 5: Approach to and relevance of proposed future research

This project was rated **3.0** for proposed future work.

- The proposed plans are a logical development upon this year's work.
- Future work continues to service CoE, as it should.
- Future plans should be given in a more detailed manner and focus on specific interesting aspects as the project end approaches. As they appear now, they seem diverse without appropriate prioritization (taking in account the limited time and funds available).

Strengths and weaknesses

Strengths

- Excellent characterization expertise and techniques capabilities (i.e., magic angle spinning (MAS)-NMR, Raman, TEM).
- High-hydrogen-content systems are being scrutinized.
- Good combination of techniques, including NMR.
- Group has excellent skills for complimenting the other CoE partners' capabilities.
- Good expertise of partner, wide range of available techniques.
- Characterization and insight into a range of storage materials. Extensive collaborations.

Weaknesses

- The implicit assumption that the only gaseous product of reactions is hydrogen needs to be verified for every transformation.
- The project is not really assessing the practical implications of the results very well. What do the scientific findings really mean relative to overcoming DOE barriers?
- Lack of focus on specific promising aspects.
- None.

Specific recommendations and additions or deletions to the work scope

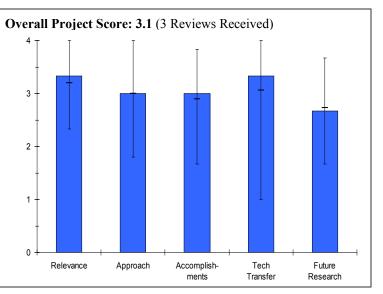
• Emphasis could be placed in the limited remaining time on scaffolding aspects.

Project # STP-42: Lightweight Borohydrides for Hydrogen Storage

J.-C. Zhao; Ohio State University

Brief Summary of Project

The overall objective for this project is to discover and develop a high-capacity, (>6 wt%) lightweight hydride capable of meeting or exceeding the 2010 DOE/FreedomCAR targets. Objectives for FY 2008 were to 1) study the desorption mechanism and explore ways to make the $Mg(BH_4)_2$ reversible, 2) explore new hydride materials, and 3) study an aluminoborane compound AlB₄H₁₁ for suitability for hydrogen storage. Objectives for FY 2009 are to 1) study $Mg(BH_4)_2$, $Mg(B_3H_8)_2$, and $MgB_{12}H_{12}$ and their amine complexes for hydrogen storage and 2) synthesize and characterize new boro-amine hydride materials.



Question 1: Relevance to overall DOE objectives

This project earned a score of 3.3 for its relevance to DOE objectives.

- This project is part of the Metal Hydride CoE and is aligned with the overall objective of the CoE and Hydrogen Program.
- The project aims at discovering and developing high-capacity, lightweight hydrides capable of meeting the DOE hydrogen storage targets for on-board vehicular applications. It is well aligned with the overall RD&D objectives.

Question 2: Approach to performing the research and development

This project was rated **3.0** on its approach.

- Well organized and focused using a systematic, clear approach for exploring two classes of materials: Mg(BH₄)₂ and aluminoborane compounds and their amine complexes. It also plans to use the mechanistic understanding it steadily gains on the complex desorption processes for developing a reversibility strategy for all borohydrides.
- The approach is well within the norm, albeit somewhat ineffective. Sometimes there are no good solutions to a thermodynamic problem. De-destabilization approach appears to have ad hoc success, at best, for complex hydrides. Having said that, this is a natural part of the scientific exploration and should not be considered as a criticism.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated 3.0 based on accomplishments.

- The project has produced many results. The PIs have been very candid about the outcomes and have correctly decided to explore other alternatives.
- Significant progress has been accomplished in line with the project objectives. Highlights include the next steps for the understanding of the "nature" of the intermediate phase, the MgB₁₂H₁₂, which is very important for reversibility and forms during the decomposition of Mg(BH₄)₂. Despite literature claims, is not anhydrous.

Equally significant was the amine complexes work and the synthesis of $Li_2B_{12}H_{12}$, which will be encapsulated into aerogels.

- Nice work on aluminoborane compounds and attempts to isolate B₁₂H1₂ compounds.
- Little progress on ammoniated borohydrides this year.

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated **3.3** for technology transfer and collaboration.

- The project is part of the Metal Hydride center and appears to have adequate communication within the team.
- Exploring strong links established within the CoE and other institutions. Of particular added value is the establishment of the Metal Hydride CoE subgroup on borohydride-amine complexes led by the PI.

Question 5: Approach to and relevance of proposed future research

This project was rated 2.7 for proposed future work.

- Sound future plans that include further synthesis work, but also mechanistic studies and catalyst screening for improving the reversibility and exploring the potential of these material classes.
- It would have been more effective to define the other possible candidates to be examined.

Strengths and weaknesses

Strengths

- The project team has strong capabilities.
- The project team has valuable experience and competence in the field and strong collaborations.
- The project is rather exploratory: it looks for breakthroughs in reversibility of borohydrides (a strength, but also a weakness).

Weaknesses

- Difficult area of research.
- The project is rather exploratory: it looks for breakthroughs in reversibility of borohydrides (a strength but also a weakness).

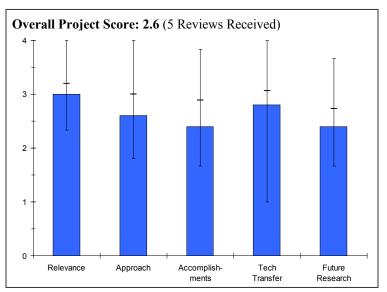
Specific recommendations and additions or deletions to the work scope

- The PIs also need to review the work that has been completed by system analysis project (ANL) to help them narrow down the practical limits of a potential successful reversible metal hydride. Optimistically, there is enough data to suggest that a good candidate would have an enthalpy less than 30 kJ/mol-H2 and equilibrium temperatures below 120°C-150°C with absorption/desorption pressure of at least 5 atm. Before embarking on a new direction or materials, it is necessary (but not sufficient) to conduct an internal assessment of the potential success of a material.
- Recommendations are to intensify collaborative efforts, coordinate the research, and ensure transfer of knowledge within the Metal Hydrides CoE subgroup of borohydride-amine complexes.

Project # STP-43: Center for Hydrogen Storage Research at Delaware State University *Andrew Goudy; Delaware State University*

Brief Summary of Project

The overall objective for this project is to establish a Center for Hydrogen Storage Research at Delaware State University for the preparation and characterization of selected complex metal hydrides and the determination their suitability for hydrogen storage. The 2008 objectives were to 1) extend the studies to include other complex hydrides that have greater hydrogen storage potential than the destabilized hydrides, such as ternary borohydride systems and 2) perform kinetic modeling studies and develop methods for improving kinetics and lowering reaction temperatures. The 2009 objective was to make a go/no-go decision. The team decided not to continue studies on ternary borohydride systems that contain



amides. The team will continue to focus on other borohydride systems with reaction enthalpies predicted to be less than 50 kJ/mol \cdot H₂.

Question 1: Relevance to overall DOE objectives

This project earned a score of **3.0** for its relevance to DOE objectives.

- The project aligns with the Hydrogen Program and DOE RD&D objectives.
- Designing or identifying new high-capacity materials for on-board hydrogen storage are a key element toward meeting DOE objectives for hydrogen storage. The mixed borohydride and destabilized materials presented in the 2009 AMR are members of a class of compounds that need to be explored because they could potentially offer sufficient capacity and reasonable thermodynamics. The kinetics measurements being performed as part of this work, using H₂ overpressure with a constant pressure driving force, have particular relevance to on-board storage. They map more directly to real storage systems than most kinetics measurements that either do not use constant pressure (e.g., PCT-type measurements) or are performed into an H₂-free atmosphere.
- The project is investigating high-capacity, complex hydrides and the use of either mixed metal cations or multicomponent systems to achieve a destabilization of Group I and II borohydrides.
- The project is somewhat relevant to the DOE Metal Hydride CoE objectives, but it is not well integrated into that effort. The University of Delaware effort is not part of the Metal Hydride CoE.

Question 2: Approach to performing the research and development

This project was rated **2.6** on its approach.

- Work was reported on various compounds. The kinetics and cyclability of these systems are being investigated which compliments similar work to that coming out of Hawaii. The project appears to be well focused.
- Synthesis and measurement approaches are conventional, producing interesting mixed borohydride materials. Expanding expertise in mass spectrometry to examine composition of evolved gases is encouraged. Approach to kinetics measurements is on the mark.
- The limited number of characterization techniques is insufficient to elaborate on what is happening in the studied systems.
- The approach is effective but could be improved.
- Even though the presentation indicates that some collaboration is taking place, the work does not appear to be well guided or supported by theory. It appears to be Edisonian in nature, based on trial and error.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated 2.4 based on accomplishments.

- The group presented results on several interesting materials including the Li-Mn-B-H system.
- Interesting thermogravimetric analysis (TGA) results have been obtained on AMn(BH₄)₃ (A=Li, Na) systems, but more characterization is needed to determine the active phase(s) in the ball milled specimens. NMR might be a good adjunct to help determine phase composition for samples where X-ray diffraction (XRD) is not fully revealing.
- Some interesting effects have been noticed during the dehydrogenation of the mixed metal borohydrides. However, there is currently no theory to explain the effects. This needs to be investigated further and developing collaborations with other CoE members might help.
- A few reactions were studied and data was collected, but there appears to be no real understanding. The assumption that back pressure in the pressure-composition isotherm (PCI) may affect decompositions is unsupported.
- Not a lot was accomplished during the past year. Progress has been slow, perhaps additional effort is needed. Chemical analysis and composition of the dehydrogenation products is not presented. There is speculation that diborane may be an issue, but this was not confirmed. No evidence is presented that indicates reversibility for these materials. On a positive note, the number of publications and presentations has increased from 2008.

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated **2.8** for technology transfer and collaboration.

- Some collaboration with University of Pittsburgh, Georgia Institute of Technology, University of Delaware, and Air Liquide is indicated.
- Collaboration can be improved by adding an industrial partner.
- Collaborations with University of Pittsburgh and Georgia Institute of Technology are indicated, but there is little evidence of this in the presentation.
- The PI has made some collaborations, but for the future direction of the project, collaborations with some other key CoE members are recommended (e.g., Professor Jensen at University of Hawaii). This will also help develop added value to the work and avoid duplication of effort.

Question 5: Approach to and relevance of proposed future research

This project was rated 2.4 for proposed future work.

- Plans are reasonable, and goals look achievable.
- Focus is on developing further systems with lower than 50 kJ mol-1 dehydrogenation enthalpies, nanostructuring these types of materials, and investigating the kinetics and cyclability. All aspects are important to the design of a practical storage material.
- The proposed future work matches well with overcoming barriers, but is vague as to the candidate systems to be examined and the methods to be used. Also, given the size of the effort, it appears somewhat diffuse, covering a broad range including synthesis and characterization of unique new materials, thermodynamic measurements, kinetic measurements, cycling measurements, and nanotechnology additions to improve kinetics. Is it possible for the PI to successfully address all of these areas? The kinetics method proposed is very appropriate to materials for on-board storage.
- The planned future work is certainly necessary, but there is some doubt as to whether it can be accomplished in the remaining time given the slow progress to date. The work plan for the Mg-LiBH system is not evident. Since this system is still being investigated in the Metal Hydride CoE, additional kinetic and thermodynamic data would be welcome.
- It was difficult to evaluate the future plans because they were generic and it was unclear where this project is going.

Strengths and weaknesses

Strengths

- Realistic approach.
- An interesting set of research objects.
- Synthesis of mixed borohydrides; approach to kinetics measurements.
- Bringing more kinetic understanding of these types of systems.

Weaknesses

- The group may benefit from a better coordination with others working in the same field (the Li-Mn-B-H system has been studied by another group who also presented a poster at this meeting).
- Full characterization of samples needs greater emphasis to determine the active compounds in ball milled samples.
- Work plan is not well defined and progress has been slower than anticipated.
- Important to avoid duplication of work in other labs.

Specific recommendations and additions or deletions to the work scope

- Work going forward could be more focused on the synthesis/characterization work on mixed borohydrides and the kinetics studies using constant pressure driving force that have led to interesting results to date. Nuclear magnetic resonance, if available locally or collaboratively, could offer a good adjunct to XRD and infrared (IR) toward characterization of the compounds present in the prepared and decomposed mixed borohydride materials.
- The future work is sensible and supported, but the PI needs to think about developing some strategic collaborations. One important addition would be to investigate the phase changes during dehydrogenation and hydrogenation.
- The project needs to narrow its focus in order to bring the work to a conclusion with meaningful results (i.e., pick a material and determine adsorption and desorption kinetics and thermodynamics).

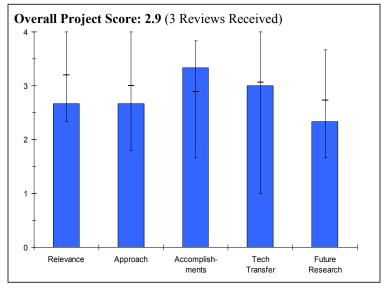
Project # STP-44: Solid-State Hydriding and Dehydriding of LiBH₄ + MgH₂ **Enabled via Mechanical Activation and Nano-Engineering**

Leon Shaw: University of Connecticut

Brief Summary of Project

This project is exploring fundamental mechanisms related to mechanical activation and nano-engineering necessary for improving kinetics of reversible hydrogen storage materials. This will be done by investigating the hydriding/dehydriding properties of LiBH₄+MgH₂ materials with different degrees of mechanical activation and nanoengineering; enhance the storage performance based on the understanding developed. The overall objectives of this project in FY 2009 are to (1) Further improve the solid-state hydriding/dehydriding properties of LiBH₄ + MgH₂ via ball milling at liquid nitrogen

temperature with the addition of transition



metals and milling additives such as boron nitride, (2) Investigate the hydriding and dehydriding reversibility of carbon aerogel confined LiBH₄ and increase its storage capacity, and (3) Demonstrate hydrogen uptake and release of LiBH₄ + MgH₂ systems with a storage capacity of ~ 10 wt% H₂ at 2000°C.

Question 1: Relevance to overall DOE objectives

This project earned a score of 2.7 for its relevance to DOE objectives.

- The project is relevant to the DOE Hydrogen Program goals. Work with the Mg-LiBH system is warranted because this material is still under consideration within the Metal Hydride CoE. Phenomenological studies on this material have some value. However, the project duplicates the effort within the Metal Hydrides CoE.
- Nothing unique was presented compared to 2008. Ball milling and nanoengineering have been attempted without sufficient reasoning.

Question 2: Approach to performing the research and development

This project was rated 2.7 on its approach.

- Gas analysis during decomposition could be helpful.
- Hydrogen uptake and release did not meet the milestone.
- The approach of incorporating nanoparticles into a support scaffold to prevent particle growth during cycling is similar to the effort in the Metal Hydrides CoE. However, there is no clear cut evidence that nanosizing particles improves the thermodynamics. Preparing material through extensive ball milling at liquid N₂ temperature does not appear to be a viable route to meet automotive quantities, even if this material can be successfully developed. Use of a catalyst may be necessary to increase reaction rates. A final dehydriding temperature of over 200°C is required to release all the hydrogen; this does not meet DOE targets. Doping with transition metals to improve kinetics seems to be more ad hoc than guided by theory.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated 3.3 based on accomplishments.

- The PI has made a good attempt.
- A substantial amount of work was reported. A partial ion exchange model was developed to elucidate the hydriding/dehydriding mechanisms. Nuclear magnetic resonance (NMR) studies at PNNL have helped to elucidate the reaction mechanisms. Some success at incorporating the hydrides in the carbon aerogel was achieved, however there is no indication that the material is stable under cycling conditions.

<u>Ouestion 4: Technology transfer/collaborations with industry, universities and other laboratories</u>

This project was rated **3.0** for technology transfer and collaboration.

- The collaborations were good.
- Good collaboration with PNNL and HRL Laboratories, LLC is evident. However, there does not appear to be good collaboration with the Metal Hydrides CoE. The PI did not offer a comparison with results reported by the Metal Hydrides CoE on similar materials.

Question 5: Approach to and relevance of proposed future research

This project was rated 2.3 for proposed future work.

- No-go decision was made.
- The proposed future work plan is very ambitious if the project will end in December 2009 as stated in the presentation.

Strengths and weaknesses

Strengths

- Good group.
- Solid-state reaction was investigated very precisely.
- Good record of publications.

Weaknesses

- The project does not appear to be very well thought out.
- Strategy for selecting additives is not explained and is unclear.
- There is no clear path to reducing the end point dehydriding temperature.

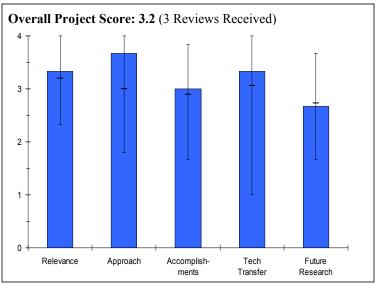
Specific recommendations and additions or deletions to the work scope

• If the work is carried on, the PI should interact with HRL to decrease the risk of duplication of effort in the nanoconfinement activity.

Project # STP-45: Standardized Testing Program for Solid-State Hydrogen Storage Technologies *Michael Miller and Richard Page; Southwest Research Institute*®

Brief Summary of Project

The overall objectives of this project are to 1) support DOE's Hydrogen Storage Program by operating an independent national-level laboratory aimed at assessing and validating the performance of novel and emerging solid-state hydrogen storage materials and full-scale systems; 2) conduct measurements using established protocols to derive performance metrics: capacity, kinetics, thermodynamics, and cycle life; 3) support parallel efforts underway within the international community, in Europe and Japan, to assess and validate the performance of related solid-state materials for hydrogen storage. Current objectives are to 1) provide an in-depth assessment and validation of hydrogen spillover in



Pt/activated carbon (AC)-bridged metal-intercalated metal-organic framework (IRMOF)-8 and AX-21 compounds; 2) assess hydrogen adsorption and spillover phenomena in catalytically doped carbon foams; 3) evaluate the thermodynamic plausibility of hydrogen spillover in catalytically doped metal-organic frameworks; and 4) continue round-robin testing in collaboration with the European Union's hydrogen storage program (NESSHY).

Question 1: Relevance to overall DOE objectives

This project earned a score of **3.3** for its relevance to DOE objectives.

- This project is focused on establishing a standardized and robust testing procedure for hydrogen storage research. This is an extremely valuable element of the DOE program because reliable, reproducible results are essential for progress to be made in achieving DOE's goals and objectives.
- This effort indirectly supports DOE targets and plans, especially in the properties of weight, volume, thermodynamics, and cycle life.

Question 2: Approach to performing the research and development

This project was rated **3.7** on its approach.

- The basic philosophy of this project is to provide a national source of testing, verification, and other contributions. This is clearly important.
- The PIs have used care in choosing materials for their experiments and in preparing samples for testing. The current experimental assessment of hydrogen uptake seems to be limited to gravimetric methods. This is a very good start, but more should be done toward understanding spurious and irreproducible results. These have not only have appeared in the literature, but these researchers themselves have experienced it for the so-called "spillover effect" materials. Adding a separate, independent measurement, such as a Seiverts method, would be an excellent way to try to get internal consistency in their hydrogen uptake results. Very nice work on kinetics and cycle life of the Mg-Li-B-N-H materials.
- The work appears to be a mixture of DOE-directed efforts, international (DOE-supported) support, private jobs, and internal Southwest Research Institute (SwRI) work. It is not clear how these distinct activity bases operate, especially relative to setting time priorities and reimbursement to the testing center.

Ouestion 3: Technical accomplishments and progress toward project and DOE goals

This project was rated 3.0 based on accomplishments.

- These researchers have seen significant variability in their own results for spillover effect materials that they have measured (e.g., the metal-doped carbon foam) that remain unexplained. Is it the material or is the measurement in question? Because the validity of results for the spillover effect interpretation of otherwise unexplainable data is very controversial among the larger hydrogen storage scientific community, it would be better if this project focused more on being an unbiased assessment of that interpretation. This project needs to help to identify what results are accurate, what measurement techniques are required to really be accurate for this kind of study on these kinds of measurements, and how spurious data can arise.
- A number of diverse activities and results were shown, but it was not made clear how these results bring us closer to meeting DOE system targets.
- Except for one slide on Pd/polyaniline, all of the DOE directed results are on Li-Mg-B-N-H (from University of South Florida [USF]). What is the basis of the extensive work on this material? The results do not seem impressive, for example, relative to simple catalyzed MgH₂. How do these conclusions relate to DOE needs?
- The NESSHY work on PdHg/carbon foams has been useful, if apparently in a negative (poor reproducibility, H₂O) sense. At last year's AMR, the presenter stated that no H₂O was desorbed on this poster.

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated **3.3** for technology transfer and collaboration.

- This project has a very good collaborative research portfolio.
- Shows H₂O dominates over H₂ desorption. The major change and its technological implications are confusing. Does the NESSHY foam now have little practical potential as a storage medium for high-purity H₂?
- While it is beneficial for privately-funded, related work to be included in DOE merit review presentations, especially when carried out on DOE contributed equipment, potential intellectual property conflicts must be considered and avoided.
- The standardization and round-robin testing should have important worldwide effects in reducing error. Has this happened to a significant degree?
- A number of collaborations are listed; however, except for NESSHY, few details and results are given. Are these collaborations generally resulting in synergy and benefit for DOE's investments in the testing center?

Question 5: Approach to and relevance of proposed future research

This project was rated 2.7 for proposed future work.

- The proposed future work is fully directed toward achieving the stated goal of developing a standardized testing procedure for such materials as the spillover effect samples.
- Only seven samples are planned for future work.
- Only one sample is scheduled for completion in June 2009.
- Project completion date is 2011, but there is no clear description of future work.
- Future work planned is only the present sample backlog. What is the justification for accepting these particular samples versus the DOE barriers?

Strengths and weaknesses

Strengths

- Standardized testing procedures are essential to good research on hydrogen storage materials, and this project is all about that.
- The concept of having a national testing lab is, in principle, sound and valuable to DOE and the entire storage materials community.

Weaknesses

- It seems that there is too much bias toward acceptance of questionable results (e.g., spillover effect) that give hard-to-understand data. This leads to expectations that the results will be (or should be) verified. When there is variation of a factor of 4 in hydrogen uptake, the presumption is that the sample is to blame rather than questioning if the interpretation of the uptake data is correct. Could there not be something other than hydrogen uptake going on in these materials that could give the results? The project needs to give much more attention to the robustness and accuracy of the experiment and its interpretation before assuming the mechanism of spillover can be applied.
- It is not clear the results so far have improved the general, national, and worldwide accuracy of testing.
- There seem to be a number of independent activities being pursued without clear justifications.

Specific recommendations and additions or deletions to the work scope

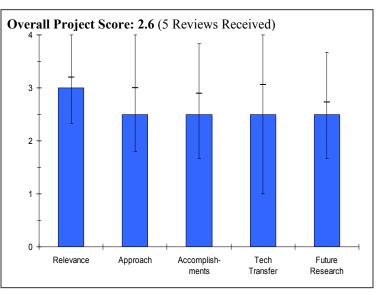
- Add more confirmation that hydrogen is really being taken up by the sample in the way assumed (i.e., spillover) via gravimetric and other methods. Explain why the conditioning is necessary for the Pd-doped polyaniline (PANI), and why the initial uptake of hydrogen is so rapid with pressure. Does this really have anything to do with the PANI, or is it merely due to Pd?
- A better mechanism is needed to decide on the value of taking on a new material. It is unclear what that mechanism should be.

Project # STP-46: An Integrated Approach of Hydrogen Storage in Complex Hydrides of Transitional Elements

Abhijit Bhattacharyya, Tansel Karabacak, Ganesh Kannarpady, Fatih Cansizoglu, Anindya Ghosh, Dustin Emanis and Mike Wolverton; University of Arkansas at Little Rock

Brief Summary of Project

The objective for this project is to find complex hydrides of transitional elements for hydrogen storage that meet the following project targets by 2010: 6% weight percent. a pressure of 100 bar, kinetics of 3 min, and a temperature of -30/50°C. Objectives for bulk materials are hydrogen storage characterization and development of materials for hydrogen storage, including 1) increasing reversible hydrogen capacity in complex metal hydrides by developing new systems including hydride phases, 2) developing catalytic compounds to enhance the formation and decomposition of complex metal hydrides, 3) investigating hydrogen storage capacity in metal- (Ti and Li) decorated polymers, and 4) investigation



of enhancement of hydrogen storage capacity in metal hydrides dispersed in a polymer matrix. Objectives for nanostructures are the 1) investigation of maximum hydrogen storage capacity and adsorption/desorption kinetics of thin films and nanostructures of magnesium alanate and magnesium borohydride, 2) utilization of glancing angle deposition technique for the growth of nanorod arrays of magnesium as a model system, 2) construction and utilization of new quartz crystal microbalance gas chamber system, and 4) investigation of effect of catalyst on hydrogen adsorption/desorption properties of Mg, magnesium alanate, and magnesium borohydride.

Question 1: Relevance to overall DOE objectives

This project earned a score of **3.0** for its relevance to DOE objectives.

- This work is very well aligned with the goals and objectives of the DOE Hydrogen Program.
- Most project aspects are aligned with DOE RD&D objectives.
- The calcium borohydride work is the most relevant to the overall DOE objectives. The Ti in polymers has theoretical work in the literature predicting high capacities, but no researcher has managed to stabilize isolated Ti atoms in such materials. The least relevant work was the magnesium nanoblades as magnesium hydride has already been deselected by the MHCoE.
- There are gaps in the consideration of volume and cost.
- This project is not very well focused.

<u>Ouestion 2: Approach to performing the research and development</u>

This project was rated **2.5** on its approach.

- This project focused on the possibility of synthesizing density functional theory (DFT)-predicted metaldecorated materials, synthesis and reversibility of Ca-B-H material, and the use of conventional metal hydride as an additive to complex hydrides. These approaches address, to a significant degree, the identified barriers of understanding physisorption/chemisorption, kinetics, and durability of hydrogen storage materials.
- This project is a mixture of various activities in macro- and nanomaterials.
- As shown by presenters' references to prior work, most of the materials being studied are also being studied elsewhere. It is not at all clear what is different in this work.

- There appears to be a lack of awareness between this project team and work going on in the MHCoE. Lack of communication with the MHCoE has meant the work has not progressed as well as it might have:
 - The group has struggled to synthesize calcium borohydride and would benefit from advice from the MHCoE into the conditions for this.
 - Ball milling Ti clusters with polymer will not achieve atomically dispersed Ti through the polymer matrix. This is the wrong type of synthetic approach.
 - The Mg nanoblades have dimensions too large for any size-induced affects on the dehydrogenation thermodynamics.
- This work was not very well thought out.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated **2.5** based on accomplishments.

- Very good work on Ca-based complex hydrides and the nanostructured glancing angle deposition (GLAD) materials, especially with the quartz crystal microbalance (QCM). However the work also demonstrated how a faulty valve can give an apparent positive result for hydrogen uptake where none occurs and that the DFT-predicted metal-decorated materials are, once again, not possible to synthesize in the laboratory.
- Presenters are to be praised for the frank admission that all experimental work on metal-decorated polymers has been completely negative. Likewise for the admission that earlier finite storage results were a result of experimental errors.
- Development of the QCM technique may be useful.
- A new synthesis method for Ca(BH₄)₂ may have been developed from NaBH₄. However, here is the best example of ignoring cost considerations. A process for the chemical synthesis of Ca borohydride from expensive NaBH₄ seems highly questionable.
- The bulk characterization of LaNi₅ is especially perplexing. The results are exactly the same as shown by many early investigators of LaNi₅. Is this a learning process using an old reference material?
- Development of the GLAD technique may have some synthesis value. Will it ever be a potential low-cost mass production technique?
- Work on GLAD nanobladed Mg is interesting, but offers no real advantages over many other Mg efforts for meeting DOE goals. Catalyzed and composite micro- and nano-Mg have shown similar (and even better) H₂ absorption improvements. Without major improvements in desorption thermodynamics (e.g., 1 bar desorption plateau pressure at <100°C), significant H₂ will have to be burned for the necessary 300°C desorption enthalpy, making it impossible to reach DOE system goals.
- There are some interesting ideas which the group may wish to pursue for destabilized calcium borohydride systems. Unfortunately, this work has been hampered by the inability to synthesize this borohydride.
- The group proved that ball milling Ti clusters with various polymers did not produce materials with any interesting hydrogen storage properties.
- The magnesium nanoblades were shown to have fast hydrogenation kinetics at low temperatures. However, the thermodynamics of the system has not been addressed; hence, the work is of low impact. N.B.: 30 nm dimensions will not lead to a change in the thermodynamic properties.
- The progress has not been good.
- Progress towards the DOE objectives has been very limited.

<u>Ouestion 4: Technology transfer/collaborations with industry, universities and other laboratories</u>

This project was rated 2.5 for technology transfer and collaboration.

- Good collaborations.
- A few collaborations listed, but not described in any detail.
- The investigators seem to have little interaction with other hydrogen storage research groups. The exchange of ideas is essential if researchers are to avoid falling into the same traps as others. The work here would be greatly enhanced if the group integrates more with the MHCoE. The MHCoE should be encouraged to offer some guidance to these investigators (if this has not already happened).

<u>Question 5: Approach to and relevance of proposed future research</u>

This project was rated 2.5 for proposed future work.

- Efforts should be focused more on the areas that are more relevant to the DOE objectives. The calcium borohydride work would appear to be the most fruitful area for investigation. The investigators have down-selected the Ti-polymer materials, which seems sensible. There was no clear idea for how the nanoblade work was going to translate to other more relevant materials. This would appear to be a weaker line of investigation, and it is recommended that the magnesium hydride nanoblade work be stopped. If this nanoblade technology can be translated to other more relevant hydrogen storage materials, then this would be of interest.
- The proposal for future work was vague.
- This reviewer is glad to see that there are apparently no further plans to work on DFT-predicted metal-decorated materials in this project. It seems that this area of modeling work was an attempt to somehow legitimize the early work on hydrogen uptake by carbon nanotubes that turned out to be only metal impurity particles that do the absorbing of hydrogen. The idea that somehow those metal particles or atoms can decorate carbon structures, remain stable, and absorb hydrogen has not been convincingly demonstrated experimentally, and consequently, is not based in reality. It seems that the "spillover" effect is another example of this. It is past the time to move on to materials that have a better chance of being real and practical hydrogen storage materials.
- The proposed future work is not very innovative or new. There is a low potential for meeting any DOE goals. Most work planned has already is repeating work already completed in various places around the world.

Strengths and weaknesses

Strengths

- Enthusiastic to get results.
- Very interesting synthesis and characterization methods using GLAD and QCM.
- The strengths in this project were limited.
- Some interesting new ideas being proposed for the calcium borohydride system backed up by an enthusiastic thrust for discovery.

Weaknesses

- Not good background to follow this area of research.
- Too much time was spent trying to create the DFT-predicted metal decorated materials in the laboratory.
- Presenters seem to be new to the field and are lacking in understanding of this field's history.
- Poorly thought out synthesis for Ti-polymer materials. Lack of awareness of current developments and perceived wisdom in the area means the group has spent time investigating systems either of low relevance to the DOE objectives (e.g., Mg nanoblades) or of theoretically predicted materials that are technically very challenging to make (Ti-polymer).

Specific recommendations and additions or deletions to the work scope

- Recommend no further work be done on DFT-predicted metal-decorated materials.
- The scope of project should be reworked for more innovation and connection to DOE goals.
- It is essential that this group build up collaborations with other key members of the CoE. This will help the group develop a more strategic focus. It is recommended that the Mg/MgH₂ nanoblade work be discontinued. The work on calcium borohydride is encouraged to continue. The group may wish to consider ways to produce nanostructured complex hydride systems.

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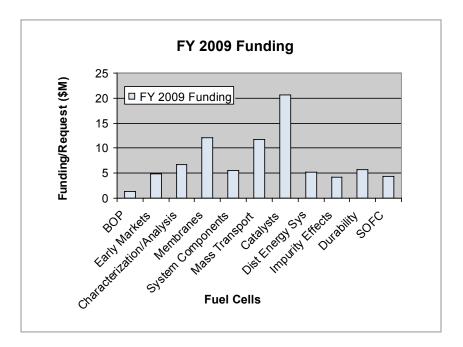
Fuel Cells Summary of Annual Merit Review Fuel Cells Subprogram

Summary of Reviewer Comments on Fuel Cells Subprogram:

Reviewers consider fuel cell development to be a critical enabling technology for the success of the Department's Hydrogen Program. Overall, the research and development portfolio was judged to be well managed, appropriately diverse, and focused on addressing technical barriers and meeting performance targets. Progress was considered remarkable. There was an undercurrent of concern about the announced program redirection and consequent effects on solid plans already in place and technical progress underway. As a result there was less confidence in future plans and prospects than in previous years. One portfolio gap appeared in several reviewer comments in the area of balance of plant (BOP) components, highlighted by the program's cost studies showing cost reduction in stack components making the BOP a significant contributor to system cost.

Fuel Cells Funding by Technology:

The Fuel Cells subprogram continues to concentrate on the critical path technology of stack components (membranes, catalysts/supports, bipolar plates/seals, water transport and management, and analysis/characterization). Additional projects address cross-cutting technologies and effects of impurities on fuel cell performance. Cost and durability of stack components continue to be a key focus of the subprogram.



Majority of Reviewer Comments and Recommendations:

This year 60 fuel cell projects were reviewed of the 63 projects presented. In general, the reviewer scores for the fuel cell projects span the range (1=poor, 2=fair, 3=good, 4=outstanding), with scores ranging from 3.6 to 1.6 for the highest and lowest scores, respectively. The average score of Fuel Cells subprogram projects was 2.9. The highest, lowest, and average scores were all lower than in the 2008

383 FY 2009 Merit Review and Peer Evaluation Report review values of 3.8, 1.9 and 3.0, respectively. The set of projects were reviewed by three to eight reviewers each, with an average over all 60 projects of six reviewers (posters had a lower average number of reviewers). Project scores reflect the technical progress made over the past year; relevance to the DOE Hydrogen Program; technical approach; extent of technology transfer; and proposed future plans. While reviewers tend to award those projects closer to commercial application with higher scores, their comments reveal that they also appreciate and support more fundamental work attacking key barriers to commercialization. Key recommendations and weaknesses are summarized below. DOE will respond to reviewer recommendations as appropriate for the scope and coherency of the overall fuel cell research effort.

Analysis/Characterization: The six projects in this category included two projects that tied for both the highest rank and second highest rank in the subprogram, with the overall category score well above average. These diverse projects were noted to strongly support the fuel cell program objectives and goals. The Oak Ridge National Laboratory microstructural characterization effort again ranked high, this year achieving the highest score in the subprogram tying with 3M and Delphi on other projects. Reviewers commend the advances in techniques and resolution, and continue to comment that correlating the microstructure of membrane electrode assemblies revealed in these images with performance data would increase the value of the effort. The National Institute of Standards and Technology neutron imaging project received the second highest score in the subprogram and demonstrated improvements in capability and resolution. The reviewers again encouraged the modelers in the fuel cell program to validate their models with real world data, and to work more closely with industry. Fuel cell manufacturers need to supply more experimental data to the modelers. The cost of an 80-kW automotive polymer electrolyte membrane (PEM) fuel cell system operating on direct hydrogen and projected to a manufacturing volume of 500,000 units per year continues to fall, and the cost studies help illuminate opportunities for cost improvement. The technical assistance to developers' activity at Los Alamos National Laboratory (LANL) is thought to provide value to the fuel cell community and was particularly noted for its collaborative approach.

Water Transport: Three water transport projects were reviewed with ratings from average to well above average. The LANL project was rated the highest, and the reviewers appreciated the scientific approach but felt that the project may be trying to cover too many phenomena, which limits depth. Reviewers recommended that both the modeling and materials effort of CFD Research Corporation and the visualization project at Rochester Institute of Technology work toward providing developers with models, recommendations, or insights that help advance fuel cell stack design and operation.

Impurities: The three impurities projects received above average scores, with the LANL effort achieving the second highest score of all the fuel cell projects. Reviewers consider these studies, on both the fuel and air sides of the fuel cell, to be very important to program success. The LANL project was lauded for improving understanding of the underlying degradation mechanisms and for suggesting/exploring mitigation strategies. The university projects were encouraged to quickly move to relevant contaminant levels and catalyst loadings, to increase modeling, and to address mitigation. Reviewers note the scope of the projects exceeds what can be reasonably accomplished with resources available. Although the researchers are sharing information and working on coordination, several reviewers recommended increased coordination to avoid duplication of effort.

Membranes: The sixteen membrane projects reviewed were ranked from well below average to well above average, with scores ranging from 1.8 to 3.4 and an average score of 2.7 against a subprogram overall average of 2.9. Giner's dimensionally stable membrane project and Vanderbilt's nanocapillary network proton conducting membrane projects received the second highest scores in the Fuel Cells subprogram, with FuelCell Energy's membrane project using humidification-independent cluster structures and 3M's project ranked just behind. The Vanderbilt project this year moved away from

sulfonated poly (arylene ether sulfone) nanocapillaries to perfluorosulfonic acid materials. The first three projects listed above met the DOE interim proton conductivity milestone at the 120°C, 50%RH conditions. As six projects pass the go/no-go milestone, some reviewers look forward to effort on development of compatible electrodes and fuel cell testing, while other reviewers find such work premature. In several projects, reviewers commented that membrane principal investigators would benefit from closer collaboration with fuel cell researchers and developers. A cost of production study of the most promising membranes was recommended for many of the projects. Reviewers provided specific recommendations to improve lower rated projects.

Catalysts/Supports: All but one of the five catalysts/supports projects reviewed received an overall rating above average, with two of the projects receiving the highest and second highest scores in the subprogram. The top-ranked 3M nanostructured thin film electrode project was particularly notable, exceeding three key DOE stack-level targets for 2015 on the single-cell level, on a mechanically-stabilized 3M membrane. The required total platinum group metal (PGM) content continues to fall as a result of subprogram research, and non-precious metal approaches show progress toward mass-activity targets. Reviewers continue to express concern about approaches that replace platinum with other PGMs. Some durability results from the non-precious metal catalyst projects are promising, but performance generally needs to be an order-of-magnitude higher before this durability matters. The reviewers commented that these efforts in alternative electrocatalysts, though high risk, represent a potential high pay-off option and should be supported in the future. Reviewers had mixed views on the conflict between improving fundamental understanding of a broad array of approaches with the desire to down select to a few candidate materials and focus effort as soon as possible. The only project in the category focused exclusively on supports scored below average, and reviewers offered a broad array of recommendations to improve the likelihood of success.

Recycling: The one remaining recycling project was evaluated and received an overall rating at the top of the range, achieving the second highest score in the subprogram. Reviewers consider PGM recovery an important aspect of the overall fuel cell life cycle, because it addresses both environmental issues and cost issues that impact the cost of fuel cell systems. BASF Catalysts has successfully completed the project, identifying and demonstrating the most efficient processes to recycle both catalyst-coated membranes and membrane electrode assemblies. Reviewers questioned the future impact of advanced catalyst forms, such as core-shell structures, and the economic impact of ultra-low PGM loadings, but generally considered BASF ready to commercialize PGM recovery whenever the market is ready.

Bipolar Plates/Seals: Two bipolar plate projects and one project on seals were reviewed in the Annual Merit Review and Peer Evaluation. These projects received average scores. Reviewers suggest increasing collaboration with stack developers and investigating remaining issues of concern, including: metal plate formability and joining; further reductions of processing temperature and cost; and the permeability, durability, and minimum thickness/formability of expanded graphite/resin plates. Reviewers believe more information on the seal materials developed must be provided if the UTC seal project is to be of use to the broader community. They also recommend permeability testing and testing under fuel cell cyclic conditions.

Water Management: Two projects in water management were reviewed. The Nuvera project received an above average score, and notably demonstrated that DOE cold-start targets can be met at the stack level. However, reviewers questioned the benefit to developers from the design and testing of a proprietary stack with limited data provided to the community, and they felt that the question of long-term durability of the stack under the start/stop protocol has not been adequately addressed. The Honeywell project received a score well below average, and reviewers questioned the value of testing of commercially available components. Reviewers noted that even if successful, the project is unlikely to improve the overall technological readiness of PEM fuel cell systems.

Distributed Energy: The ten distributed energy projects reviewed were generally scored below average; however, the Materials and Systems Research Solid Oxide Fuel Cell (SOFC) hybrid plant for the coproduction of electricity and hydrogen, and the UTC stationary PEM power plant verification project, scored notably above average. Distributed energy fuel cell applications are growing in program emphasis, and this year present a very diverse set of projects at widely varying levels of technical maturity and system development. Effort ranges from the fundamental to field testing of pre-commercial systems. Across the projects, reviewers noted both significant progress and significant problems and provided recommendations for the improvement of individual projects in approach, collaborations, and future planning.

Auxiliary, Off-Road, and Portable Power: Three auxiliary power projects, one off-road application project, and one portable power project were reviewed this year. The Delphi SOFC auxiliary power unit (APU) for heavy-duty trucks tied for the highest ranked project in the subprogram. Reviewers found the progress commendable, including two new on-vehicle demonstrations since the last review, and judged the project generally on track for success. The Cummins Power Generation SOFC heavy truck APU project was also rated above average, showing good progress, though the current design misses targets in several areas. The remaining projects in this category were generally rated below average. The IdaTech methanol-fueled PEM golf course maintenance vehicle received mixed reviews, with a lack of test data collection and analysis noted. The remaining projects, a solid acid fuel cell stack and a silicon-based SOFC for portable electronics, both demonstrated progress. However, they were judged to be relatively immature, and technical detail in the presentations was lacking.

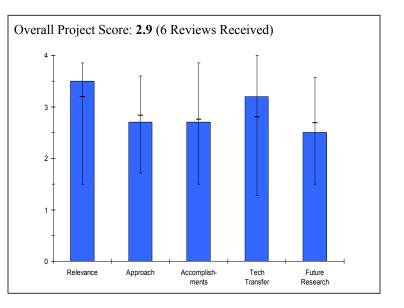
Cross Cutting: The five cross-cutting projects reviewed this year generally scored well below average, and this category had the year's lowest ranked project from Microcell Corporation for commercial scaleup of a microfiber fuel cell, which was scored at 1.6 (below a rank of 2.0, or "fair"). The remaining projects in this category are all university-led, most of which tend to collect a number of disparate tasks spread across a number of investigators under a project umbrella. Although reviewers generally agree that the individual tasks address important issues in fuel cell development, reviewer comments indicate a lowlevel and diffuse effort on a broad number of technical areas does not constitute a well-defined, coordinated project likely to make progress toward targets.

Project # FC-01: Lead Research and Development Activity for DOE's High Temperature, Low Relative Humidity Membrane Program

James Fenton; University of Central Florida

Brief Summary of Project

The objectives of this project are to 1) investigate new polymeric electrolyte/phosphotungstic acid membranes; 2) develop standardized characterization methodologies, including conductivity, mechanical, mass transport, and surface properties of membranes; 3) provide the High Temperature Membrane Working Group (HTMWG) members with standardized methodologies; and 4) organize HTMWG biannual meetings. Fuel cell performance will be evaluated and the durability of membranes will be predicted. Membrane electrode assemblies (MEA) will be fabricated and evaluated.



Question 1: Relevance to overall DOE objectives

This project earned a score of 3.5 for its relevance to DOE objectives.

- This program supports the DOE R&D objectives.
- It was not clear whether this membrane development program was geared towards stationary or transportation applications. At 120°C and low relative humidity (RH), heat rejection and operation of the stack will be favorable for transportation applications with pure hydrogen. However, for stationary applications, the stack must operate at 40°-45°C higher than 120°C to avoid CO sensitivity, assuming they use natural gas (NG) or propane and a low-cost fuel processor.
- The project is critical to the Hydrogen Program and its need for membranes that can operate at higher temperatures under low humidity conditions. However, listing the electrolyte/phosphotungstic acid membrane development first in the list of objectives suggests a questionable set of priorities. Working with the HTMWG members is surely the first priority, as well as helping with standardized measurements or otherwise. This project has not lived up to its promise with regards to providing support for the HTMWG members and has shown that standardized measurements and biannual meetings are not sufficient to generate the necessary collaborative and collegial spirit to maximize the benefits of the HTMWG members' efforts. The phosphotungstic acid work is worthwhile, but not enough to merit dividing the team's attention. It is recommended that the team returns to the original proposal and revisits some of those ideas to generate more collaboration.
- The project goals are aligned with DOE targets and goals, and the project is relevant to DOE objectives.
- Tasks 3-7 are critical to facilitating the common conductivity testing of all the membranes in the HTMWG. Without this testing, it would be impossible to compare performance from one project to the next; furthermore, the tasks have addressed issues in conductivity testing and are intended to enhance it.
- Tasks 1 and 2 are dedicated to membrane development for fuel cells, which like all other membrane projects, is at least relevant.

Question 2: Approach to performing the research and development

This project was rated 2.7 on its approach.

- This program should be focused on meeting conductivity, mechanical properties, and chemical stability targets. Doing electrode development and evaluating fuel cell performance is premature in a materials-development program such as this.
- Given the scope of the project, it appears very well designed.
- The project needs to improve interactivity with other HTMWG members. The approach is a little too split between the project team's ideas on membranes and other's ideas. More assistance should be offered to other group members on more issues than just conductivity and MEA manufacture. For example, there seems to be little on mechanical properties, swellability, or gas cross-over. How are these measurements to be done? More leadership by others is necessary so that it occurs more frequently than just twice a year.
- The project team's work in the function of HTMWG lead is good. The approach to obtaining high temperature membranes led to an improvement by an approximate factor of two over Nafion®.
- The approach of adding heteropoly acids (HPAs) to perfluorosulfonic acid (PFSA) is basically reasonable, though more attention should be given to leaching prevention strategies. However, so far HPAs have not provided substantial improvement, especially at low RH, and it is not clear that the investigators have a good approach to further attacking the problem.
- The membrane development work lacks novelty. The literature contains many attempts to combine HPAs with PFSAs.
- The project does not show a convincing effort to defend against two of the most probable failure modes associated with HPAs: swelling and leaching of the HPA, with exception of the use of a reinforcing material.
- The project exhibits nice consistent effort to generate conductivity data with partner membranes, despite the fact that in-plane conductivity will mask anisotropy.

Ouestion 3: Technical accomplishments and progress toward project and DOE goals

This project was rated 2.7 based on accomplishments.

- Several of the partners have made good progress in meeting targets.
- It appeared that significant improvements have been made. Conductivity of membranes from all but one of the high-temperature membrane projects was already higher than Nafion®, with two of them already exceeding the target, and a third one being close to the target.
- Progress towards the HTMWG barriers as a whole is fair, but not compelling. This project's progress towards 50% RH is fair, but reaching this goal entirely seems rather problematic. Can a thinner membrane be used? The area specific resistance (ASR) is a good measure only if the gas crossover numbers are known. No real mention of this in the presentation.
- A technique was developed to measure HPA in the membrane and ensure it remains there during processing. Conductivity results are less than desired, but still exhibited an improvement by an approximate factor of two over Nafion®. The project team has developed thru-plane conductivity/ASR measurement with collaborators.
- The project exhibits some improvement over Nafion®, but is still not very close to the 120°C target and has no clear path to get there.
- None of the data clearly show that the addition of HPA increases the conductivity of membrane samples.
- No swelling data was reported.
- Some slides were missing important information, such as temperature.
- By this stage in the project, we should know something about the degree to which the HPAs leach from the Florida Solar Energy Center (FSEC) series membranes.
- The project team gave a good effort to produce a multi-port system for *in situ* testing.

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated **3.2** for technology transfer and collaboration.

- The project team collaborated well; however, more interaction with industry partners such as GM, Ford, and 3M would be useful.
- For a complex project with various stake holders like this, collaboration and coordination appeared to be at a very healthy level.

- Collaboration appears strong in the presentation, but really needs to be dramatically increased if the project is to be the lead project charged with coordinating the efforts.
- Overall, collaborations with membrane working group members appear to be good.
- This project has done an excellent job at staying consistent to its original intentions, especially while working with a large number of partners. Some may criticize the use of the in-plane method, and some may criticize the use of PFSA ionomers for all *in situ* testing, but the project has still managed to produce the results that it was assigned to do.

<u>Question 5: Approach to and relevance of proposed future research</u>

This project was rated **2.5** for proposed future work.

- As mentioned above, emphasis should be on conductivity and other material properties. Fuel cell testing at this early stage will not provide useful information for most of these new materials.
- The project team should add some sort of accelerated endurance testing for the membrane, as well as testing of the membrane as an MEA, to its future work plan.
- Future work plans appear to be confined to MEA preparation, without much fundamental basis for the proposed methods. Each polymer delivered from another group will need to be treated differently. This is not addressed.
- Redirection to stop membrane fabrication seems appropriate when test results are compared to milestone targets and other results in the high-temperature membrane projects. It is appropriate to begin planning for durability testing and integrating the new membrane working group project's membranes into MEAs.
- It seems unlikely that proposed future work, which mostly seems to involve varying processing and casting parameters, will result in sufficient improvement.
- The test system shown for running multiple fuel cells at one time appears promising.
- Future work on partner membranes was not clearly outlined; however, one slide implies that both mechanical and chemical durability tests will be pursued, which is good.
- The project should offer specific definition on ASR based on a specific protocol, and then seek the research community's feedback, rather than allow the community to define it.

Strengths and weaknesses

Strengths

- Several of the partners have made good progress in meeting targets.
- The team took a methodical approach.
- Standard procedures for conductivity are good.
- There was good collaboration between BekkTech, Scribner, and the University of Central Florida (UCF).
- The project team exhibited a strong ability to gather samples from the research community, perform needed testing, and fabricate test devices.
- The project team attempted to use reinforcement in membrane fabrication.

Weaknesses

- This program should be focused on meeting conductivity, mechanical properties, and chemical stability targets. Doing electrode development and evaluating fuel cell performance is premature in a materials development program such as this.
- The end user, or customer, was vaguely defined.
- The MEA standard procedure was not necessarily good. We need more research on what is important about polymer structures.
- Collaboration with other DOE workers in the membrane area seems to be weaker than this project requires, and leadership is not provided.
- Membrane development work has not increased high-temperature/low RH conductivity as much as desired.
- There was a lack of novelty in new membrane fabrication.
- There was a lack of initiative in addressing known membrane failure modes, such as swelling and leaching, within the opening stages of the project.
- The project team needs to more clearly define some future protocols.

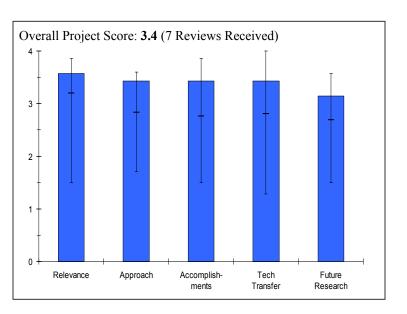
- The project team needs to work with partners to understand and address material shortcomings to push as many new materials as far as possible. This will increase the likelihood of new and improved commercially viable membranes being developed.
- The plans should include fuel cell level testing to ensure that there are no interface level issues when these membranes are used in an MEA.
- The decision for UCF to stop membrane development work and concentrate on testing is appropriate.
- The Florida Solar Energy Center should eliminate development of its own membrane materials and focus on its other roles in the HTMWG.
- The project team should eliminate new membrane fabrication (which has been done).
- The project team should add emphasis on *in situ* testing of partner membranes and focus on the three ideal functions of the membrane: proton conduction, gas separation, and prevention of electrical shorting. This would create a wide temperature range before and after a stress test (e.g., open circuit voltage (OCV) or RH cycling). In other words, create a simple grid of measurements by which every membrane can be evaluated under *in situ* conditions.

Project # FC-02: Dimensionally Stable Membranes

Cortney K. Mittelsteadt, William Braff, Shelly VanBlarcom, and Han Lie; Giner Electochemical, LLC Fred Johnson and Israel Cabasso; SUNY-ESF

Brief Summary of Project

The ultimate goal of the project is to meet performance targets with film that can be generated in roll at DOE cost targets. The Year 2 milestones were achieved and interim conductivity targets have been met. Improvements in fuel cell performance have been shown, including electrodes. A realistic pathway for meeting cost targets can be seen for both paths. To reach the ultimate DOE goals, Giner needs to incorporate the low equivalent weight (EW) materials that have been developed at the State University of New York-Syracuse (SUNY).



<u>Ouestion 1: Relevance to overall DOE</u> <u>objectives</u>

This project earned a score of **3.6** for its relevance to DOE objectives.

- Dimensionally stable, high-temperature membranes are vitally important for fuel cell vehicle (FCV) commercialization. Whether or not FCV commercialization is still important to the DOE is another matter.
- High membrane conductivity over the range of operating conditions is critical to achievement of DOE targets. This project is focused on high-temperature and low relative humidity (RH).
- An important and essential aspect of the objectives of this effort is the high-volume supported membrane production capability development. This effort, together with the objective of meeting or exceeding the performance requirements, fully supports the DOE hydrogen R&D objectives.
- The project actually addresses the three primary barriers of durability, cost, and performance.
- Work is in line with Task 1, Barriers A, B, and C, to develop membranes that meet all targets.
- Membrane swelling remains an issue; hence the relevance of this task is undeniable. The composite membrane approach is a viable path to perhaps preventing membrane thinning, which is also observed in some failure modes.
- Improved conductivity, high-temperature, and low RH membranes are included in Hydrogen Program and DOE RD&D objectives. These are not the most critical material needs for enabling fuel cell commercialization.

Question 2: Approach to performing the research and development

This project was rated **3.4** on its approach.

- Unfortunately, Giner's unique laser etched reinforcement layer technology is not economically feasible due to an intrinsically high cost for the laser etching. Therefore, Giner is now working on commercially available support materials with ionomer from collaborators. It is unclear, with the 3DSMTM support material, what inhouse technology Giner is bringing to this work.
- Using a mechanical support structure to allow lower EW ionomer has shown merit. The support structure prevents macroscopic swelling in the x-y plane.
- The performance of the 3-D stable membranes is impressive, particularly at 50% humidity, in this internally well-integrated project. The connection to other projects in the Hydrogen Program is less clear.
- Work is based on a previously established concept. The approach suggests a good chance for success. The 2DSMTM is a clever way to use less of the expensive ionomer and the better performing low equivalent weight

materials. The rationale of their approach seems logical and solid, and it is pleasing to see a possible alternative to the laser drilling.

- The approach is excellent, and the use of insoluble highly proton-conductive ionomers in a commercial 3D support should achieve the project goals.
- The approach appears very methodical, and it appears that testing the membrane in fuel cell embodiment and considering/factoring in production cost early on is a thoughtful approach.
- The project team employed a very strong approach using high-acid content ionomers and supported materials in which the mechanical properties are provided by the support. Down-select to a single approach, such as 3DSM, which should allow for more significant advances. Addition of Millipore as a team member supplying 3D significantly strengthens project.

Ouestion 3: Technical accomplishments and progress toward project and DOE goals

This project was rated **3.4** based on accomplishments.

- Proton conductivity measurements are showing progressively better values approaching the DOE target; however, the key to achieving the goals will solely lie with the ionomer producer, as mechanical minimums are not required by the DOE. In the case of 3DSM, support is provided from outside the company.
- Giner has met the Year-3 go/no-go target for high-temperature (120°C) and low-RH conductivity (50%).
- Data show the possibility of meeting the final target at 25% RH.
- So far, this program is one of the very few that has exceeded the DOE goal for conductivity at low RH.
- Fuel cell performance gains with the 2DSM are quite good with the 700 EW ionomer. Humidity cycling passes for all approaches and is giving a very good result. The new casting approach for the 2DSM is clever and encouraging. The project team should resolve the issue between its measurements and those of BekkTech.
- This project exceeded the go/no-go decision point target of 0.1 S/cm at 120°C and less than 50% RH.
- Technical progress appears consistent with expectations at this phase. The project team should make an effort to get rid of water and find a new mechanism for transport of protons.
- The project's progress over three years has been strong. In comparing this year's presentation to last year's, advances achieved in the last year seem a little limited focusing mainly on fuel cell performance and 3DSM advances. The fuel cell performance was deemphasized, and rightly so. The 3DSM results are interesting, show promise, and likely suffered from "learning pains;" but they show limited progress. The team should make more significant advances along these lines in the coming year. The results of the overall project are strong and show materials with significant property improvements.

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated **3.4** for technology transfer and collaboration.

- Based on the results, it appears interaction is high. This type of close collaboration is highly necessary, as both the ionomer and 3DSM comes from someone other than Giner.
- Giner knows its technical limitations and has partnered with appropriate organizations to fill in the gaps. He is working closely with GM and other partners including a porous support developer (Millipore) and a monomer synthesis organization (SUNY).
- Testing of SUNY polymers provides evidence of collaboration; however, the relation to GM was not clarified in the presentation.
- The program could benefit from collaboration with a larger film manufacturing company with large scale experience in film casting. This would provide not only experience, but also an understanding of cost and quality control issues.
- There have been collaborations with polymer chemists at SUNY and an industrial original equipment manufacturer (OEM) in GM.
- The amount of collaboration appears healthy but exhibits a strong dependency on SUNY for low EW materials.
- It was demonstrated that collaboration exists with SUNY. GM was mentioned several times during talk, and the addition of Millipore, a leader in porous membrane technology, significantly enhances the project.

Question 5: Approach to and relevance of proposed future research

This project was rated **3.1** for proposed future work.

- This program should focus on 2DSM with the funding of program DE-FG02-05ER84322. Giner's unique technology is 2DSM/laser etching, and finding a cost effective manufacturing process is very important. If 3DSM technology is used with outside ionomer, the unique sales point of Giner is lost.
- Future *in situ* fuel cell results will be beneficial in understanding the true potential of the material.
- A down-select to 2DSM or 3DSM should be done soon.
- Working on cost and manufacturability is appropriate and important.
- More effort on mechanical testing and RH cycling is needed.
- Future work was appropriate. Efforts should be devoted to enhancing performance at lower RH levels.
- It is not clear what the criteria will be to down-select between the 2DSM and the 3DSM approaches. What advantage does the project team expect with the 3DSM over the Gore membrane?
- The down-select approach to go forward will demonstrate cost feasibility, fuel cell performance, and RH cycling durability.
- I agree with the proposed future work, and propose additional thoughts on eliminating water as a medium for proton migration. Also, along with fuel cell performance, some endurance run is also essential to prove the feasibility of the down-select solution.
- Down-selecting to a single support membrane structure was presented clearly and with good rationale. Focus on high-acid content polymers continues to be appropriate. Advancing to even higher acid contents (by shorter side chains) was mentioned but not discussed as a topic of further study.

Strengths and weaknesses

Strengths

- Strengths include: 2DSM, strong collaborations, and a strong team at Giner.
- Identification of highly conductive membrane at low RH is a major accomplishment.
- The project team shows novel approaches with logical, easy to understand potential benefits.
- They seem to have achieved a practical solution for the required membrane performance.
- The project team has taken a methodical approach.
- This is one of the best high-temperature membrane projects. It has shown clear advances using relevant materials and methods, as well as provided increased understanding/insight of high temperature, low RH conduction.

Weaknesses

- Using 3DSM support materials and outside ionomer, it remains unclear to the reviewer what technology Giner brings to the table. Giner must focus on 2DSM with key ionomer producers.
- The project team needs an independent projection of cost, including the cost of the synthetic processes.
- The project team shows a lack of large scale manufacturing experience.
- I am still not convinced that the 2D laser-drilled support will ever be cost competitive or able to be mass produced. More information is needed here.
- Perhaps not a weakness of the project, but coming down on the cost curve appears to be a challenge.

- DE-FG02-05ER84322 should become fully funded so that Giner can fully focus 2DSM materials. Fuel cell experiments should shed more light on the potential of this material.
- The SUNY synthetic effort needs to be enhanced, so that larger quantities can be available for membrane production and in-cell evaluations.
- Cast and cure of the 2DSM approach should continue and perhaps be expanded to include a broader array of processing methods.

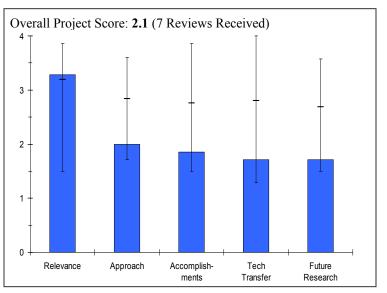
- The material should be evaluated at all temperatures relevant to the automotive industry, including temperatures as low as -20°C with a concentration on 95°C. That is, temperature and RH cycling down to -20°C and from 20%-100% RH should be done.
- None.
- Acid strength arguments for pursuing perfluorosulfonic acids (PFSA) are supported by data, but not proven. For an increased understanding of these systems, other conductivity data as a function of hydration number for related compounds such as methane sulfonic acid, perfluoro ethyl sulfonic acid, perfluoro propyl sulfonic acid, and perfluoro benzyl sulfonic acid, would be extremely interesting and insightful from a fundamental understanding point of view, and would provide enhanced justification of acid choice for ionomers.

Project # FC-03: New Polymer/Inorganic Proton Conductive Composite Membranes for PEMFC

Serguei Lvov, Mike Chung, Sridhar Komarneni, Zhicheng Zhang, Elena Chalkova, Chunmei Wang, Jeong Lee, Wentian Lin, Young Dong Noh, Yunchul Cho, Kanchan Grover, Joo Young Kim, and Mark Fedkin; Pennsylvania State University

Brief Summary of Project

The overall objectives of this project are to 1) contribute to DOE efforts developing high-temperature proton exchange membranes for transportation applications; and 2) develop a new composite membrane material with hydrophilic inorganic particles and vinylidene fluoride / chlorotrifluoroethylene (VDF/CTFE) polymer matrix to be used in proton exchange membrane fuel cells (PEMFC) at -20°-120°C and relative humidity (RH) of 25-50%. The main project objectives of the last year were to 1) develop a proton conductive inorganic/polymeric membrane for a PEMFC operating at elevated temperatures up to 120°C and significantly reduced RH and 2) increase durability with



improved fuel cell performance. Tasks for the last year included the 1) synthesis and characterization of functionalized polymeric materials suitable for the desirable composite membranes; 2) synthesis and characterization of inorganic proton conductive materials suitable for the desirable composite membranes; and 3) fabrication and characterization of composite membranes and membrane electrode assemblies for PEMFCs in automotive applications.

Question 1: Relevance to overall DOE objectives

This project earned a score of **3.3** for its relevance to DOE objectives.

- The project is relevant to DOE's 2010 and 2015 low RH/high-temperature membrane R&D objectives.
- The tasks are aligned with the low RH/high-temperature project goals.
- The intent of the project is relevant to DOE's Hydrogen Program.
- The development of new membranes is aligned with DOE R&D objectives.
- The project's goals are limited to immediate achievement of shorter-term milestones with what appears to be a dead-end for the really desirable milestones. This is a pity, as the project held the potential for some basic investigation into polymer-surface interactions that could have been generally applicable and useful to the entire High Temperature Membrane Working Group (HTMWG) program.
- The project's goals and targets are aligned with DOE program goals and objectives.
- The project relevance is high because it involves fuel cell membranes with high conductivity at high temperature and low RH.
- In as much as the project attempted to fabricate proton-conducting membranes for PEMFCs, it was entirely relevant to the DOE objectives. If it had succeeded, it could have been critical.

Question 2: Approach to performing the research and development

This project was rated **2.0** on its approach.

• The approach of synthesizing crosslinked membranes with a crosslinked hydrocarbon backbone, which is known to be unstable to free radical condition, was not appropriate for the intended fuel cell application.

- The sulfonated polyethylene (PE) polymers have formed a crosslinking group with benzylic hydrogen, which is very well known to be unstable under free radical conditions. The synthesis of such crosslinkers with benzylic hydrogen was not appropriate for the intended fuel cell application.
- Although neat phosphosilicate has the potential to meet low RH/high-temperature conductivity, since none of its diluted composite showed better performance with Nafion® binder, this indicates limitation of phosphosilicate use under DOE conditions.
- It is not clear how holding water more tightly will contribute to membrane conductivity. The researchers should provide experimental or theoretical evidence that these inorganic additives can provide enhanced conductivity. Inorganic materials that bind water tightly often do not contribute much to enhancing conductivity.
- Aliphatic HCs typically do not have adequate chemical stability for use in PEMFCs. Stability experiments need to be done to show if these materials will survive.
- The presentation does not demonstrate how fundamental principles are used to design the materials to achieve the goals. This seems very empirical which is not helpful to the overall program.
- Chemical stability of polyolefin has not been demonstrated in fuel cell conditions; PE background should be susceptible to peroxide attack.
- At the low wt% inorganic additive (lower volume percent), the membrane can only be acting as a water storage material; otherwise, a template for organizing the Nafion® will not offer an alternative conduction pathway as postulated, because there is not enough inorganic additive to conduct over any appreciable length before the conduction pathway is interrupted by Nafion®.
- The approach was not particularly creative. The materials to be examined, as neither the polymers nor the inorganic additives, represent a step-jump forward in potential fuel cell performance and durability. The organic and inorganic materials were not highly conductive.
- Adding inorganic proton conductors is a poor approach when the inorganic components themselves have conductivity far below the 120°C target. Increasing water retention with hydrophilic dopants is a more credible approach.
- The original intents of the project were to fabricate membranes with functional groups that were known to not be stable for PEMFC environments.
- The switch to polyolefins still leaves the prospect of instability to oxidizing/reducing environments.
- Phosphosilicates chosen to enhance proton conductivity do not demonstrate sufficient proton conductivity on their own at 120°C and 25% RH.
- No strategy was given regarding the stabilization of inorganic additives in the membrane.
- All measurements focused on 120°C, although many fuel cell applications require lower temperatures during operation.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated 1.9 based on accomplishments.

- A considerable amount of work had been conducted towards the sample preparation and testing, but, due to the less effective approach, no success was realized.
- Under DOE's condition of 120°C, all the test samples showed performance as being the same or below Nafion® membrane.
- No conductivity was realized by improving the approach of phosphosilicate-based Nafion® composite.
- No progress has been made towards meeting the high-temperature membrane conductivity objective of the project.
- The materials produced in the program met the 30°C conductivity target, but showed no improvement at 120°C. The fuel cell testing is interesting, but an explanation should be offered as to why there is this difference. The "re-cast Nafion®" control had an unusually low open circuit voltage (OCV).
- Some reasonable technical progress was made but there is no sense of great insight into membrane structures, proton conduction mechanisms, or how the next set of milestones will be achieved. The project seems to have very limited goals, and hence has very limited achievements. Much more extensive insights could easily have been found in this project, and it is disappointing that the participants were so unadventurous.
- The project team has only achieved limited improvements in conductivity compared to Nafion® with dopants. Progress on the HC membranes being investigated has been slow, and they are not developed enough yet to

make membranes comparable to Nafion® in performance, so the overall idea of a composite HC membrane with inorganic testing has not been tested.

- The technical accomplishments were not impressive. Conductivities were no better or only slightly better than commercial Nafion®. The addition of inorganic particles resulted in a lower membrane conductivity. Fuel cell current-voltage data were presented. The improvement in fuel cell performance with the PI's new membranes could not be explained.
- None of the tested materials have had significantly better performance than Nafion®, and most have had worse performance.
- Proton conductivity targets were not met at 120°C.
- Proton conductivity targets were not met at lower temperatures for materials still discussed in this year's presentation.
- The combination of best inorganic additives (P-Si) with updated functionalized polymer (PE-based) was not completed.
- The lowest swelling in the project was for Nafion®/P-Si composites, which were not the intended membranes.
- No demonstration was made in which materials had the prospect of durability.

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated 1.7 for technology transfer and collaboration.

- There is no industry, national laboratory, or other university involved in this project.
- Most of the work was only conducted by Pennsylvania State University (Penn State) groups.
- There is no indication of any technology transfer prospect from the present project.
- There appears to be no outside collaboration.
- Not much interaction is taking place with other institutions apart from the obligatory one with BekkTech. This is very disappointing, particularly as interactions with other groups could have helped this project live up to its true potential.
- Collaborations outside of Penn State are limited and appear to be only for membrane testing.
- Collaborations/partners were only with researchers from Penn State.
- The only collaboration involved in the project was the one that was enforced on all membrane projects (BekkTech).

<u>Question 5: Approach to and relevance of proposed future research</u>

This project was rated 1.7 for proposed future work.

- The reason is not clear for proposing the crosslinkable polyolephynes, when it is clear that this approach is not showing any sign of membrane conductivity improvement.
- Sulfonic acid functionalized inorganic additives could be a potential route of making membranes with higher conductivity, if they help in enhancement of the ionomer conductivity. The present data suggest the inorganic additives do not help in increasing the conductivity of Nafion® ionomer.
- Cross-linking is a good approach.
- The chemical stability of the HC polymer needs to be addressed first.
- The project is at an end, but suggested future work is totally uninspired.
- Given the lack of progress with the polyolefin materials tested to date and results from block copolymer systems in other work, it appears unlikely that these systems will be able to achieve high enough ion-exchange capacity (IEC)/low enough equivalent weight to meet the conductivity targets.
- Nothing new here: The project has been completed, so future work is irrelevant.
- Proposed plans are either very similar to approaches already taken by several others in the case of increased sulfonic group concentrations (so there would be no point in duplicating this effort), or not a significantly different from what they have already tried in the case of increasing water retention (so unlikely to lead to significant conductivity improvement).
- The PI indicates that P-Si would be combined with PE-based polymers if more time was given, which is good.
- It is entirely speculative as to whether future efforts would be able to generate sufficient proton conductivity, lower swelling, prevent leaching of inorganics, and prevent brittleness.

Strengths and weaknesses

Strengths

- This is a good academic project for helping students get introduced to the field of fuel cells.
- The program provides hands-on membrane synthesis and fuel cell testing opportunities to students.
- The program also covers diverse areas of polymer synthesis, material development, and electrochemical testing in a single project.
- The project has the capability of providing real insight in the fields of polymer-particle interactions and solidstate proton conduction.
- The fuel cell results are promising, although they cannot be explained and, thus, it appears to be difficult to move forward with new-generation materials.
- The project allows for the ability to survey a wide variety of chemistry.
- The project has moved away from prior membrane systems where swelling was excessive.
- The project conducts systematic elimination of inorganic candidates based on the inability to conduct higher than Nafion® at varied weight percents.

Weaknesses

- The approaches to enhance membrane conductivity are not effective.
- The material selection of conductivity enhancement to the ionomeric membranes under dry condition was not adequate.
- Benefits of different ionomeric binders, such as HC-based ionomers with phosphosilicate inorganic salts, should have been explored.
- Aliphatic HCs typically do not have adequate chemical stability for use in PEMFCs. Stability experiments need to be done to show if these materials will survive.
- There appears to be no outside collaboration.
- The project exhibits timid objectives, poor collaborations, no sense of vision, and is limited to meeting short-term goals.
- The weaknesses are the absence of new materials with dramatically improved properties, and the resulting low/disappointing conductivity data at high temperature/low RH. There was no additional membrane property data, such as gas crossover, water uptake, or mechanical properties.
- None of the approaches tried so far have yielded significant improvement, and plans for future work are unlikely to change this.
- The project is unable to begin with a functionalized polymer system that either had a well-understood prospect for durability, or that brought some novel means of water retention or proton conduction.
- No effort was given towards understanding whether additives could be immobilized.
- The overall approach was more Edisonian than it should be. Ultimately, there needs to be well-established reasons for choosing the chemistry of the membrane beyond the overall goal of dispersing proton-conducting additives within a polymer backbone.
- The swelling issue was addressed too late.

- The crosslinkable polymer possessing aromatic crosslinkers with benzylic hydrogen should be deleted.
- The team should explore new inorganic proton-conducting materials capable of enhancing proton conductivity to the ionomers under dry operational conditions.
- The stability of the inorganics towards hot water needs to be shown.
- The team needs to be more adventurous and show better direction.
- The stability of the polyethylene-derived materials in the fuel cell environment is questionable. The reviewer recommends testing some of these materials in a fuel cell environment, or *ex situ* in Fenton-type reagent before continuing this line of work.
- There needs to be a new direction and focus for this project, in order to attain the DOE target of 0.1 S/cm at 120°C and 50% RH.

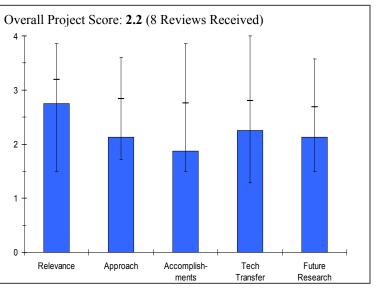
- If the project were to move on, collaboration with an industrial partner would be a necessity. Such a partner would provide guidance on what swells, leaches, enables conductivity, etc.
- An industrial partner might also be able to give advice on crosslinking or membrane reinforcement.

Project # FC-04: Poly(cyclohexadiene)-Based Polymer Electrolyte Membranes for Fuel Cell Applications

Jimmy Mays and Suxiang Deng; University of Tennessee Mohammad Hassan and Kenneth Mauritz; University of Southern Mississippi

Brief Summary of Project

The objective of the project is to synthesize and characterize novel neat and inorganically modified fuel cell membranes based on poly(1,3-cyclohexadiene) (PCHD). To achieve this objective, a range of materials incorporating PCHD will be synthesized, derivatized, and characterized. Successful completion of this project will result in the development of novel and potentially inexpensive polymer electrolyte membranes engineered to have high conductivity at elevated temperatures and low relative humidity (RH).



Question 1: Relevance to overall DOE objectives

This project earned a score of 2.8 for its relevance to DOE objectives.

- Low-cost and high-temperature membranes are a vital technology needed for fuel cell vehicle (FCV) commercialization.
- Membranes that operate at high temperature and low RH are in line with DOE targets and objectives.
- This program is scheduled to end. Stated objectives support DOE objectives, but the work appears to not meet the go/no-go milestone. Also, in its synthesis activities, it is not geared to address the synthesis of actual membranes, but rather membranes that are intrinsically unstable.
- The project addresses the three most critical barriers of cost, performance, and stability.
- The development of low-cost membranes is critical for FCV commercialization.
- Work is in line with Task 1, Barriers A and B, to develop membranes that meet all targets.
- The project goals of fabricating and characterizing a high-performance polymer electrolyte membrane for high-temperature/low RH fuel cell operation are highly relevant to the DOE.
- Improved conductivity, high-temperature, and low RH membranes are included in the Hydrogen Program and DOE RD&D objectives. These are not the most critical material needs for enabling fuel cell commercialization.

Question 2: Approach to performing the research and development

This project was rated **2.1** on its approach.

- The PI knows that disulphide bonds and remaining chlorine atoms on cyclohexadiene are highly susceptible to hydrolysis (disulphine bonds) and platinum poisoning (chlorine), but chose to ignore this for the sake of "synthetic ease." Therefore, the reviewer does not understand the purpose of this research as it has neither reached the DOE's proton conductivity requirements, nor will it have the necessary durability. Furthermore, if it were to have succeeded, it is not apparent how the knowledge obtained would have been transferred to a more robust chemistry.
- The program is focused on the technical targets of increasing membrane conductivity over a wide operating range.
- Adding titania is questionable based on data presented on water uptake.
- Some mechanical properties are measures, but interpretation and relevance need to be clarified.

- The work is focused on model systems that have insufficient stability. The easiest synthetic path was chosen at a loss of relevance. Although the "right" crosslinking was mentioned, no argument was presented that the current work would be relevant to this.
- One concern is with the expected stability of the HC membranes from peroxide and free radical attack.
- Another issue is catalyst membrane integration when an HC membrane is used.
- The project seems focused on only one HC monomer. Are there others nearly as low cost that might work better?
- The approach of copolymerization with poly(ethylene glycol) (PEG) is a good idea for improving conductivity.
- The PI is applying relevant diagnostics such as water adsorption/desorption and dynamic mechanical analysis (DMA).
- The concepts being generated have extremely high swelling, and no viable path was presented to reduce swelling.
- Novel chemistry was based on polymerizing cyclohexadiene, and it is not clear how this would ever make an oxidative stable film. What advantages does this approach have over other HC technologies?
- The PI focused on a low-cost polymer for his membranes. The use of derivative forms poly (cyclohexadiene), however, is suspect; S-S bonds for crosslinking are prone to hydrolysis, and PEG is oxidatively unstable.
- The pursuit of polycyclohexadiene as an ionomer material is limited because the backbone will have poor durability in fuel cell environments. The addition of PEG as a block component and disulfur as a crosslinker have stability issues, but was at least addressed in as far as perfluoro PEG and other crosslinkers could be investigated. Still, the backbone polycyclohexadiene is unstable and the pursuit of these materials is unlikely to help achieve DOE targets particularly in the area of durability.
- The high water uptakes and stiff mechanical properties are unlikely to meet RH cycling requirements.
- The project focused too much on physical characterization of materials.

<u>Ouestion 3: Technical accomplishments and progress toward project and DOE goals</u></u>

This project was rated 1.9 based on accomplishments.

- The membranes did not meet DOE proton conductivity targets.
- The membranes will not meet durability needs due to known chemical weaknesses.
- Nafion® conductivity was matched, but neither the interim conductivity milestone of 30°C and 80% RH, nor the Year 3 decision point of 120°C and 50% RH, were met.
- Work proceeded along the "easiest" lines with loss of relevance. Even with the introduction of less appropriate PEG moieties, the performance did not meet the conductivity goals.
- No direct swelling data vs. water uptake have been shown yet.
- The membrane conductivity at 120°C is comparable to many other approaches.
- There is a concern as to why the polarization curves with titania in the Nafion® were so bad. This has been tried by others many times.
- The project team should be utilizing fuel cell testing resources sooner and more often for functional performance feedback and guidance.
- The conductivity has been significantly improved.
- Why does the addition of titania not reduce the ion exchange capacity (IEC)?
- The combination of high-swell and high-dry modulus is the worst case scenario for mechanical durability under RH cycling.
- Oxidative stability is a concern.
- New polymers were produced, but none of these met the performance metrics, and many were similar at best to Nafion® in conductivity under some conditions.
- Membranes were made and some characterization data was collected. Water swelling in some membranes was very high. Some results could not be explained (e.g., same water absorption isotherms at 25°C and 80°C). Some polymer components may not have the requisite chemical stability. No membrane attained the DOE target of 0.1 S/cm at 120°C and 50% RH.
- The project was unable to meet conductivity targets or significantly improve on Nafion®, and it has therefore been chosen for a no-go decision. The addition of titania as an additive or PEG as a block showed modest changes in properties, but nothing suggesting high-conductivity goals could be met with further effort.

<u>Ouestion 4: Technology transfer/collaborations with industry, universities and other laboratories</u>

This project was rated **2.3** for technology transfer and collaboration.

- Collaboration between the University of Tennessee (UT) and the University of Southern Mississippi (USM) is high (even the talk was split between the two). Other than that, there were no other partners with a role. Perhaps an industrial partner would have been beneficial to the program.
- The team does not include commercial stack developers/integrators.
- The participation of ORNL and USM has been helpful.
- Work seems to proceed with little evidence of direct collaboration.
- It is not clear what the role of ORNL has been. It seems the project could really benefit from more fuel cell testing expertise.
- Jimmy and Ken have a nice collaboration, but it would be nice to see some industry input.
- This project involves two universities and a national lab, but no industrial partners neither an automotive original equipment manufacturer (OEM) nor a membrane electrode assembly (MEA) manufacturer.
- The primary collaboration was with Ken Mauritz at USM, who performed some membrane characterization experiments.
- The project team comprises two teams, one for synthesis and the other for characterization. While this is a logical combination, the need for and value of characterization provided in this project is limited.

Question 5: Approach to and relevance of proposed future research

This project was rated **2.1** for proposed future work.

- A fundamental shift in chemistry is needed before the occurrence of further optimization of the reaction conditions or optimization of the composition.
- The PIs need to remove chemically weak points from membranes as soon as possible; otherwise the project is not relevant to the program and should be shifted to Basic Energy Sciences.
- The DOE project ends in August 2009.
- The project needs chemical durability data, such as Fenton's test, the open circuit voltage (OCV) hold test, and mechanical durability data, such as RH cycling.
- More attention to cost is needed.
- It is not clear what will be new in the synthesis routes that will improve progress towards the DOE goals for high temperature.
- The top priority should be to reduce extremely high water uptake.
- The project team should focus on making thinner membranes (~25 um) to approach area specific resistance targets.
- The project will be terminated, and wrap-up activities look reasonable.
- Future work lacked specifics as to how the PI will reach the DOE conductivity target. The project is concluding, so future work is not relevant.
- The project is 99% complete, making this category largely irrelevant. The future work proposed suggests pursuing similar electrolytes for Li batteries. This makes some sense as similar materials like PEG or polyethylene oxide are used commonly in these applications.

Strengths and weaknesses

Strengths

- A strong synthetic PI and an excellent membrane morphology PI are working on this project.
- The project team is using relevant diagnostics such as water uptake and desorption as a function of temperature and RH.
- This is a novel polymer system.
- The polymer will probably be low cost, but it might not have the required properties and durability.
- The project team is also using chemistry that allows reasonable control of blocks.

Weaknesses

- The chemistry chosen at the beginning of this project makes it a dead-end, which will be of little use to the fuel cell community unless it is modified shortly.
- The project shows a lack of relevance.
- There has been no fuel cell testing expertise on the project to provide valuable functional performance properties.
- The membranes have an extremely poor combination of high swell and high modulus, with no significant plans given for reducing swell. Adding titania doesn't appear to help much.
- It never looked like it would work, and it didn't after the first three years.
- The chemical durability of the PI's membranes is questionable. The inability to fabricate a membrane with high proton conductivity is a project weakness.
- The primary weakness is the use of a backbone not inherently stable in fuel cell operation and membranes of conductivity properties that are unremarkable.

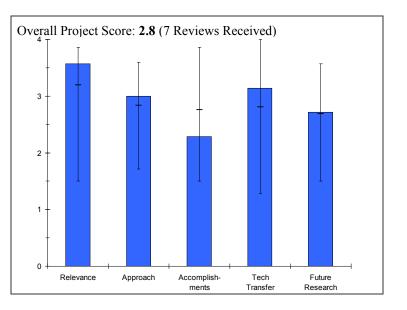
- The project is complete at this time. For future funding opportunities, chemistry building blocks must be changed and industrial partners should be brought in.
- The decision to terminate is appropriate.
- This reviewer concurs that the project will be terminated.
- This project is ending, but more fundamental membrane synthesis/fabrication work is recommended, with less emphasis on complicated/sophisticated characterizations (e.g., dielectric spectroscopy).
- For materials with poor chemical stability and questionable mechanical properties, these do not merit further investigation. This conclusion is also based on the observed properties reported and have been properly down-selected.

Project # FC-05: Advanced Materials for Proton Exchange Membranes

James E. McGrath and Donald G. Baird; Virginia Polytechnic Institute and State University

Brief Summary of Project

The objectives of this project are to 1) design, identify, and develop the knowledge base to enable proton exchange membrane films and related materials to be utilized in fuel cell applications, particularly for H₂/air systems at 100°-120°C/low relative humidity (RH); 2) nanophase separated hydrophilic-hydrophobic thermally stable multi-block copolymers; 3) correlate water diffusion coefficients with proton conductivity under partially hydrated conditions; and 4) relate thermodynamics of nanophase formation to ordered morphology and to conductivity, diffusivity, and novelmembrane self-assembly.



<u>**Ouestion 1: Relevance to overall DOE**</u> <u>objectives</u>

This project earned a score of **3.6** for its relevance to DOE objectives.

- The project is relevant to the objectives of DOE's Multi-Year R&D Plan.
- The initial activities were very much aligned to DOE's goal, but in the later part of the project, the focus became a bit distracted from the goal.
- Improvement of low RH membrane conductivity is critical to the success of DOE's Hydrogen research initiatives.
- This program supports the DOE R&D objectives.
- Work is in line with Task 1, Barriers A, B, and C, to develop membranes that meet all targets.
- The project goals align with DOE objectives, but the switch to polybenzimidazole (PBI)-phos acid block copolymers is not in line with objectives to be able to use these membranes in the presence of condensed water.
- The project goals of fabricating and characterizing a high-performance polymer electrolyte membrane (PEM) for high-temperature/low RH fuel cell operation are highly relevant to the DOE.
- The project aims to produce membranes that meet conductivity targets for proton exchange membrane fuel cell (PEMFC) commercialization. For that reason, every task of the project fits the DOE R&D objectives, and if successful, could be critical to the Hydrogen Program.

Question 2: Approach to performing the research and development

This project was rated **3.0** on its approach.

- The approach of making low equivalent weight (EW) HC based membranes with a high concentration of sulfonic sites is a good strategy for retaining membrane conductivity at low RH and high-temperature operational conditions.
- The approach of making nanophase separated sulfonic acid membranes to control membrane swelling and retain better conductivity is the right approach.
- The approach of surface fluorination of HC membranes to improve membrane compatibility with perfluorosulfonic acid (PFSA)-based electrodes is good.
- However, the approach of making PBI-biphenyl sulfone (BPS) copolymer does not fit with the goal of this project. Phosphoric acid-doped PBI can meet DOE's goal of low RH/high-temperature conductivity. So why bother making PBI-BPS copolymer, when it still needs acid doping? This approach is not good.

- The block co-polymer approach is very systematic and holds promise for meeting DOE goals.
- Obviously, applying the knowledge of the McGrath group to this problem allows one of the greatest minds in polymer science to systematically improve the science. Proton conductivity can be understood in terms of morphology and the other desirable properties of the film. Unfortunately, the target was only based on proton conductivity, and perhaps too much time was spent making the perfect PEM in the first three years.
- The approach has led to membranes that have good mechanical properties and durability, but less than desirable conductivity. The choice to pursue phosphoric acid doped membranes that will likely not be stable in contact with liquid water is problematic for automotive applications. Polymer processing work is a bit premature since polymers do not have desired conductivity.
- The approach of using biphenyl sulfone H form (BPSH)-type polymers is moderately innovative, but much of the project tasks appear to be logical extensions of the PI's prior research. There was no truly creative tasks and/or materials described in the PI's approach.
- Not enough attention has been paid to improving membrane conductivity, which should be focused on at this stage more than other membrane attributes.
- The approach has generally been the highlight of this project, since, in principle, the project should be able to generate a wealth of fundamental knowledge. A well-defined, multi-block copolymer with variable lengths of hydrophobic and hydrophilic blocks is an ideal system for realizing trends for conductivity and mechanical properties vs. variations in the two block lengths.
- The project begins with a polymer system where some rationale for expected durability does exist.
- In the absence of success with the original approach, other approaches were added (addition of PBI and fluorination processes) with dubious implications for cost and commercial acceptance.

Ouestion 3: Technical accomplishments and progress toward project and DOE goals

This project was rated 2.3 based on accomplishments.

- In terms of conductivity improvement, not much progress has been made towards the goal since last year.
- Except for Hydroquinone-Based Poly(arylene ether sulfone) (HQSH)-BPS, none of the membranes showed better membrane conductivity than Nafion®.
- However, under the DOE goal of 120°C and 50% RH, the conductivity of HQSH-BPS is very close to the Nafion® membrane, and significant conductivity improvement is needed to meet DOE's goal.
- This work gives insight into structure-property relationships for block copolymer ionomers. The demonstration of low XY swelling is important for durability in fuel cells. Conductivity targets were not met, but a systematic study of these systems should provide improved conductivity and valuable insight for future development work.
- Adequate proton conductivity was not demonstrated. Many other useful PEM attributes were achieved.
- Progress in increasing conductivity at low RH has been slow. Conductivity has not improved much over the course of the project. In general, these materials have conductivity which exhibits a higher dependence on RH than Nafion® conductivity. The team has not looked into the effect of the anisotropy of their membranes on conductivity.
- Many of the technical accomplishments were not connected to the overall goal of fabricating a fuel cell membrane with a conductivity of 0.1 S/cm at 120°C and 50% RH. Direct methanol fuel cell DMFC crossover and fuel cell performance data are not relevant. Similarly, it is not clear why acid doped BPSH-PBI blends and surface fluorination were studied. The effort was much too broad, without an organized plan to achieve the DOE conductivity target.
- Membranes have been developed that have reasonably good properties for fuel cell applications, as demonstrated by the fuel cell testing and durability testing; however, the conductivity just isn't where it needs to be.
- The ability to adjust both conductivity and swelling with block length was shown for multiblock copolymers.
- Multiblock copolymers did not meet conductivity targets at any temperature.
- A PBI-based system that demonstrates 80 mS/cm at 80°C without phosphoric acid (PA) is intriguing, but RH needs to be specified.
- Some idea of the cost implications for fluorination must be understood before conductivity/dimensional stability enhancements can be considered promising. As a fundamental study, however, this does offer some useful insight.

<u>Ouestion 4: Technology transfer/collaborations with industry, universities and other laboratories</u>

This project was rated **3.1** for technology transfer and collaboration.

- There is good interaction with different industry, academics, and national lab groups.
- The demonstration of large quantity polymer synthesis at Akron Polymer Synthesis (APS) is relevant to the focus of the project.
- The overall team has done well with the intended research on high-temperature membrane development.
- Work with an industrial membrane/membrane electrode assembly (MEA) developer would benefit this program.
- The project team is collaborating with national labs and industry.
- Collaborations were listed, but the actual collaborative work was not clearly identified in the project presentation.
- Effective use of technical abilities of partners has been made, particularly with LANL.
- Akron appeared to be successfully leveraged for membrane fabrication.
- The difference between Arkema and Giner contributions was not entirely established in the slide materials.

Question 5: Approach to and relevance of proposed future research

This project was rated 2.7 for proposed future work.

- Post-fluorination of random and block copolymers will not provide low RH conductivity of the membrane, and so they are not relevant to the goal of this project.
- High ion-exchange capacity (IEC) crosslinked polymers are known to be unstable under a free radical environment: therefore, crosslinking homo and multi-block copolymers may not be the right strategy to achieve a low RH/high-temperature membrane.
- The biphenyl system has potential for further gains in conductivity. The fluorination of polymers is an interesting approach for membrane stabilization.
- The wrap-up activities seem adequate.
- Future work covers a variety of areas. The reviewer suggests that future work focus on high IEC crosslinked materials.
- The listed future work was very general and non-specific. This project is ending, so "future work" may not be relevant.
- Future work plans are reasonable, and there is slight hope of reaching targets, but there is still a long way to go.
- Lowering EW of the multi-block copolymers in order to return to the original goals of the project is a worthwhile exercise.
- In general, the question of what controls conductivity at low RH (in particular for sulfonic acid PEMs) is not only good to address for this project, but could have been a great project unto itself if the DOE had begun three years ago. This is one of the fundamental questions that the DOE Hydrogen Program should answer.
- It would be interesting to see if future work would include non-PA PBI-based membranes.

Strengths and weaknesses

Strengths

- This is a new approach to solve the problem of low RH membrane conductivity.
- The synthetic method is novel, and it is a valuable contribution to the development of ionomer chemistry.
- The concept of nano-phase separation and correlating this fact to the membrane conductivity at low RH is a well-thought-out concept.
- This work gives insight into structure property relationships for block copolymer ionomers. Demonstration of low XY swelling is important for durability in fuel cells. Conductivity targets were not met, but systematic study of these systems should provide improved conductivity and valuable insight for future development work.
- This is one of the few projects to try and optimize all PEM properties.
- BPSH materials represent a class of polymers with some potentially useful/interesting properties.
- The PI exhibited enormous skill and expertise.

- The original approach allowed levers of control for membrane conductivity, dimensional stability, and mechanical properties.
- The original membrane concept had a previously identified rationale for stability.
- This incorporation of collaborations can competently produce membrane samples and perform testing.

Weaknesses

- The BPSH type HC ionomer seems to have limitation in membrane conductivity under low RH conditions.
- Anchoring BPSH to other base polymers, such as PBI, will not add any conductivity effect to the copolymer, unless the copolymer is doped with acid. This is not a viable approach and doesn't meet the goal of the project.
- Surface fluorination may help to improve the MEA interface, but it is not going to improve the membrane conductivity to the order of magnitude presently needed for BPSH-type polymers.
- It is not clear that this approach would ever have met the target, but a valiant effort was made nonetheless.
- Progress in increasing conductivity toward the target was low. The project lacked a focus on increasing the conductivity at high temperature and low RH.
- The obvious weakness is the PI's inability to attain the DOE's go/no-go conductivity target of 0.1 S/cm at 120°C and 50% RH.
- The project exhibits insufficient focus on strategies for improved conductivity.
- The original concept is unable to meet conductivity targets.
- The ideas generated after not reaching the conductivity targets might not be commercially accepted.
- The opportunity to fundamentally address low-RH conductivity for -SO₃H membranes was not taken.

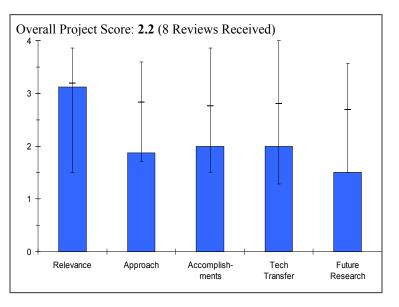
- It may be necessary to incorporate proton-conductive and water-retaining inorganic salts, such as hetropolyacid or phosphosilicic acid, to make the BPSH composite a more viable approach to improve membrane conductivity under low RH.
- Further development of crosslinked materials may not help in attaining the goal of the project.
- This project should be considered for continuation if possible.
- If the focus remains dual-use (for automotive and other applications), it is recommended that the project team delete the work on phos-acid doped membranes. If stationary systems become more of a focus, the phos acid doped PBI-block copolymer systems may be worth investigating.
- N/A since this project is ending.
- The project has ended, but hopefully the investigators can continue with other funding sources. With a tighter focus on strategies to improve conductivity, there is promise for development of high-performance materials.
- If this project were to continue, instead of scrambling for "what works," it would be interesting to see further progress framed in terms of fundamentals. For example:
 - What is responsible for conductivity at low RH? adjust such elements as EW, block lengths, processing solvent, and morphological parameters;
 - If fluorination works, why? Then an industrial partner could attempt to answer whether a low cost means exists to realize it; and
 - Further efforts to demonstrate stability are always good.

Project # FC-06: Protic Salt Polymer Membranes: High-Temperature Water-Free Proton-Conducting Membranes

D. Gervasio, C.A. Angell, R. Marzke, and J. Yarger; Arizona State University W. Youngs; University of Akron

Brief Summary of Project

The objective of this project is to make proton-conducting solid polymer electrolyte membrane (PEM) materials having 1) high proton conductance at high temperature (up to 120°C); 2) effectively no co-transport of molecular species with proton; 3) reduction of fuel cell overvoltage; and 4) good mechanical strength and chemical stability. PEMs are being made based on "solvent free" protic ionic liquid concepts, which can be used to model membrane factors such as stability and conductivity, and to act as plasticizers in membranes. Acid and base moieties and polymers are varied to optimize properties in two kinds of PEMs. Proton conductivity will be characterized by electrochemical impedance spectroscopy from -20° to 120° C.



Question 1: Relevance to overall DOE objectives

This project earned a score of **3.1** for its relevance to DOE objectives.

- High-temperature membranes, which do not rely on water and function at all temperatures, would be an amazing breakthrough for the fuel cell community especially for vehicles.
- The relevance of this project is high. Conductivity at low relative humidity (RH) and high temperature has been one of DOE's key technical targets.
- The project is highly exploratory in nature, and although the objectives are stated in accordance with DOE objectives, the actual work is not proceeding along those lines.
- The project addresses two of the major barriers: durability and performance.
- Developing a PEM that does not rely on water for proton transport would enable higher temperature operation and a potentially simpler water management system.
- This project is very relevant. It works on removing water as the limitation of membrane performance. This is a critical barrier for use of fuel cells in vehicles. The observation of better catalytic activity is also important. The project is aimed at very relevant objectives; however, in the execution, the relevance sometimes seems to be lost. It would be best to simply focus on the method of proton conductivity first, and then make the appropriate membranes. Some of the materials chosen are unlikely to be stable, so the relevance of choice of materials might be questionable. This does not matter if the basic mechanism of proton conduction is elucidated.
- The reviewer has some doubts about the project relevance. The reviewer thought the project goals were to fabricate and characterize a high-performance polymer electrolyte membrane for high-temperature/low RH fuel cell operation. The PI wrote that his goal was to fabricate an anhydrous proton-conducting electrolyte membrane. Such a membrane would operate at a very high temperature. It is unclear whether this is what DOE wants. The reviewer questions this goal because a fuel cell operating temperature of 275°C is outside the targets set in the DOE Multi-Year R&D Plan.
- Membranes with improved conductivity that function under high-temperature/low-RH conditions are included in the Hydrogen Program's and DOE's RD&D objectives. These are not the most critical material needs for enabling fuel cell commercialization.

Question 2: Approach to performing the research and development

This project was rated **1.9** on its approach.

- While the concept is an excellent one, the PI may not be pursuing this in the best way. The first step should have been to screen and pick the best protonic salt based on proton conductivity. The second step should have been immobilizing the best salt to prevent water solubility, while maintaining the proton conductivity. The third step then should have been the fuel cell experiments. Too much time was spent on the third step and not enough on the first two.
- The original ionic liquid formulations did not meet DOE targets.
- The new indium tin phosphate (ITP) approach shows high conductivity, but crossover and mechanical strength of the pure ITP may be issues. Blending with poly-vinyl pyridinium phosphate (PVPP) may reduce crossover, but conductivity may also be reduced.
- It is unclear what membrane/electrode interface issues will arise with an ITP membrane, or how they will be addressed.
- It is interesting to look at ITP materials and composites, but the conductivity of these compounds appears to be substantially below what is needed. There appears to be no clear path for improvement, so the team should, instead, switch to some other as yet unidentified compounds.
- The concept of a non-aqueous proton conductor is good, but the approach seems to be too diverse and unfocused. At such an early conceptual stage, it might be more productive to take a model system and study it in depth to better understand the fundamental prospects and limitations. This should be combined with bonafide material property and even fuel cell functional property evaluation to prove feasibility and identify the most significant problem areas.
- Protic ionic liquids (pILs) have demonstrated the ability to conduct protons.
- There has been too much focus on fuel cell testing, and not enough focus on proving proton conduction in actual films.
- ITP is not recommended because of H₃PO₄ release and likely severe performance loss over time.
- The approach is okay, but seems to be unfocused in many places and trying to do too much at once. The ITP work seems like a diversion. Showing such apparently poor polarization curves is not very helpful at this time. The project team should concentrate on the proton conduction mechanism first, and then add the other issues.
- The use of pILs is an interesting approach. Unfortunately, the PI was not able to achieve the DOE conductivity target of 0.1 S/cm at 120°C and 50% RH with such materials. It was not clear why the PI switched to the use of ITP. While a purely inorganic film (very thick) met the DOE conductivity target, an ITP/polymer composite exhibited a low conductivity (0.01 S/cm). The reported fuel cell performance of the ITP membrane electrode assembly (MEA) was very poor. The focus of looking for membranes that operate without water at 275°C does not seem to be appropriate for this DOE program.
- The project has significant weaknesses, but may have some impact on overcoming barriers. The investigation of pILs is of interest from a fundamental proton transport standpoint, but is unlikely to yield materials suitable for commercial applications. The addition of ITP adds a material that shows significantly more promise, but these studies do not build on previous studies, and seem like a subset of results already reported by Hibino and coworkers.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated 2.0 based on accomplishments.

- Decent progress was made in finding a protonic salt and immobilizing it with PVPP; however, more work should have gone into further optimization of this system with *ex situ* testing such as PC and water soak testing, and not fuel cell testing.
- IV Curves with an OCV of 0.8V and 30 mA/cm² at 0.4V does not help the fuel cell community, nor does it help develop this material from a basic membrane understanding perspective.
- The original membrane technology did not meet the DOE targets.
- Target conductivity has been realized with pure ITP, but ITP issues are not insignificant.
- It would appear that the current emphasis on doped tin metaphosphates may not be effective at room temperatures. It is also not clear how ionic liquids could lead to an appropriate fuel cell membrane. This work

appears to be an extension of some other work by some of the investigators on ionic liquids. The relevance to the Hydrogen Program is unclear.

- There is a fundamental problem of some kind preventing their oxygen reduction reaction (ORR) with the protic salt-based electrolyte. The cyclic voltammogram on slide 13 may imply a fundamental issue with catalyst poisoning.
- Fuel cell performance examples are low by up to two orders of magnitude. Something is very wrong, and the PI should get help to understand if this is just their inexperience or a fundamental limitation with the technology.
- The claim on slide 6 to have made a neat ITP membrane with conductivity that exceeds the DOE targets by such a large amount, at 120°C and totally dry, is remarkable. The presentation should have focused on this, and then tried to explain why fuel cell performance on slide 29 is so terribly bad. Is the water generated in the fuel cell hurting the electrolyte?
- The fuel cell tests showed extremely poor results.
- The liquid electrolyte conductivities do not meet DOE targets, bringing to question why immobilized ILs have any chance to meet targets.
- ITP results must be verified and proved stable.
- Good progress has been made in making polymers. There are concerns about stability, particularly with regards to the pyridinium ions which are known to be easily oxidized; however, the structural effects on proton conduction mechanisms should be useful.
- The DOE conductivity target at 120°C and 50% RH was not met. Too much of the work focused on nonmembrane work, e.g., cyclic voltammetry studies of ORR, hydrogen pump experiments, and studies of liquid electrolytes. For non-leachable membranes, the proton conductivity was quite low (<10⁻² S/cm, as shown in slide 24).
- There are several scientifically interesting results presented. In particular, the high open circuit voltage (OCV) demonstrated for some liquid studies and voltammetry showing currents at high potentials, although these are not represented in any of the polarization curves presented.
- The results for liquid systems show poor performance and no clear path for stable, realizable systems.
- The ITP-based systems show similar results compared to those shown by Hibino with no clear insight/rationale as to how or why further improvements to this system should be expected by this team's work.

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated **2.0** for technology transfer and collaboration.

- Some collaboration exists with the University of Akron (UA), but the reviewer does not fully understand their role in the project.
- Collaborations do not include stack developers or integrators.
- Collaboration was not addressed in this presentation, but may be presumed to have occurred.
- It is not clear what the contributions of the other, limited collaborators were.
- There is a collaboration with UA, but the project could benefit with industry collaboration and support from someone with MEA preparation experience.
- The collaborations are okay, but could be better. It is not clear who is doing what or what kind of feedback is coming from the Florida Solar Energy Center (FSEC) and partners.
- The collaborative work appears to be minimal.
- There is some collaboration. This topic is not particularly relevant for grading this project.

Question 5: Approach to and relevance of proposed future research

This project was rated 1.5 for proposed future work.

- Future work should focus on the fundamentals of this material and really understanding the proton mechanism and its potential in an idealized form. An outside modeling group could potentially be involved to find out.
- This group should not conduct fuel cell testing until acceptable proton conductivity and water non-solubility are achieved.
- Future work should focus on ITP and blends.

- Much of the future work seems to continue study of the failed ionic liquid systems.
- The work is highly and broadly explorative. Program reformulation is required to focus on materials that can actually serve as fuel cell membranes. In view of the poor cell performance of just the ionic liquids, it is not clear why the work merits further effort. A better case needs to be made.
- The project should focus more on why the electrode kinetics are so bad. It is a much bigger issue than the membrane conductivity, and it needs to be understood before more effort is put into the membrane alone. The membrane has to be integrated with the catalyst and other components to work effectively, but when the combined system is one to two orders of magnitude below expected performance, it is not simply a matter of tweaking the MEA making. Something more fundamental may be at play that needs to be understood.
- There has been too much focus on fuel cell testing.
- The decision to focus on non-leachable PEMs is good.
- Before too much work is done on ITP, the PI should be absolutely sure that it is not releasing phosphoric acid.
- The future plans are very unclear. It is unclear where this project is going. The ITP work is most confusing.
- The future work is suspect. pILs do not seem to work. ITP is not a viable option when mixed with a polymer binder (conductivity is too low). The PI should not focus on anhydrous fuel cell operation at a very high temperature. It seems that the PI has abandoned the DOE target of 0.1 S/cm at 120°C and 50% RH.
- The proposed future work seems to hinge critically on polyphosphazene development, poly vinyl pyridine (PVP) and PVPP as binders with ITP. These aspects were not well explained during the presentation, and are somewhat confusing from the presentation text. It seems that the motivation is based on an assumed interaction between ITP and these polymers with no presented basis. ITP is not an ionic liquid it is a solid, which is key in the way it behaves in terms of its conduction process. If the polymer was co-synthesized, or the ITP particles dissolved, the positive properties observed would likely be destroyed. If the ITP particles remained intact, the polymer would serve only as a binder and would not be expected to result in positive effects.

Strengths and weaknesses

Strengths

- The concept of immobilized protonic salts is a great concept and should be funded by DOE.
- The project team took an imaginative approach.
- The concept is high risk, but with a potentially high payoff.
- It is one of the few projects that focus on anhydrous proton conductors.
- The project exhibits very relevant goals and objectives. The project addresses issues that are of fundamental importance to the program.
- The PI seems to be well versed with a variety of analytical electrochemical techniques.
- The team is investigating non-typical materials with interesting properties.

Weaknesses

- The approach is weak, with too much emphasis on fuel cell data.
- Poor materials performance suggests that the approach is not going to lead to the desired results.
- The team does not have enough experience with whole MEA performance requirements.
- No fundamental work has been done to suggest that pILs have the potential to meet DOE proton transport resistance targets.
- The project team is too scattered; it is trying to do too much. It does not help the cause to show polarization curves that are not good without adequate explanation of why they are so poor.
- The PI appears to be focusing on H₂/O₂ fuel cell operation under anhydrous conditions at 275°C, but the DOE fuel cell operating conditions were 120°C and 50% RH.
- A lack of scientific basis for the guidance of future work is a major weakness. The poor OCV of the ITP systems and the liquid nature of the pIL systems result in materials that are further weaknesses.

- The project team should add a modeling group to understand the full potential of this material.
- The project team should spend more time on the fundamental side and material development.
- The project team should stop doing fuel cell experiments.

- So far, the results do not support continued work on the ITP blend materials.
- The project team should focus on establishing a solid, credible benchmark performance with the ITP system, and go from there.
- There should not be any more fuel cell testing until stable membranes are prepared with conductivity within 1/10 of DOE target conductivity.
- The project team should concentrate on making solid polymer electrolytes that have the required conductivity and forget about the rest for the moment. Any changes in the structures should be designed to elucidate the mechanisms of conduction.
- The PI did not present any evidence that the use of tethered acid and base groups will yield a membrane with the requisite proton conductivity at 120°C and 50% RH. The PI needs to provide a clear and convincing path to achieve high conductivity. At the present time, it is questionable if this project will yield useful fuel cell membranes.
- The addition of ITP adds a relevant material to the study; however, these results are essentially completely independent of prior reported pIL studies and do not show signs of advancing beyond other reported studies on similar systems (Hibino). Arguments can be made for this project as meeting DOE conductivity targets based on conductivities of phosphoric acid, but it reflects a poor metric for the go/no-go decision on these projects as this project should have been held to a higher standard.

Project # FC-07: Fluoroalkyl-Phosphonic-Acid-Based Proton Conductors

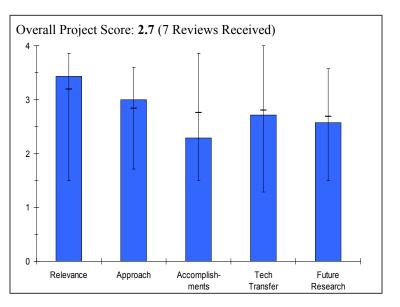
Stephen Creager and Darryl DesMarteau; Clemson University Oleg Borodin, Grant Smith, and Gregory Voth; University of Utah

Brief Summary of Project

The overall objective for this project is to provide new electrolyte materials for use in next-generation hydrogen fuel cell-powered sources, especially for automotive transportation applications. The specific objectives of this project are to 1) synthesize and characterize new proton-conducting electrolytes based on the fluoroalkylphosphonic acid (FPA) functional group; and 2) create and apply new computer models to study proton conduction in FPAbased electrolytes.

Question 1: Relevance to overall DOE objectives

This project earned a score of **3.4** for its relevance to DOE objectives.



- The project supports DOE's Hydrogen Program.
- All the aspects of this project are aligned to the hydrogen vision and DOE RD&D objectives.
- This program supports the DOE R&D objectives.
- The relevance of the project is undeniable, but it may be time to do a risk assessment.
- The program addresses important questions regarding proton-conduction mechanisms and polymer structures. The combination of synthesis and modeling is very powerful and appropriate for addressing the objectives of the Hydrogen Program.
- The project addresses appropriate DOE barriers. Membranes that operate under hotter and dryer conditions are critical to fuel cell vehicle commercialization.
- The project intends to develop a new family of proton-conducting membranes for proton exchange membrane fuel cell (PEMFC) applications. As such, the project is entirely relevant to DOE R&D objectives and maintains the possibility of becoming important.

Question 2: Approach to performing the research and development

This project was rated **3.0** on its approach.

- The approach of this project is very valid.
- The project is related to the common belief that the phosphonic acid polymers may have better low relative humidity (RH) conductivity than sulfonic counterpart as proton transport occurs without any assistance of water.
- The approach of studying the model compound is a good way to predict the behavior of phosphonic acid fluoropolymers.
- The use of phosphonic acids in fuel cell membranes has been proposed many times. This is a well designed, systematic study which can show if this is a promising path.
- The approach appears systematic, but conductivity targets are not being met. There may be too much emphasis on the computer models. It is unclear why the PBI approach is not being pursued.
- The approach is okay, but perhaps light on the synthesis and measurement part. The modelers seem to be far ahead of the ability to make and measure the materials. The lack of investigation of bases other than the amphoteric phospohorus groups and water is curious. One would think it probable that the modelers could

easily throw in some heterocylic bases to the mix to see what effect would be expected. The program seems a bit inflexible.

- The approach is focused on trying to obtain conductivity under hotter and drier conditions. Modeling is useful, but not developed enough to provide results to guide the synthesis effort yet.
- The general approach of employing perfluorophosphonic acid membranes, supported by computational studies and examination of model compounds, is sound.
- The beginning approach of this project was simple and strong, i.e. replace the sulfonic acid group in a perfluorosulfonic acid (PFSA) membrane with a phosphonic acid at the termination point, to see whether there are advantages for conductivity, particularly as they relate to enhanced proton hopping.
- The project has sought to verify directions for enhanced conductivity through both molecular dynamics modeling and model compound studies.
- While the model compound studies do compare phosphonic/phosphinic species to sulfonic, the molecular dynamics studies unfortunately do not.

<u>Ouestion 3: Technical accomplishments and progress toward project and DOE goals</u></u>

This project was rated **2.3** based on accomplishments.

- So far, the progress made has not been focused towards the DOE goal of low RH membrane.
- Very little progress was made for the development of synthetic pathways for phophonic acid bearing fluoropolymers.
- The conductivities of the polymers are the same as the Nafion® membrane. So far, no improvement of the phosphonic acid approach has been demonstrated.
- While conductivity targets were not met, progress was made in preparing lower equivalent weight (EW) samples and understanding the ionomer morphology.
- It appears to be a high-risk project, as the conductivity target was not met. The membrane became brittle and failed during conductivity testing at BekkTech.
- Much progress has been made in synthesis and modeling. The results are useful in the study of proton transfer mechanisms. There seems to have been some disconnect with the Topic 2 program at the Florida Solar Energy Center (FSEC).
- The team has prepared new phosphinic and phosphonic acid derived membranes. Conductivity of these materials has not been as high as desired, and has been substantially lower than Nafion®. Improvements in morphology have not yet led to the improvements in conductivity deemed necessary. Decreased EW from the two acid groups on the phosphonic acid does not seem to be as beneficial as would be expected; a more detailed comparison of phosphinic and phosponic acid membranes may shed some light on this.
- Some progress has been made, but conductivity is still far below targets.
- Molecular dynamics were able to agree that certain model compounds would show proton hopping (CF₃PO(OH)₂), but not for all model compounds that showed proton hopping.
- Desired membrane structures appear to have been produced, but further chemical identification would be helpful to confirm this.
- The project failed to achieve conductivity targets. It is clear that further optimization in terms of casting solvent, EW, means of crosslinking, etc. need to be pursued aggressively. In some cases, this is necessary just to be able to do a conductivity measurement.

<u>Ouestion 4: Technology transfer/collaborations with industry, universities and other laboratories</u>

This project was rated **2.7** for technology transfer and collaboration.

- Good collaborations were carried out between different research groups.
- Good coordination has been carried out between industry, national labs and the University of Utah.
- The collaboration with Giner is a plus. Collaboration with a PFSA manufacturer will help a lot in moving this program forward more quickly by allowing the controlled preparation of low EW membranes and other samples for conductivity optimization.

- This is a good fundamental study; however, more consideration is perhaps necessary with keeping the real customer in mind. The project team should go back and make the same recommendation as was made last year, to consider collaboration with an industrial partner.
- Good collaborations have been made with lots of good groups, but the collaboration with FSEC and its subcontractors seems not to have been good. It should be expected that materials like these will behave differently from Nafion®, and there should have been much communication to avoid the problems that occurred.
- Collaboration between team members has been good. Collaboration with High Temperature Membrane Working Group and others is apparent.
- An industrial partner could be extremely useful to this membrane fabrication aspect of this project. The services provided by Giner and JEOL were not applicable towards membrane fabrication.
- Perhaps greater use of nuclear magnetic resonance (NMR) expertise could have been applied towards the membrane samples.

<u>Ouestion 5: Approach to and relevance of proposed future research</u>

This project was rated **2.6** for proposed future work.

- The combination of sulfonic and phosphonic acid in the same polymer will result in lowering the effective EW of the ionomer. Instead, why not to use low EW sulfonic acid polymer?
- Crosslinked polymers are not stable in a free radical environment. Why pursue the crosslinked polymer route?
- The researchers seem to be on the right path to optimize this system. Greater focus should be placed on lower EWs and methods to increase phase separation (domain structure).
- The risk level for the proposed future work is unclear.
- Future plans are not well laid out and do not overcome the limitations of the system.
- Plans for work with higher acidity fluoro-sulfonimides are intriguing.
- Incorporating superacid moieties into perfluorophosphonic acid membranes is a logical path to improving membrane conductivity.
- Introducing the sulfonimide chemistry would likely prove to be a distraction. This might be better contemplated after 3M has finished its project on similar chemistry.
- It is agreed that crosslinking needs to be a future activity, but particular modes of crosslinking should be targeted.

Strengths and weaknesses

Strengths

- Phosphonic acid based fluoropolymer is a novel route to address low RH membrane conductivity challenges.
- There is a good combination of synthetic and modeling groups to address the wide scope of this project.
- The use of phosphonic acids in fuel cell membranes has been proposed many times. This is a well designed, systematic study which can show if this is a promising path.
- The project uses an approach of fundamental study supported by modeling and experiments.
- The project exhibits good fundamental studies on important issues, with good synthetic skills and strong modeling.
- The project has a strong team of theorists and experimentalists.
- It seems to be a well-thought out and logical approach to achieving high conductivity at low RH.
- The project has a simple and strong premise.
- The project has the ability to predict conductivity using molecular dynamics and model compound studies.
- The project also has the ability to still produce desired membrane chemistry despite earlier setbacks related to keeping monomers in solution.

Weaknesses

- As expected, phosphonic acid fluoropolymers did not show high membrane conductivity under low RH conditions.
- The addition of sulfonic acid groups to phosphonic acid polymers is not expected to enhance proton conductivity of the membrane to the same extent as low EW sulfonic acid polymers.
- This program needs to show greater progress towards meeting conductivity goals.
- The project requires improved gap analysis and consideration for practical use.
- It is perhaps weak on measurements and definitely somewhat inflexible in trying to overcome limitations.
- The relative knowledge of perfluorophosphonic acid materials is not as developed as that for sulfonic acid derivatives.
- Despite a promising approach, a lack of positive results so far makes the technical viability questionable.
- The lack of industrial collaboration made it tough on the project to be more nimble about optimizing membrane fabrication such as casting solvent and EW.
- There is a lack of molecular dynamics comparison to sulfonic acid groups.
- More information about the membranes should be reported, including swelling, NMR identification, and perhaps mechanical/thermal characteristics.

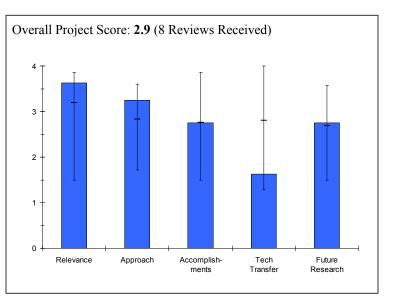
- The crosslinked membrane approach may not give free radical stability to the membrane, so there is no point in carrying out this task.
- It will be interesting to see whether acid-containing inorganic composites with phosphonic acid-based fluoropolymers will help in enhancing the membrane conductivity.
- I would like to see a greater focus on lower EWs and methods to increase phase separation (domain structure)
- The team should consider a membrane with PBI.
- While performance of perfluorophosponic acid derivatives is of interest, the poor conductivity seen to date suggests that this may be more appropriate for Basic Energy Sciences-type studies rather than the more near-term applications oriented EERE funded projects.
- Temptations to dive into other forms of chemistry beyond the original project premise should be avoided.
- An industrial membrane collaborator should be added to optimize the membrane faster.

Project # FC-08: Rigid Rod Polyelectrolytes: Effect on Physical Properties Frozen-in Free Volume: High Conductivity at Low RH

Morton Litt; Case Western Reserve University

Brief Summary of Project

The objectives of this project are to 1) synthesize polyelectrolytes that reach or exceed DOE low humidity conductivity requirements; 2) use materials and synthetic methods that could lead to cheap proton exchange membranes; 3) understand structure/property relationships in order to improve properties; and 4) develop methods to make these materials water insoluble and dimensionally stable with good mechanical properties. Case Western Reserve University has decided to work with poly(pphenylenes) with one and two sulfonic acids per ring. These have lower equivalent weights (EWs) and cannot hydrolyze.



Question 1: Relevance to overall DOE objectives

This project earned a score of 3.6 for its relevance to DOE objectives.

- With a stable and low relative humidity (RH)/high temperature, the membrane supports the Fuel Cell Program at DOE.
- The relevance to obtaining low RH/high-temperature membranes is high.
- The team took a well-formulated and innovative approach and fully supports DOE objectives.
- Developing membranes with high conductivity at low RH is critical to automotive proton exchange membrane fuel cell (PEMFC) commercialization.
- This program supports the DOE R&D objectives.
- This work is in line with Task 1, Barriers A, B, and C to develop membranes that meet all targets.
- It is a relevant project with an out-of-the-box concept.
- Membranes with improved conductivity that function under high temperature / low RH are included in the Hydrogen Program and DOE's RD&D objectives. These are not the most critical material needs for enabling fuel cell commercialization.

<u>Ouestion 2: Approach to performing the research and development</u>

This project was rated **3.3** on its approach.

- The project is another DOE funded HC membrane using poly(biphenyl [di]sulfonic acid) membranes. While the concept is worthwhile, the reviewer does not see this as a long term solution to fuel cell membrane commercialization.
- The performance is too low, the cost is too high, and the membrane lacks the required durability (the membrane is water soluble or disintegrates in water).
- The rigid rod structure is intended to provide permanent volume for water, even at low RH. Conductivity results are very good.
- Mechanical and chemical durability have not been sufficiently addressed.
- The rod polymers are very promising. The project team needs to construct some fuel cell-type membranes to verify how these would function in an actual fuel cell configuration.
- Trying to improve mechanical stability is an excellent approach.

FY 2009 Merit Review and Peer Evaluation Report

- The team has taken a very novel approach towards producing a highly conductive polymer.
- This is probably one of the few legitimate hydrocarbon films that has a shot at achieving program objectives. The team is currently concentrating on making water insoluble films.
- This project has an interesting concept; however, there are uncertainties about the risk level for this approach.
- The high conductivities of the novel ionomers presented are promising for developing materials with decreased conduction losses. Developing ultra-high acid loaded polymers is interesting and has largely been shown viable through the approach presented. The focus needs to shift further to producing materials with improved mechanical properties.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated 2.8 based on accomplishments.

- Proton conductivity targets were met with a water soluble membrane or a membrane which disintegrates in water. Benchmark material used by the PI is Nafion® 117. For the amount of money spent by DOE, the reviewer does not see anything in this presentation that is unique or has not already been attempted.
- Excellent conductivity has been achieved.
- Mechanical and chemical durability have not been sufficiently demonstrated.
- Perpendicular conductivity is presumed to be higher than the in-plane conductivity, based on the rod orientations, but this assertion needs to be demonstrated experimentally.
- There were a few new ideas for mechanical stabilization via copolymer development, but there was little new data, and little progress toward making a membrane that is mechanically stable in water.
- The conductivity results are very impressive. The work towards producing materials that can be tested in fuel cells should be accelerated. The oxidative stability of the pendent aliphatic groups should be studied.
- Very high proton conductivities were demonstrated, and the project comfortably met the go/no-go criteria.
- The team performed a good analysis and material characterization; however, physical properties are major limitations now.
- There were a few more "new results" in this year's presentation compared to the prior year's presentation, but there is still less progress advancing this promising area of science than would be expected at this funding level. The graft copolymer approach shows some promise at improving properties, but further advances are necessary in the area of mechanical properties/durability.

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated **1.6** for technology transfer and collaboration.

- Collaboration with outside companies remains non-existent.
- There were no industrial collaborators because the membrane is at a very low level.
- The program should have had more collaborators from the beginning.
- There seems to be very little outside collaboration, although "interest from GM and 3M" is encouraging.
- Collaborations were not addressed in the presentation, and cannot be judged from the material provided.
- Professor Litt could benefit significantly by collaborating with experts in block polymer synthesis.
- It would be beneficial to this team to work with an industrial partner who can do a more in-depth evaluation of these materials
- Interest from 3M and GM is not the same as working with 3M or GM. The PI must involve industrial collaborators who can give relevant advice and aid in the commercialization of the material.
- The project may benefit from collaboration with any of the major industry partners.
- There have been relatively few interactions; however, they are not particularly needed at this point in time.

Question 5: Approach to and relevance of proposed future research

This project was rated 2.8 for proposed future work.

- Future work is as expected for this type of material, e.g. increase molecular weight (MW) and graft copolymers. One highlight would be to use these ionomers with Professor Pintauro's electrospinning technique.
- More work on the mechanical and chemical properties of the materials should be done. Approaches to solving these issues are not compelling.
- Future work is well planned and builds on the present results.
- The proposed focus of copolymerizing sulfonated poly(p-phenylenes) with non-soluble copolymers is warranted.
- The focus on making higher MW polymers is also directionally correct.
- The grafting work does not seem to show much promise.
- The project shows very good direction towards improving mechanical properties, although chemical stability (oxidative) should be evaluated. More emphasis on fuel cell testing would be appropriate at this stage.
- It really looks like a serious effort is being made to make these materials practical.
- The risk of the proposed approaches for improving mechanical properties is not known.
- Work should move beyond the current studies suggested involving an increasing degree of sulfonation. The past year showed advances in this area without major impact on performance. The suggested approaches that involve copolymer synthesis by Suzuki reactions are quite reasonable. No direction is shown as to the approaches that will be followed, but rather a list of many possible studies is presented.

Strengths and weaknesses

Strengths

- There is a potential for collaboration with Professor Pintauro; the electrospinning technique is very unique and could be of high value.
- It is an innovative approach that actually works.
- Professor Litt has demonstrated the best conductivity of High Temperature Membrane Working Group projects.
- The conductivity results are very impressive.
- There was good emphasis on understanding structure-property relationships.
- The hydrocarbon material was very highly proton conductive.
- The project team took an out-of-the-box approach, and exhibits a fundamental understanding of the mechanism.
- Extremely high conductivities were demonstrated.

Weaknesses

- The chemical backbone is not unique; sulfonated polyphenyl has been extensively studied and does appear to have the inherent properties needed for fuel cell vehicle membrane requirements.
- This project desperately needs partners for synthesis and durability issues.
- The project shows no obvious weaknesses.
- Poor polymer synthesis expertise to make high MW copolymers.
- There are still issues with making water insoluble materials.
- This project could perhaps use a more holistic approach, where all requirements are addressed relatively simultaneously.
- This project is very slow in advancing the technology. The particularly impressive conductivity results are now more than two years old, and relatively little has happened in advancing these materials since their creation.

- At this funding level, more output is expected. The focus should be on creating a membrane with a relatively high proton conductivity and decent mechanicals. This would speed up collaboration with Professor Pintauro.
- This work is yielding excellent results. Fuel cell testing should be planned, and equipment made available to do this.
- The project team should obtain through-plane conductivity data because membranes are not isotropic.
- The project team should to add more polymer synthesis expertise to the project.
- Work with an industrial partner who can do more in-depth evaluation of these materials would be beneficial to this program.

- More morphological studies and RH and temperatures cycling are necessary.
- These synthesis studies are often slow and laborious, but the focus could be modified to focus on more processable systems as mechanical properties seem to be a limitation of these materials. These are extremely promising materials, and it is suggested that the project team introduces a separate mechanical component (either through support incorporation or producing blocks) and/or some backbone flexibility without diluting acid concentration substantially (at least within the conducting domain).

Project # FC-09: NanoCapillary Network Proton Conducting Membranes for High Temperature Hydrogen/Air Fuel Cells

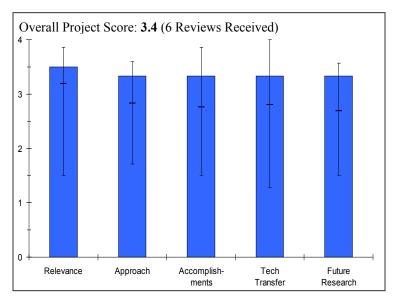
Peter Pintauro; Vanderbilt University Patrick T. Mather; Syracuse University

Brief Summary of Project

The objective of this project is to fabricate and characterize a new class of NanoCapillary Network proton conducting membranes for hydrogen/air fuel cells that operate under high-temperature, low humidity conditions. The 2008-2009 project goal was to fabricate membranes with a proton conductivity of 0.10 S/cm at 120°C and 50% relative humidity (RH) in preparation for the Year 3 DOE go/no-go decision.

Question 1: Relevance to overall DOE objectives

This project earned a score of **3.5** for its relevance to DOE objectives.



- The project is aligned with DOE's RD&D objectives.
- The focus of this project is to develop a low RH membrane, which is aligned with the hydrogen vision.
- All the tasks in this project are focused towards the low RH, high-temperature membrane initiative.
- This project is very relevant to DOE's objectives, and on track to meeting all of them.
- The program investigates novel ways of making membranes with controlled channel structures of perfluorosulfonic acid (PFSA). This method provides interesting ways of making membrane structures; however, it is not clear how this will work in the membrane electrode assemblies (MEA) and the Norland embedding material must be suspect if it is a polyurethane. Although the program is not very profound in its goals and objectives, it is of considerable benefit to the Hydrogen program.
- The project is aligned with DOE goals and targets and addresses appropriate barriers.
- This project fully supports DOE RD&D objectives by attempting to create a novel membrane for proton exchange membrane fuel cells (PEMFC). If successful, it will be critical to the Hydrogen Program.

Question 2: Approach to performing the research and development

This project was rated **3.3** on its approach.

- The approach of transporting protons through proton conductive fibers is interesting.
- The concept seems to be an inverse concept of reinforced membrane, and the non-conductive NOA63 seems to be a good mechanical reinforcement material.
- The limitation of proton conductivity in 3M 733 equivalent weight (EW) material indicates that densification of the fiber is needed.
- The use of sulfonated polyhedral oligomeric silsesquioxanes (SPOSS) seems to be boosting the proton conductivity.
- This is an interesting, almost systematic approach, by decoupling conductivity and mechanical strength. The project team needs to incorporate fuel cell level testing and understand the impact of trace impurities, thermal cycling, and robustness of the membrane over longer periods of operations.
- The approach is slightly pedestrian beyond the initial premise. One would like to see more work on variation of the channel dimensions, EW, and other additives besides SPOSS. There is a suspiciously empirical feel to this

that is troubling. One would like to see a bit more fundamental objectives, such as the mechanism of proton transport. Also, there really is no mention of how to make these work with electrodes.

- The project team changed course away from polysulfones when it was seen that they would not meet the 120°C target and moved to PFSA materials. The approach is flexible and may be useful for other ionomers as well as PFSAs.
- The team took a very well-organized approach to addressing technical barriers, and it was logical throughout.
- While some doubts still exist about whether the volume consumed by the non-conducting resin will prevent commercialization, the approach still remains simple and novel: electrospun PFSAs provide conductivity while the embedded resin provides mechanical support.
- This year's approach was excellent; the electrospinning of PFSAs was well worthwhile.

Ouestion 3: Technical accomplishments and progress toward project and DOE goals

This project was rated **3.3** based on accomplishments.

- Good progress has been made during the last year.
- Achievement of the DOE goal by a sample 4 mm thick NFN-02 is impressive.
- The spinning method seems to be very versatile and capable of making fiber with many different ionomers.
- The team has made impressive progress and is on track to meeting all its objectives.
- The team has made good technical progress in achieving the set objectives, but it needs to set some more ambitious goals for the future otherwise, this will just be another membrane that is not quite as good as Nafion[®]. The mechanical properties are described as good or better without any discussion of what is wanted. Some better thought into this would be good.
- The project team met the very aggressive DOE milestone of 0.1S/cm at 120°C and 50% RH. Flexibility of the approach increases chances of meeting all the DOE membrane targets simultaneously.
- So far, the project is meeting all its milestones, and the membranes also have good mechanical properties.
- This project made quite a leap forward this year with the electrospinning of PFSAs. Conductivity measurements showed that the DOE 120°C target was achieved. It should be noted, however, that a more realistic 120°C target (25% RH) would not have been met, and that the target at 80°C was not met.
- Swelling and gas crossover data were not reported in the slides. In the future, the project should be sure to present a "scorecard" of membrane attributes to make sure everything is covered.
- The sample thicknesses are still too large.

<u>Ouestion 4: Technology transfer/collaborations with industry, universities and other laboratories</u>

This project was rated **3.3** for technology transfer and collaboration.

- The inclusion of two industrial partners, 3M and Nissan, is good for the progress of the project.
- It would have been nice to have a national lab and university involved in the project.
- There appears to be strong collaboration with 3M.
- The program has good collaborations with industry, but not many with other academics that might increase the curiosity into the fundamental mechanisms. This should be emphasized in the future.
- There have been collaborations with an MEA manufacturer and an original equipment manufacturer (OEM). The project team initiated work with Nissan this year. The team is working with 3M, and with Professor Litt to try to incorporate his high-conductivity material.
- The project team has exhibited good collaboration with 3M.
- The project team has very effectively worked with 3M as a collaborator. It was 3M who provided the PFSAs that helped greatly in achieving the DOE 120°C conductivity target.
- Collaboration from Nissan does not yet appear to have generated much data.

Question 5: Approach to and relevance of proposed future research

This project was rated **3.3** for proposed future work.

- The proposed future work is aligned with the present issues faced in the project.
- The exploration of insoluble SPOSS material will be helpful in controlling the conductivity of the membrane.
- The development of core-shell fibers and use of inorganic fillers are good strategies.
- Proposed future work should help the project achieve all its technical milestones.
- Future work will no doubt be useful, but it could be improved with more fundamental work on proton conduction mechanisms and how such elements as channel size and EW affect it.
- Future work is focused in the right areas looking at the durability of SPOSS and Norland Optical Adhesive (NOA), and options to replace these, and looking at further options in PFSA materials.
- A number of good ideas were presented for further development. It is good that there are multiple pathways under consideration for further improvement of membrane performance, and also that stability is being addressed.
- The future work section correctly recognizes that the use of SPOSS is likely a liability, and that it should ideally be replaced.
- The future work section also correctly regards the resin with suspicion.
- A baseline of the chemical and mechanical stability of present materials (in DOE Accelerated Stress Tests, ASTs) would be good. Or, if speculation is strong enough, it would be good to present some commentary on why these ASTs would not work with materials as they are (e.g., swelling is too high so the mechanical test would fail quickly).

Strengths and weaknesses

Strengths

- Developing wired matrix for proton conduction is a very interesting and novel concept.
- The feasibility of the concept has been demonstrated well.
- Improvement of the membrane's mechanical strength by using NOA63 polymer matrix is a good concept.
- The project team has had early success with decoupling membrane conductivity and stability functions and working on areas to build on this success.
- It is an excellent concept and rapidly produces new ways of affecting morphology.
- The flexibility of the electrospinning approach allows the benefits of a composite membrane to be seen with materials with poor mechanical properties.
- It is a novel concept unlike other projects.
- This is a teachable project that has embraced feedback from reviewers to create even better materials than before.
- This is also an evolving project that realizes the drawbacks of particular components, but has a solid plan to address them.
- The project has shown the use of quick technical decisions to make challenging tasks (e.g., electrospinning of PFSAs) work out.

Weaknesses

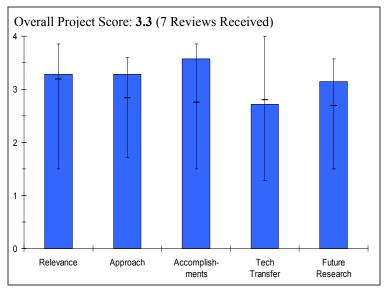
- The project team needs to find a non-leachable SPOSS type proton conductor to have a practical membrane.
- The chemical stability of NOA63 is still an issue.
- SPOSS is expected to deform the fibers upon prolonged RH cycling.
- The team needs to improve the NCM surface to enhance the membrane electrode integration.
- The reviewer didn't get a good feel for cost.
- There has not been enough fundamental thought to what is going on. This has the feel of an engineering project where not too much inquiry into the basics is going on.
- The durability of SPOSS and the inert membrane filler NOA have not been demonstrated.
- There is a lack of reporting certain attributes that reviewers need to know about, e.g., swelling and gas crossover.
- The membrane thickness is a weakness.
- It is still unknown whether a chemically stable embedding resin will be found.

- The project team needs to focus on cost and ability to manufacture in large volumes, along with performance in fuel cell environment.
- The team needs to add aq modeling components and force the program to look into basic mechanisms, such as how the channel dimensions affect the behavior.
- The team also needs to work with lower EW material being made at 3M, and material being made for Giner at Syracuse if possible. Look at polyPOM materials as additives.
- Once it is known that a fairly durable PEM has been fabricated (which has not yet necessarily happened), it would be good to have *in situ* DOE accelerated stress tests performed.
- While it is good that 3M has contributed the PFSA for electrospinning, it might also be wise to add their services in order to figure out how to decrease the thickness of the membrane. It might also be interesting to see how lower EW PFSAs perform in electrospinning trials.

Project # FC-10: High Temperature Membrane with Humidification-Independent Cluster Structure *Ludwig Lipp; FuelCell Energy, Inc.*

Brief Summary of Project

The objectives of this project are to: 1) develop polymer membranes with improved conductivity at up to 120°C; 2) develop membrane additives with high water retention and proton conductivity; 3) fabricate composite membranes; and 4) characterize polymer and composite membranes (in-plane conductivity). FuelCell Energy, Inc. has 1) fabricated three polymer iterations, six nanoadditive batches and more than 10 composite membrane batches; 2) improved mC^2 uniformity and conductivity with concurrent process simplification; 3) integrated additive functionalization and composite membrane fabrication; and 4) demonstrated >2ximproved conductivity at 120°C over 2008 (>3x higher than NRE-212[®]).



Question 1: Relevance to overall DOE objectives

This project earned a score of **3.3** for its relevance to DOE objectives.

- A high-temperature membrane that operates at low relative humidity (RH) is one of the key technologies needed for the commercialization of fuel cells.
- High conductivity at all operating conditions is critical to achieving overall DOE targets of cost and performance.
- This project is fully in line with DOE objectives.
- It appears to address only one critical barrier of one membrane electrode assembly (MEA) component.
- High-performance membranes are critical to automotive commercialization, but lack of specifics doesn't allow others to benefit from fundamental knowledge gained from the work done.
- There appears to be good alignment with DOE's current objectives. A broader consideration should include the ability to operate at higher temperatures to have low CO sensitivity required for stationary fuel cell systems operating on infrastructure fuels.
- Membranes with improved conductivity that function under high temperature/low RH are included in the Hydrogen Program and DOE's RD&D objectives. These are not the most critical material needs for enabling fuel cell commercialization.

<u>Ouestion 2: Approach to performing the research and development</u>

This project was rated **3.3** on its approach.

- While the PI does not divulge the details of their approach, the concept of adding a variety of technologies, e.g., co-polymer, support polymer, water retention additive, and proton conductivity enhancer, to obtain a viable fuel cell membrane is good approach.
- Unfortunately, the reviewer has no idea what these various technologies really are.
- The necessary functionalities such as water retention, conductivity, and strength, are being provided by additives to form a composite membrane.
- Complicated systems usually lead to high cost.

- The project has overcome significant technical barriers. The disclosed material was, however, short on details because of the proprietary nature of the additives. Some of these additives are known to be very expensive, so new synthetic routes may also need to be developed.
- The approach appears to be a truly "engineered" membrane physical versus just chemical. It appears to be quite successful in breaking down the overall functional performance properties into separate characteristics.
- The approach is hard to judge without knowing anything about the materials, other than it seems to work for getting good conductivity at low to moderate RH. The approach may not be compatible with durability or cost targets. There is no way to know without knowing what the materials are or having any durability data.
- The project team has taken an excellent problem solving approach. Considering all required functions of strength, water retention and protonic conductivity early on allows for narrowing down to a comprehensive solution.
- The approach involves a multicomponent system containing a support, low equivalent weight (EW) ionomer, water retaining additive and proton conduction enhancing additive. The multicomponent approach seems to provide additive or synergistic effects based on conductivities reported. Evaluation of the approach is limited as it is unclear what additives are being investigated and how they work.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated 3.6 based on accomplishments.

- Based upon the PI's results and the results at BekkTech, the research obviously meets or exceeds the DOE's targets; however, the PI did not discuss the mechanical nature/swelling of the membrane, which could be the potential weak point.
- All project targets, goals, and decision points have been met to date.
- The amounts of additive have not yet been optimized.
- Swelling may need to be addressed.
- The performance of the composite membranes, particularly at 50% humidity, is spectacular.
- The project shows very encouraging results and is meeting all program milestones, but it still needs to demonstrate that fuel cell performance will not have any surprises. Also, other membrane durability tests have not been carried out yet.
- The conductivity results are very good as verified by BekkTech. If the materials turn out to be durable, I'd say progress was outstanding.
- The project team has made excellent progress. The reviewer is curious to see the actual fuel cell performance and endurance data.
- Of the conductivity results reported to date, the recent results are impressively high. Other data regarding the materials is lacking in the presentation. In particular, water uptake and mechanical properties would be useful as only conductivity is reported anywhere without any information on durability/leaching.

<u>Ouestion 4: Technology transfer/collaborations with industry, universities and other laboratories</u>

This project was rated 2.7 for technology transfer and collaboration.

- Collaboration with various institutions appears to be very high; however, as everything is highly confidential, the reviewer does not know who they are: a polymer company, nano-materials company, or university? Are they receiving DOE funding?
- Although impressive progress implies impressive partners, the partners are not named and, therefore, cannot be rated.
- Collaboration was not addressed and cannot be judged.
- It appears they brought together the key technology experts to methodically address their membrane component/functional requirements, but why aren't the collaborators fully identified?
- The unnamed collaborators seem to work together to provide a product with good conductivity. It's impossible to know the value of partners as no specifics were given.
- There was excellent collaboration among vendors, material experts, academia, and test entity probably the best of any team.

• There were relatively little interactions; however, they are not particularly needed at this point in time. A partner is mentioned as contributing to the project, but no further information regarding this partner is given. This makes an assessment of the value of this teaming arrangement difficult.

Question 5: Approach to and relevance of proposed future research

This project was rated **3.1** for proposed future work.

- The proposed work is based upon existing/established membranes and is well thought out.
- Fuel cell experiments with performance and durability experiments are on the agenda, which is excellent at this stage of development.
- Future work is right on the mark, addressing durability/stability, cell performance, cost, scale-up, and synthesis simplification.
- The accomplishments to date are extraordinary, and definitely warrant continued and intensified development efforts.
- The project team needs to demonstrate compatibility with catalyst electrodes to identify any future issues.
- The two areas of recommended future work are durability testing and high-temperature fuel cell testing.
- Further polymer optimizations should only be made while taking durability under consideration. Performance is already satisfactory.
- I agree with proposed future work. The ability to manufacture in high volume and low cost needs to be a consideration.
- It is not certain how the project has resulted in the conductivity reported, and this makes future advances uncertain. Further optimization is the first bullet noted in future work, but conductivity does not seem to need significant advances. Durability is noted but not discussed, and at the present time it is uncertain what the durability concerns are.

Strengths and weaknesses

Strengths

- The approach is based upon what the reviewer can see is very sound and logical, and results support this fact.
- The additive approach works.
- The PI's company has a strong background of practical understanding of fuel cells and what is required for commercialization.
- The project team has made a membrane with good conductivity.
- The project team has taken a highly methodical and holistic problem-solving approach. They are staying focused on project goals and optimizing around meeting objectives.
- The team has taken a combined approach that seems to be yielding enhanced benefits from additive approach, particularly high conductivity.

Weaknesses

- The only weakness (and I'm not even sure if it a weakness) is the secrecy of the project. Does this work help the overall industry or only the company itself? Does that matter?
- The lack of identification of partners and chemical/structural constituents prevents full analysis of the project.
- Cost issues may need to be addressed.
- There is a lack of disclosure of materials.
- There is a lack of mechanical and swelling data on membranes.
- There is a lack of durability data.
- There is also a lack of cost analysis.
- I can't think of any. This is probably the best project!
- There is a lack of technical data, other than conductivity and a lack of information regarding materials and scientific basis for advances. This makes the project more difficult to evaluate and is frustrating, as three years into the project they still haven't discussed any materials from even initial studies.

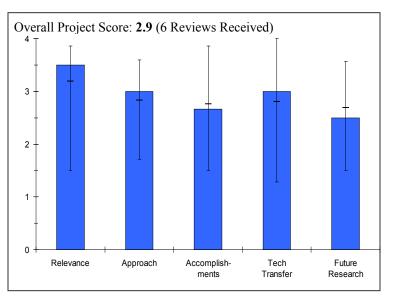
- The team should continue as planned; *in situ* fuel cell experiments are the planned next step to look at performance and durability. It will be very important to learn from these experiments and cycle back to the beginning if the results do not meet expectations.
- The reviewer recommends continued evaluation of longer term tests, and possibly stability testing with Fenton's reagent.
- The team should run DOE specified durability tests. Further recommendations will fully depend on the durability data.
- The team should provide a cost analysis or, better yet, have an independent party such as TIAX or DTI do it.
- The project team should move beyond conductivity to other properties.

Project # FC-11: Novel Approaches to Immobilized Heteropoly Acid (HPA) Systems for High Temperature, Low Relative Humidity Polymer-Type Membranes

Andrew M. Herring; Colorado School of Mines(CSM) Mathew H. Frey; 3M Corporate Research Materials Laboratory

Brief Summary of Project

The overall objective of this project is to fabricate a hybrid heteropoly acid (HPA) polymer from an HPA functionalized monomer with >0.1 S/cm at 120°C and 25% relative humidity (RH). The objective for 2007 was the synthesis and optimization of hybrid HPA polymers for conductivity from room temperature to 120°C. The 2008 objective was the synthesis and optimization of hybrid HPA polymers for conductivity from room temperature to 120°C with an understanding of chemistry/morphology conductivity relationships using a model system. The 2009 objective was to optimize hybrid polymers in more practical systems for proton conductivity and mechanical properties.



Question 1: Relevance to overall DOE objectives

This project earned a score of **3.5** for its relevance to DOE objectives.

- The project is very relevant to the Hydrogen initiative and supports DOE RD&D objectives.
- This project is focused on meeting DOE objectives on low RH membrane conductivity.
- The project addresses important issues of particular relevance to the Hydrogen Program. It attempts to study the factors that are important in controlling proton transport under low RH conditions, as well as simply trying to meet milestones. This is important, as meeting the 25% RH goal looks difficult for this system, and fundamental studies will be necessary to meet the goal.
- The project is aligned with DOE goals and milestones, and it addresses relevant barriers.
- The project goal of fabricating and characterizing a high-performance polymer electrolyte membrane for high-temperature/low RH fuel cell operation is highly relevant to the DOE.
- The project, like many other membrane projects, is attempting to produce a membrane for polymer electrolyte membrane fuel cells (PEMFC). The production of membranes that can operate at high temperature and low RH is central to DOE Hydrogen Program goals.

Question 2: Approach to performing the research and development

This project was rated **3.0** on its approach.

- The approach taken for achieving the goal is unique.
- The incorporation of HPAs in PFSA-type materials to enhance low RH conductivity is a good approach.
- However, the incorporation of HPAs into other types of host polymers, which are unstable under free radical environments, may not yield a practical membrane.
- Ultra-violet (UV) curable polymer host materials may contain leftover free radicals, which may degrade the polymer under fuel cell conditions.
- The approach seems fair. Use of the polyacrylate polymers is okay and justified by the need to make membranes and get on with the polymer properties. The design space is rather mysterious and not well defined.

The axes are not understandable; however, at some time the durability needs to be addressed. It is also unclear on how the membranes will function with the electrodes. Some ideas for this might be useful.

- Initial work has been done and has resulted in easier-to-produce, quicker-to-make polymer linkers, which allowed quicker progress and enabled the team to meet the conductivity target with a totally new polymeric ionomer system. With this newer system, this was the appropriate approach, and allowed them to demonstrate that they can approach the targets with this new type of ionomer system. This is a good mix of synthetic work with advanced characterization techniques, which allows the team to understand its system, as well as other systems that have been studied for much longer.
- The use of HPAs is interesting, but there are many potential pitfalls, including membrane brittleness, leaching of HPAs from the membrane, the thermal stability of such HPAs, and the method of mixing such inorganic materials with a polymer.
- The approach is good novel, well-designed, and feasible although it would have been better if a stable comonomer had been used from the start.
- While the approach recognizes that a water soluble group such as an HPA would be best situated as an immobilized part of a polymer chain, issues of swelling and morphologically derived conduction inefficiencies still remain as hazards.
- The project shows that its approach is changing; however, positioning the HPAs as pendant groups off a main chain might return HPAs to a vulnerable position.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated 2.7 based on accomplishments.

- The project has achieved the conductivity objectives, but has not addressed the mechanical properties of the membrane.
- The HPA co-polymer (slide-14) did not show good conductivity above 100°C.
- It seems that the HPA polymer hybrid material is behaving similar to perfluorosulfonic acid (PFSA)-type material and losing its conductivity above 100°C.
- Many measurements have been taken, and some reasonable progress on how morphology affects conductivity has been made. The low RH results are a bit worrying, and some more work on the polyoxometalate (POM) mechanisms might be useful.
- The project team has achieved the very aggressive DOE milestone of 0.1 S/cm at 120°C and 50% RH, and developed a totally new class of polymeric protonic conducting materials.
- The data presented by the PI is confusing. No BekkTech conductivity data were presented and some data were confusing: PolyPOM75v membrane loses all its water at 56% RH for all temperatures (slide 12), and thus has no conductivity at this RH, but PolyPOM80v has a very high-proton conductivity at 120°C and 50% RH. It is unclear why this is the case. The two membranes are similar. In addition, the use of acrylate polymers because of their poor chemical stability is questionable. It is unclear why the team has not used 3M's perfluorosulfonic acid polymer since 3M is a collaborator on the project.
- The project is meeting conductivity milestones, which is good, but it needs to accelerate efforts to provide good chemical and mechanical stability.
- Numerous drawbacks are found with the original strategy, including membrane brittleness and low conductivity at low RH.
- Some promise is found with certain samples achieving 0.1 S/cm at 120°C/50% RH, and with the use of UV polymerization.
- Although it can be said that certain conductivity measurements achieved their goal, not enough is known about the membranes, particularly with respect to swelling and leaching. Furthermore, chemical identification (NMR, IR/Raman) within a fairly complex system would be useful.

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated **3.0** for technology transfer and collaboration.

- The project involves good industry and academic collaborations.
- Involvement of some national labs could have been better.

- Partners are well coordinated, but collaboration with the Topic 2 group is not well presented. Outside collaborations are not prominent, and could be increased in order to attack the low RH problem which looks to be big.
- The project team is collaborating with 3M.
- There seems to be a good collaboration with 3M.
- Interaction between CSM and 3M has been fruitful.
- 3M has played a consultant role for a while, but it appears a more earnest role is just beginning, as indicated by the future work.

Question 5: Approach to and relevance of proposed future research

This project was rated 2.5 for proposed future work.

- The proposed research is very vague.
- No clear direction in the future work on improving the membrane morphology is given.
- There is no clear indication on the types of monomer to be used. It is understandable that the monomer structure could be proprietary, but the nature of materials could have been mentioned.
- Future work is a bit mysterious and not easy to judge. How is the morphology to be improved? The details on this are fuzzy.
- Future work with 3M offers the potential for a link to fluorinated linkers and fuel cell testing. More information on monomer systems to be used would be helpful. Whatever information can be provided without divulging intellectual property (IP) would help (are they using hydrocarbons, fluorocarbons?).
- The future work slide was very general and lacked specifics. There were no mechanical property measurements in the 2009 AMR presentation and no plans to make such measurements next year. Mechanical tests on the membrane (both wet and dry) should be carried out next year. Also, the water swelling and chemical/thermal stability of the membranes should be evaluated.
- Future work plans are logical and sound, but the lack of detail makes this one a bit hard to judge.
- The prospect of positioning an HPA as a pendant group off a main group may not be appealing. The HPA may be more susceptible to leaching, and the channel size may have to be increased, in which case perhaps conductivity would require greater RH. This is all just speculation, but there is no assurance that the new possible structure will work.
- Thankfully, the old concept has not been entirely tossed aside. It would be interesting to see if 3M could still find a way to keep the old system from being mechanically unstable.

Strengths and weaknesses

Strengths

- The team has taken a good approach by harvesting the low RH conductivity property of HPA.
- The team shows good collaboration with an industrial partner.
- The project team has taken an interesting approach of making HPA hybrid material using UV curable polymers.
- The team has a good combination of industrial and academic workers.
- Polymer chemistry and HPA chemistry give the prospect of a genuine breakthrough in proton conduction mechanisms that could solve the low RH issue.
- The team has a good mix of synthetic work and characterization which allows them to have a better understanding of their system. The presence of 3M provides the polymer experience necessary to advance the project, and the material offers the potential for very low RH conductivity.
- The team has taken an interesting approach that appears to be working.
- The team has strong collaboration with 3M.
- The team has attained high-conductivity measurements despite complex chemistry and numerous materials drawbacks.
- The team is collaborating with 3M.
- Certain prospects still exist for improving membranes, e.g., UV polymerization.

Weaknesses

- There are no clear directives towards the future work.
- Using UV-curable host polymers to make the HPA hybrid membrane is not very practical.
- The second generation hybrid material (slide 18) may result in poor mechanical properties of PFSA membrane due to the bulky size of HPA incorporated between the polymer chains of the backbone polymer.
- The team should move on from polyesters. Future plans are veering into secrecy at an inopportune time. More progress needs to be made on the basic HPA polymer interactions before drawing a secrecy veil around the work. The team did not show where the membrane electrode assembly (MEA) work is planned. Durability issues need to be more explicitly addressed.
- There are many unanswered questions, such as why there are no BekkTech third-party proton conductivities, and seemingly confusing data, e.g., the difference in properties of polyPOM75V and polyPOM80v.
- The PI has not yet addressed any critical issues regarding the chemical stability of his polymer and the mechanical properties of his polymer-HPA materials.
- The project has exhibited sample brittleness and the possibility of other material disadvantages.
- The project has also exhibited low conductivity at low RH.
- The general concept of using HPAs is risky due to swelling, leaching, etc.

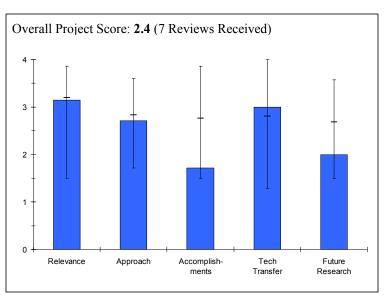
- How is the MEA to be prepared with these materials?
- The group should begin to address mechanical properties and durability issues.
- The group should clarify the results obtained to date, and ensure that reproducible membranes can be made. It is unclear why the PI is planning to look at morphology. He already has met the DOE conductivity target, and should focus on chemical/thermal and mechanical stability.
- Work focused on the original concept should continue, but with more intense collaboration from 3M to resolve brittleness, low conductivity at low RH, uniformity of the material, and other problems.
- Perhaps some theoretical work previously applied to other membrane projects could be used here to help predict the degree of proton hopping to be expected for distinct membrane structures.

Project # FC-12: Improved, Low-Cost, Durable Fuel Cell Membranes

James Goldbach, David Mountz, Tao Zhang, Wensheng He, and Michel Foure; Arkema

Brief Summary of Project

The objectives of this project are to 1) develop a membrane capable of operating at 80°C at low relative humidity (RH) (25-50%; 2) develop a membrane capable of operating at temperatures up to 120°C and ultra-low RH of inlet gases (<1.5 kPa); 3) use commercially available matrix materials as a low-cost approach; and 4) elucidate ionomer and membrane failure and degradation mechanisms via ex situ and in situ accelerated testing. Mitigation strategies will be developed for any identified degradation mechanism. M41 was shown to have superior durability in accelerated in situ testing and shown to operate down to 65% RH. Initial M70 membranes show an order-of-magnitude increase in conductivity versus M43.



Question 1: Relevance to overall DOE objectives

This project earned a score of **3.1** for its relevance to DOE objectives.

- Low-cost and durable membranes are critical to achieving DOE targets.
- The project does not clearly address DOE objectives, as the project targets are for performance at 80°C rather than 120°C.
- The project focuses on just one fuel cell membrane electrode assembly (MEA) component the membrane. This may not be adequate to show ultimate feasibility.
- Mechanically robust and low-cost membranes are critical for automotive fuel cell commercialization.
- Work is in line with Task 1, Barriers A, B, and C, to develop membranes that meet all targets.
- The project goals of fabricating and characterizing a high-performance polymer electrolyte membrane for high-temperature/low RH fuel cell operation are highly relevant to the DOE.
- Membranes with improved conductivity that function under high temperature/low (RH) are included in the Hydrogen Program and DOE's RD&D objectives. These are not the most critical material needs for enabling fuel cell commercialization.

Question 2: Approach to performing the research and development

This project was rated **2.7** on its approach.

- It is not clear how membrane conductivity can be maintained when a substantial fraction of the material is composed of an insulating material such as Kynar®.
- However, the Kynar does help with mechanical and chemical durability.
- Biphenyl sulfone H form (BPSH) probably does not have the necessary conductivity to achieve DOE targets.
- Large volume production of the BPSH-Kynar blends appears to be feasible, but performance of the membranes is significantly below target.
- Focusing on commodity Kynar is a good cost strategy, but the downside is that it may limit options for meeting the performance and durability goals.
- Blending polyelectrolytes with polyvinylidene fluoride (PVDF) is a solid approach to make a durable, potentially high performing, and low-cost membrane.

- Working with highly functionalized polyelectrolytes is also a good approach.
- The choice of ionomers so far has been poor. Ionomers with a chance of meeting the targets should be used.
- The use of polymer blends is a sound approach, although not particularly novel. A focus on low-cost approaches is important and worthwhile.
- Investigating Kynar (PVDF) as a potential cheap/durable polymer is sensible for a company with PVDF experience. The use of polymer blends is worthy of investigation, but testing to-date has not shown significant promise, as current low RH conductivity is poor.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated 1.7 based on accomplishments.

- Arkema has increased the conductivity an order of magnitude over the early formulations, but it is not clear how continued optimization of blends of Kynar with M7x or BPSH can realize another order of magnitude to reach the DOE high-temperature/low RH targets.
- Conductivities are way below what is needed for these blends.
- Given where the project was with the M4X series, the M70 is showing much improvement, but it is only just matching the old Nafion® standard.
- It would be good to have already demonstrated some fuel cell performance with the M70 membranes. If they had membranes for the conductivity measurements, then why were the fuel cell measurements not done as well?
- The rate of progress of the program is low.
- While they have tested a lot of membranes, none approach the low RH resistance targets.
- I commend the PIs for running RH cycling and open circuit voltage (OCV) hold tests, and showing very good durability in both tests.
- It was also nice to see some results on the sensitivity to Kynar content.
- Proton conductivity is still very low, and a lot of time is being wasted testing the materials for properties that can be optimized after the conductivity targets have been met.
- Membranes that have been made to-date lack the requisite low humidity conductivity. A conductivity of two mS/cm at 50% RH is unacceptably low. New membranes have a conductivity less than that of Nafion® for all values of RH. BPSH/Kynar blends do not appear to be promising; a highly charged water soluble BPSH must be crosslinked to prevent solubilization, and this will undoubtedly lower proton conductivity and make the polymer highly brittle. It is unclear why durability tests were performed on the M41 membranes when they have insufficient proton conductivity.
- The approach presented has not met low RH conductivity of even Nafion®, and remains far from DOE targets. Performance of membrane materials in MEAs is not presented particularly for durability studies. The comparably funded project by 3M shows greatly improved conductivity and extremely long durability. Membrane development on the materials presented by this lead organization has been funded by DOE for several years, and the current level of advancement is disappointing for the significant investment.

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated **3.0** for technology transfer and collaboration.

- A stack manufacturer would add to the project team capabilities.
- Collaboration was not addressed.
- It is not clear what, if any, contributions were made by the University of Hawaii.
- They could benefit from much more fuel cell functional property testing.
- The collaborations provide access to many ionomer and catalyst materials for membrane and MEA development.
- The transmission electron microscope (TEM) work at Oak Ridge National Laboratory provides useful insight into blend morphology and miscibility.
- Hawaii's role is unclear.
- The project team exhibited a good mix of university, national lab, and industrial partners.

- There are quite a few collaborators on this project. Most appear to be peripherally involved with the work, and do not directly assist in formulating new membranes and new membrane morphologies (e.g., they provide polymer catalyst samples or they do TEM studies; membrane fabrication and morphology control studies are done solely by Arkema).
- The project has strong partners, such as Johnson Matthey of Oak Ridge and Jim McGrath; however, it is not clear how Johnson Matthey interacts.

Question 5: Approach to and relevance of proposed future research

This project was rated 2.0 for proposed future work.

- For the time left on the project, the future plans are appropriate. The latest formulations will be optimized and more completely characterized.
- There is a lack of clarity of what to do next, or lack of intention to come closer to the DOE targets.
- The team seems to be satisfied with the commercial viability of current status.
- Testing should be done extensively now on their best membrane option in fuel cells as a function of membrane thickness as well as polymer composition and morphology, and fuel cell testing conditions (temperature and RH) to really establish a benchmark of this technology approach and reveal both operating windows of opportunity and material issues and gaps.
- There was nothing specific in the future work plans to suggest they have a good idea for how to improve low RH performance.
- Emphasis should be put on using highly conducting ionomers, and understanding proton conductivity from -20° to 120°C at dry conditions. A detailed understanding of morphology, chemistry, and transport is needed so that the conductivity in these materials can be understood and optimized.
- The PI could not explain why the proton conductivity of Arkema membranes with the low EW polymer was much lower than that of Nafion®. Without a firm understanding of why the Arkema membranes do not perform up to expectations, it is difficult to see how improvements can be made.
- Future work focuses on many of the same ("continued") studies. The specific approaches proposed are vague and seem to hinge on the hope that crosslinkable end groups could allow higher conductivity and reduced water uptake by using BPSH-100. It seems highly unlikely that this change alone would result in the significant advances necessary to yield new materials with competitive properties.

Strengths and weaknesses

Strengths

- Large quantities appear to be easily produced.
- The project team shows a strong technological understanding of polymer properties and processing, particularly with their core technology, Kynar.
- The project team performs durability testing.
- The project team has access to McGrath ionomers.
- A low cost potential exists.
- PVDF blending capability exists.
- Arkema and the PI are experienced in using PVDF in various types of membranes. PVDF is an attractive material for blended fuel cell membranes.
- Cheap/chemical resistant polymer systems could lower the cost of fuel cell ionomers.

Weaknesses

- There are large quantities of membranes of questionable utility.
- There has not been enough functional property and durability testing in full MEA configurations to understand water management properties.
- There has also been very little progress towards main objective (low RH conductivity) with little demonstrated fundamental understanding as to why conductivity is so low.
- The project team made a poor choice of ionomers for blending.

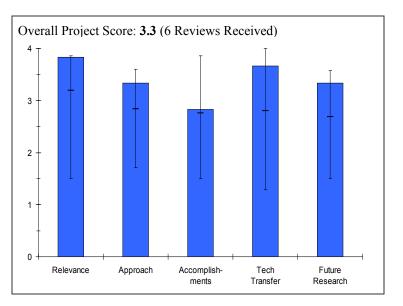
- Proton conductivity on new membranes is very low (much lower than Nafion® 212). A credible strategy for overcoming this weakness was not presented.
- Fuel cell testing has been too limited, and the approach taken has not addressed a key issue of low conductivity at low RH.

- It is not advisable to continue this project in view of poor results and the lack of a clear path to improvement.
- The project team should work with McGrath's partially fluorinated block copolymers.
- The project team should do more fuel cell testing (H₂/Air) with these materials as conductivity can be misleading.
- The project team should also concentrate on meeting proton conductivity targets first. A go/no-go point that requires a material substantially improved versus Nafion® 212 should be developed.
- No additions/deletions to the project scope are recommended.
- The team should focus on higher acid content polymers and crosslinkable end groups, and it should stop studies with ionomers with lower acid content than BPSH-100.

Project # FC-13: Membranes and MEAs for Dry, Hot Operating Conditions Steven Hamrock; Fuel Cell Components

Brief Summary of Project

The objective of this project is to develop a new proton exchange membrane (PEM) with higher proton conductivity and improved durability under hotter and dryer conditions compared to current membranes. Fuel Cell Components is developing new membrane additives for both increased conductivity and improved stability/durability under dry conditions. Experimental and theoretical studies will be conducted of factors controlling proton transport both within the membrane and mechanisms of polymer degradation and membrane durability in a membrane electrode assembly (MEA).



<u>**Ouestion 1: Relevance to overall DOE**</u> <u>objectives</u>

This project earned a score of 3.8 for its relevance to DOE objectives.

- Membranes that can operate stably with high conductivity over the entire range of expected temperature and humidity are critical to DOE goals.
- The project is in alignment with DOE's objectives.
- The project addresses all the relevant DOE targets of looking at membrane performance at high temperature/low RH and durability.
- Improved membranes with wider operating window, higher performance, and better durability are critical to the Hydrogen Program.
- This project is highly relevant to the Hydrogen Program. It systematically seeks to attack the issue of conductivity at low humidity by lowering membrane equivalent weight (EW), while still maintaining a mechanically stable structure.

Question 2: Approach to performing the research and development

This project was rated **3.3** on its approach.

- 3M is paying a lot of attention to durability under cycling conditions.
- 3M is addressing composition, additives, synthesis, and manufacturing methods, and theoretical analysis to support the project. It is not clear how or if these approaches will be down-selected or combined.
- The approach to nailing down and optimizing a system appears to be too broad. The number of options should be narrowed down after performing appropriate risk analysis.
- The project team is looking at stability, durability, and performance. It builds on strengths of the current 3M ionomer, while investigating the limits of that chemistry. The combination of theory, synthetic work, and characterization help understand effects of crystallinity, EW, and acidity on conductivity and physical properties.
- The approach covers all critical areas and provides good balance between new materials development, fundamental understanding, scalability, and stack performance.
- The approach is very ambitious in terms of the broad range of materials and additives being investigated.
- The approach appears complex, but is very simple: reduce EW while maintaining mechanical stability, which is the essence of most of the decent membrane projects.

- The approach makes room for all the major techniques for achieving the above: blends, polymer modification, reinforcement, and crosslinking. Not all these methods receive equal treatment, however.
- The polymer modification part is the best conceived. As groups are added as chemical handles (increasing EW), more conductive groups are added (returning to low EW).
- Other efforts (SSC, tethered HPAs) are interesting, but not yet integrated into the mainstream of the project.

<u>Ouestion 3: Technical accomplishments and progress toward project and DOE goals</u></u>

This project was rated 2.8 based on accomplishments.

- Membranes have been fabricated that approach 0.1 S/cm at 50% RH and 80°C.
- Mechanical stability under RH cycling is a serious issue.
- Reasonable progress has been made. The team needs to narrow down the scope to start hitting project goals.
- The team has demonstrated membranes in an MEA with durability exceeding 10,000 h. They have determined EW-conductivity relationships for the baseline 3M ionomer. They have prepared derivatives of the 3M ionomer for bis-acids with increased conductivity compared to the base ionomer with the same backbone.
- The project has shown conductivity meeting DOE 2010 targets with low EW polymers.
- The project has given impressive fuel cell durability data.
- The team is meeting or approaching conductivity targets, although mechanical and chemical stability are still a concern.
- The synthesis progress in its own right has been good, although bottom-line conductivity results have not been delivered. For example, the ortho/meta bis-acid membranes have been fabricated, but conductivity measured at 80°C/50% RH is still 40-60 mS/cm.
- An urgent need still exists to show that the ortho/meta bis-acid membranes have not become low enough EW that they are on the "wrong side" of the solubility threshold.
- Electron spin resonance (ESR) shows that the base 3M 825 EW membrane is more resistant to radical attack, but it is not entirely understood yet why.
- Additive A appears to extend lifetime, but the test used for lifetime is still more of a load cycle than a drive cycle.

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated 3.7 for technology transfer and collaboration.

- The team includes an auto original equipment manufacturer (OEM) and all other disciplines necessary.
- The project appears to have strong collaboration, but the scope of collaboration appears too broad for the given scope.
- The project team has collaborated with several top-name people.
- The collaborators have provided important input and feedback.
- 3M has assembled a wide range of collaboration, some of which is more useful than others.
- GM, BekkTech, and the University of Detroit-Mercy all have clear and necessary tasks.
- Colorado School of Mines (CSM) and the University of Tennessee (UT) are providing solid contributions modeling morphology, but it still remains up to the project leadership to integrate this better into the rest of the project.
- Case Western Reserve University (CWRU) appeared to be used early on to look at proton diffusion at low humidity, but this has not been repeated yet for the newer membranes.

Question 5: Approach to and relevance of proposed future research

This project was rated **3.3** for proposed future work.

• The team is addressing mechanical durability and water solubility by several approaches including theoretical analysis.

- The scope of future work is too broad, and requires a more holistic approach to meet all requirements as opposed to targeting individual product attributes.
- The team needs a comprehensive plan to address the barriers by characterizing various important underlying aspects of performance and durability.
- The team clearly needs a lot of planning for future work. Their strategy is very ambitious essentially to examine every possible route to improve performance and stability they can think of, which is a lot; if they are able to achieve this level of effort, then good results are likely.
- There are a lot of tasks in the future work, split amongst a number of parties. The challenge will be to create some coherent sense out of all the disparate parts.
- The emphasis needs to remain on making a stable, high-conductivity, low-EW membrane. Towards this end, the morphological studies need to be getting used to better direct the polymer modifications. Reinforcement may be important at some point if the chemical stability offered by additives is not sufficient. The project's success will depend on keeping about 7-8 "plates spinning."

Strengths and weaknesses

Strengths

- The project team has taken a diverse approach.
- The team has used a good combination of synthetic work, characterization, and theory.
- The team has taken several parallel and complimentary approaches to increasing performance and durability.
- They have used interesting and systematic work to develop new polymers.
- Investigators have lots of ideas, and are effective in the examination of multiple strategies for improved performance and durability.
- The team has come up with creative, well-conceived ideas for polymer modifications.
- The team has exhibited a wide range of collaboration that includes modeling, *in situ* testing, and analytical expertise.
- Background demonstrates deep understanding of what the problems are.

Weaknesses

- The cost discussion is weak.
- The scope is too broad.
- The project has not yet delivered a higher conductivity membrane with lower EW that has been shown to not be soluble.
- The project contains a lot of separate parts that have not all delivered as much as can be expected.
- There could still be a number of issues that are, as of yet, untouched in the material presented (swelling, leaching, catalyst poisoning, etc.).

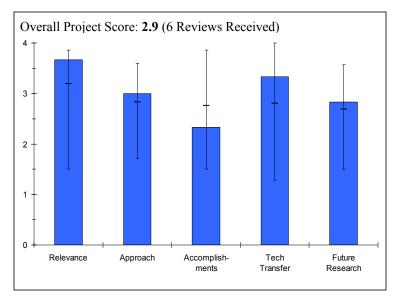
- The team needs to ensure consideration for high-volume manufacturing and cost, while staying focused on solving technical problems.
- The blends made so far do not look promising; the team should consider establishing a go/no-go milestone for this approach in 2010.
- The project should remain focused on polymer modifications and morphological refinements until conductivity goals are met, with a secondary focus on the solubility/RH cycling of the highest conductivity/lowest EW materials made to date. All activities are details in comparison.

Project # FC-14: New Polyelectrolyte Materials for High Temperature Fuel Cells

John B. Kerr; Lawrence Berkeley National Laboratory

Brief Summary of Project

The objectives of this project are to 1) develop knowledge that leads to materials that can meet the performance needs at acceptable cost; 2) create fuel cells that operate efficiently without external humidification at operating temperatures between -40°C and 120°C; 3) develop durable water-free membrane materials that meet the 2015 DOE targets as set out in the Multi-Year R&D Plan; 4) achieve conductivity of 0.1 S/cm at operating temperatures ($\leq 120^{\circ}$ C) and inlet water vapor partial pressures <1.5 kPa; 5) demonstrate durability with cycling >5,000 hours at over 80°C; and 6) achieve oxygen and hydrogen crossover currents ≤ 2 mA/cm^2 .



Question 1: Relevance to overall DOE objectives

This project earned a score of 3.7 for its relevance to DOE objectives.

- A non-water dependent proton conducting membrane, which works well from -20°C up to 120°C, would be an amazing breakthrough for the fuel cell community.
- The project is relevant to the high-temperature membrane development requirement to meet overall DOE objectives.
- The goals and objectives of the project are designed satisfactorily.
- The multi-year plan is in line with DOE RD&D objectives.
- Anhydrous proton-conducting membranes can enable higher temperature fuel cell operation enabling potentially simpler and less expensive systems.
- The work is in line with task 1, barriers A, B, and C, to develop membranes that meet all targets.
- Membranes that can operate in a wide range of conditions, including 120°C and low relative humidity (RH), are critical to meeting the performance and system cost targets for stationary and automotive fuel cells.
- The objective of this project, to fabricate durable membranes that operate in a fuel cell without external humidification at moderate temperatures (at most 120°C), is highly relevant to DOE.

Question 2: Approach to performing the research and development

This project was rated **3.0** on its approach.

- The approach is sound with a strong synthetic approach to prepare tethered imidazole membranes. The PI understands the strengths and shortcomings of imidazole and is making the necessary adjustments.
- The blending of imidazole with perfluorinated sulfonic acid (PFSA) type materials, however, seems rather banal compared to the rest of the program, and it is unclear how much value it is in both the near term and long term.
- The project has been designed appropriately to address the technical barriers of low RH conductivity.
- The approach of the project is good and its outcome will address some of the key technical barriers.
- The technical feasibility of the synthetic route to an oxidatively stable ionomeric polymer is doubtful.
- The oxidative stability of the new polymer should have been considered.
- The grafted imidazole polymer possesses benzylic hydrogen, which may affect the durability of the membrane.
- Developing a material that can use Grotthus-hopping within a polymer is a unique approach.

- This is a truly novel approach borrowing heavily from technology used in the battery industry. The team could potentially develop a truly anhydrous proton conductor.
- The water-free membrane is a very ambitious goal, and the primary focus on synthesis and conductivity is appropriate.
- The use of membrane-bound (grafted) heterocycle acids and bases, ionic liquids, and doped polymers is not a new approach; other researchers have investigated similar approaches, with limited success. It appears that the PI is mostly working on polymer synthesis.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated **2.3** based on accomplishments.

- For the amount of funding this project has received, it appears that the rate of progress is quite low. An undergraduate summer student performed the largest amount of work. While the reviewer understands the difficulty of synthesis for this type of chemistry, the work thus far is lackluster.
- The conductivity efficiencies of proposed new polyelectrolyte material are not known.
- If the new polyelectrolyte functions, as proposed by the team, then the benefit would be immense.
- The blend of Nafion® and grafted imidazole polymer may not possess phase compatibility.
- The technical progress had been good, and the development plan is satisfactory.
- Polymers were made to enable conductivity measurements, which is a major step forward from last year.
- Conductivities with free-acid electrolytes are below DOE target conductivity at 120°C, and significantly lower at lower temperatures. No rationale is given to lead one to expect that the systems with polymer electrolytes would have higher performance. Nafion®-containing membrane conductivities are still at least an order of magnitude too low.
- Modeling results do not clearly establish that DOE target conductivities are possible with this approach.
- Oxidative stability to Fenton's test was done, but not sufficient to prove oxidative stability.
- As would be expected from this team, there is a large amount of good science. Unfortunately, the conductivities achieved are still rather low.
- The project team has made good progress, but membrane conductivity needs significant improvement to reach targets.
- The PI's results are not particularly encouraging. The measured proton conductivities are generally low (too low for the membranes to be used in a fuel cell).

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated **3.3** for technology transfer and collaboration.

- Collaboration can be seen with LANL for the membrane electrode assembly (MEA) fabrication, and 3M for their PFSA material; however, the overall level of effort seems to be quite minimal.
- The project has good collaborative effort for the proposed development work.
- There has been good technical interface and information-sharing among the concerned groups.
- The project has an industrial partner as well as other national laboratories.
- Overall, the project possesses good teamwork.
- The team with 3M, LANL, and Berkeley provides a comprehensive skill set including world class materials, synthesis, modeling, and characterization capabilities.
- It appears as though this team of national lab/university/industry is working very well together.
- There has been good interaction with partners and analytical facilities.
- There is some collaboration with other national labs, such as ORNL and NIST. Michael Guiver of the National Research Center in Canada provided polymers for testing. More collaborations are needed. Why not collaborate with other high-temperature membrane researchers?

<u>Ouestion 5: Approach to and relevance of proposed future research</u>

This project was rated **2.8** for proposed future work.

- Proposed future work is in line with the project. The addition of molecular dynamics modeling to understand the potential proton conductivity limits of this material would be highly useful for the go/no-go decision.
- The future research with imidazole end group modification of PFSA polymer would not give a stable membrane.
- The siloxane modified route to new polyelectrolyte is not expected to give an oxidatively stable polyelectrolyte.
- Working with 3M, low EW PFSA and functionalized block copolymers to blend/attach/copolymerize with imidizoles is a good path forward.
- Fenton's test is not recommended. The team should wait until stable membranes can be made and then run DOE open circuit voltage test.
- Approaches towards practical proton conductivities should be emphasized. There needs to be more studies involving water and fuel cells that make water, because it will not do any good if an anhydrous proton conductor is developed that is sensitive to moisture in a bad way.
- It is a good plan with go/no-go decision criteria in place.
- It is not clear if the proposed future work will produce a usable fuel cell membrane. It is doubtful that a conductivity of 0.1 S/cm at 120°C and <25% RH can be attained by continuing to attach imidazolium groups to polymers. The PI did not explain the connection between the future work on membrane fabrication and the future work on the oxidative stability of polymers. Why work on the latter when the membrane properties are not yet at DOE targets?

Strengths and weaknesses

Strengths

- The PI is a world leader and this project is a great concept that, if successful, will be very valuable to the fuel cell community.
- It is a good group with a solid knowledge base of fuel cell fundamentals.
- There is good interaction between the collaborative groups.
- The team has taken a good fundamental approach in understanding the major technical barriers of low RH proton conductivity.
- The team has exhibited excellent collaboration.
- The team has improved and reduced focus from last year to imidizole/sulfonic acid systems.
- The team's very high level of scientific understanding should lead to a truly unique material that could be a practical proton conductor.
- The team is using novel polymer chemistry combined with known materials and techniques.
- The PI has a good reputation in the field of membrane fabrication. The PI has pursued many different approaches.

Weaknesses

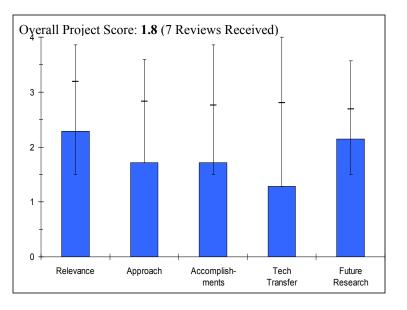
- Progress to date with this level of funding is quite low.
- No measures have been in place to evaluate the oxidative stability of the proposed electrolyte materials.
- The new polyelectrolyte material may be interesting to study, but it is not expected to give the long-term stability under fuel cell conditions.
- The oxidative stability of the polymers developed in this project is doubtful.
- The materials-to-date are still relatively poor conductors.
- The materials do not run well when wet.
- There is not enough thought towards practical proton conductivity.
- The proton conductivity results to-date are not encouraging. The PI's primary approach (tethering imidazoles to polymers with acidic functional groups) has not produced interesting materials with the potential for use in a fuel cell.

- The work should continue as planned. The hiring of motivated/well-qualified scientists for this project is highly important for the overall success. To-date, the work done is below where it should be.
- The PI should consider evaluating the oxidative stability of any new polyelectrolyte material.
- The backbone change to manipulate the polymer morphology should be reconsidered, and the approach should be changed to synthesize oxidatively stable polyelectrolyte.
- The team should include mechanical and swelling characterizations of membranes.
- The team should study conductivity versus RH, not just temperature. The materials might actually work okay at 50% RH, but there is no data.
- Modeling efforts should be increased to understand fundamental limits of the approach.
- The project team should look at the effect of moisture.
- It is not clear why the PI is looking at the oxidative stability of membranes with imidazolium groups when such membranes do not possess the requisite proton conductivity for use in a fuel cell. Similarly, MEA fabrication studies with hydrocarbon polymers appear to be premature. The PI should focus on new membranes with properties (e.g., proton conductivity) that are much improved as compared to what has been achieved so far on this project.

Project # FC-15: Development of Novel PEM Membrane and Multiphase CFD Modeling of PEM Fuel Cell Susanta K. Das and K. Joel Berry; Kettering University

Brief Summary of Project

The overall objectives are to develop a 1) novel proton exchange membrane (PEM) for fuel cells; and 2) multiphase computational fluid dynamics (CFD) model of a PEM fuel cell for improved water and thermal management. Objectives for 2008-2009 were to 1) perform real-time membrane testing for a single cell, and stack and real-time testing for stability and materials properties for a low-cost, highperformance membrane; and 2) conduct a performance evaluation for different parametric conditions for the integrated multiphase CFD model for PEM fuel cells.



Question 1: Relevance to overall DOE objectives

This project earned a score of 2.3 for its relevance to DOE objectives.

- This project partially supports the Hydrogen initiative and the DOE RD&D objectives.
- The major focus of the project should have been on the membrane conductivity at low RH, high temperature (120°C, 50% RH). There is no consideration of this goal.
- Membranes are not tailored for automotive (dry) conditions.
- CFD tools are not novel.
- The membrane development work addresses the DOE R&D objectives. The researchers have not made it clear how the work on the control strategy for the stack addresses the barriers listed.
- The project looks at new membranes that need water for conductivity. CFD modeling was used to predict water flow in cell to optimize performance. This project does not try to make a membrane that works at reduced RH.
- Membranes for high-temperature operation and water and thermal management are important issues and are aligned with DOE goals and objectives.
- The project goals of developing a novel PEM for fuel cells and developing a multiphase CFD fuel cell model for improved water and thermal management are highly relevant to DOE. These two project tasks are very different, and one does not support the other.
- The project title and intent was definitely relevant, but the execution was not because the membrane work was too early stage and the CFD modeling was simplistic.

Question 2: Approach to performing the research and development

This project was rated 1.7 on its approach.

- The nature of the membrane material and its synthetic approach is not clear.
- The CFD approach to provide a better gas diffusion layer (GDL) and flow channel designs is good.
- More information on the membrane material would have helped in understanding the approach to solve the membrane conductivity barriers.
- Membrane materials were not disclosed, so synthesis approach cannot be effectively judged.
- The conductivity method is questionable and, after three years, has still not been benchmarked against accepted direct current (DC) or impedance-based methods.
- The results were not reported in units that allow comparison to literature data or those from other DOE projects.
- Conductivity model fits data too well to be meaningful and provides no fundamental basis.

- It is not very clear from the information presented if these materials are suitable for use in PEM fuel cells.
- The measurements are unusual and probably not useful. The induction time just shows that the membranes are very swellable and take up lots of water. The approach is not designed to solve DOE's stated goals.
- Non-standard approaches are used for proton conductivity presented in nonstandard units. This makes it difficult to compare to other materials. Unusual dependence of resistance on temperature observed for Nafion® suggests there is more being measured with their technique than membrane resistance; others do not see this unusual dependence. The membrane properties desired are higher conductivity under hotter-drier conditions. Their technique does not allow one to determine conductivity under drier conditions.
- Chemical and mechanical durability of membranes are also important issues. They are not addressed at all here. Without any knowledge of the chemistry of the membrane begin presented, durability is of concern.
- The modeling appears to lack validation with experimental data.
- It was very difficult to assess the PI's approach. Very few details were presented regarding the composition of the PEM. A standard AC impedance method was not used to characterize the membrane, for reasons not well understood. It was not clear how the PI's CFD modeling work differs from that of other investigators.
- The first half of the presentation was on membrane development, but membrane chemistries were not revealed nor were the membranes compared to others (except for a simplistic and erroneous comparison to Nafion® 212). The error was a comparison based on electrolysis (for conductivity and resistance) rather than direct fuel cell comparisons. What about comparisons to other polymer systems, too? And why not use accepted fuel cell characterizations?
- CFD's work, as explained during the presentation, was simplistic and the questions from the audience were not answered satisfactorily.

Ouestion 3: Technical accomplishments and progress toward project and DOE goals

This project was rated 1.7 based on accomplishments.

- The conductivity of styrene-acrylonitrile-vinylsulfate (SAS)-type membranes should have been measured in true fuel cell conditions.
- The measurement of proton diffusion is not the correct way of measuring the proton conductivity of the membrane.
- The proton transport can happen if there is a pinhole in the membrane leading to leakage of HCl acid to the water chamber.
- No temperature or RH cycling work was done.
- No new membrane data was shown since last year's review except one set of conductivity curves from BekkTech.
- No new dynamic model simulation data was shown either.
- Based on the data presented in the "conductivity test" developed by Kettering, they may be measuring the permeability of the membrane to chloride. The conductivity data from BekkTech was far below the target.
- Measurements seem to be inappropriate and most unusual. Conclusions drawn are not straightforward and probably incorrect. Membranes need to have conductivity measured by standard methods. The PI seems to pay no heed to other groups working in the field.
- Measurements suggest they may have very good conductivity under high (100%) humidity conditions. This is not the area of interest. There also appears to be some other factors being measured, since the temperature dependence of the Nafion® resistance shows an unusual temperature dependence not observed in other studies. It is not clear that they have isolated protonic mobility from other mobile species (Cl-) in their measurement. Initial tests from BekkTech show less than stellar conductivity under lower humidity conditions.
- Some results (e.g., the dependence of temperature on the maximum in the proton transfer capacity) could not be explained. It was not clear how water uptake was measured, or if the PI's membrane is a satisfactory proton conductor.
- Solid work, if we were focused on developing HCl electrolysis membranes, but our focus should be on fuel cell membranes. The speaker revealed that no fuel cell tests were conducted on these membranes and no fuel cell data (of substance) was presented.
- Unusual and unexpected "humps" in the Nafion® 212 resistance measurements were not explained when the question was posed. There may be experimental errors in the resistance curves were presented.

<u>Ouestion 4: Technology transfer/collaborations with industry, universities and other laboratories</u>

This project was rated **1.3** for technology transfer and collaboration.

- There is no collaboration with any of the leading national labs.
- There is no interaction with any other academic institutions.
- Bei-Tech provides polymer membranes. No other collaborations were evidenced.
- The researchers need to work with someone who has expertise in evaluating fuel cell membranes.
- Collaboration is non-existent.
- BekkTech was mentioned as a collaborator, but the team was having difficulty getting conductivity measurements from them, so collaboration appears to be ineffective. They do not appear to have other collaborators. Collaboration with others in the field would be useful in validating their measurement technique or in allowing them to measure their membrane's conductivity using standard techniques/protocols.
- There was essentially no collaboration. The slides list Bei-Tech as a collaborator for polymer membranes, but their role on the project is not clear.
- The only collaboration involved the Bei-Tech membranes, but beyond the supply of the membranes, no useful data (to build further work on) was presented.

Question 5: Approach to and relevance of proposed future research

This project was rated 2.1 for proposed future work.

- The crosslinked membrane stability in the fuel cell environment may be a problem.
- The team needs to do temperature and RH cycling to understand membrane stability.
- The conductivity must be reported in S/cm or resistance as ohm-cm² and compared to literature data.
- Membrane durability should be considered and evaluated (mechanical and chemical).
- CFD work needs a stack partner for relevance and validation.
- Future plans are not well developed. No viable follow-on is proposed.
- The project is near completion and plans are to wrap-up.
- There was no connection between present results and future work. For example, the PI lists as future work: polymer crosslinking to make the membrane chemically inert towards reactant gases; however, no data were presented showing polymer degradation. Also, it was not clear why the PI wants to map water history.
- The approach was good because the team was finally going to move to fuel cell tests.

Strengths and weaknesses

Strengths

- The project team conducted good CFD modeling work.
- There was industry engagement in membrane fabrication.
- The CFD modeling work appears to be sound, although the reviewer is not an expert in this area.
- The team had a solid defense of their system as an electrolysis membrane based on a single-cell test.

Weaknesses

- The team lacked the use of proper membrane evaluation methods.
- There was no fuel cell performance data for SAS membranes.
- There is a need to get true conductivity data of SAS membranes.
- Based on the data presented, the "conductivity test" developed here may be measuring the permeability of the membrane to chloride. The conductivity data from BekkTech was far below the target.
- The approach is wrong. The execution appears to be done in the absence of checking with the literature. The nature of the membrane is not revealed. It appears to be a mystery. If this is patented, then why is there not a proper description of the membrane materials? The project does not try to address DOE goals.
- There was a lack of information on the proprietary membrane composition. Unusual non-standard techniques were used to evaluate membranes under conditions that we are not very interested in. These techniques cannot obtain information on proton conduction in the region we are most interested in.

- The membrane fabrication and characterization work is weak. Critical details were missing from the presentation. Standard methods for evaluating the membrane were not used. Membrane performance that was presented was confusing and could not be explained adequately.
- Apparently, very early-stage work was done with no cross-references to an established body of literature on the many polymer chemistries explored by other researchers. A defense of why they chose their membranes (with a revelation of the chemistry) would have been a necessary first step.
- Work displayed shows relative "immaturity" of the team in this arena.

- The team should include real fuel cell and membrane conductivity measurement methods in this project.
- The project is to end next month. Please do not renew.
- This project should be discontinued.
- There is a disconnect between the membrane fabrication work and the CFD modeling. My recommendation is that the membrane work be dropped from this project.
- Drop funding for this effort, unless further basic background work is conducted or presented. Include a body of past literature research and why they chose the membrane for scale-up relative to the many membrane developments already underway. The team should also include fuel cell test data.

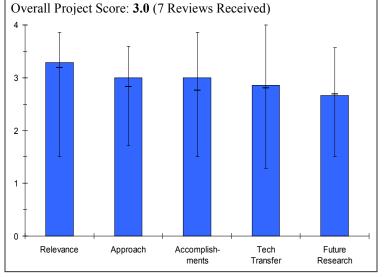
Project # FC-16: Applied Science for Electrode Cost, Performance, and Durability

Christina Johnston, Eric Brosha, Fernando Garzon, Andrea Labouriau, Marilyn Hawley, Rex Hjelm, Yu Seung Kim, Kwan-Soo Lee, Nate Mack, Bruce Orler, Tommy Rockward, Dennis Torraco, and Cindy Welch; Los Alamos National Laboratory

Piotr Zelenay and Karren More; Oak Ridge National Laboratory Bryan Pivovar; National Renewable Energy Laboratory Hui Xu; FuelCell Energy

Brief Summary of Project

The overall objective of this project is to assist the DOE Hydrogen, Fuel Cells & Infrastructure Technologies Program in meeting cost, durability, and performance targets by addressing issues directly associated with electrodes. For 2009, LANL will 1) explore the impact of solvent choice in catalyst ink on fuel cell performance; 2) relate the structural and chemical properties of the ionomer in different inks to electrode performance and structure; and 3) initiate use of bilayer/gradient structures in electrodes.



<u>Ouestion 1: Relevance to overall DOE</u> <u>objectives</u>

This project earned a score of **3.3** for its relevance to DOE objectives.

- The objectives of this project align well with the DOE program. Membrane electrode assembly (MEA) optimization is often an overlooked area of research, which can provide substantial performance and durability improvements without changing the basic components, such as membranes, electrodes, ionomers, and gas diffusion layers (GDL).
- The project directly addresses a fundamental understanding to correlate electrode processing with performance to provide insight for improved performance and durability, and to a lesser degree, potentially reduced cost.
- A fundamental basis for optimizing electrode structure based on physical properties of the components is critical for developing new electrode materials.
- Work is in line with task 2, barriers A, B, and C, to develop electrodes that meet all targets.
- This program is indeed relevant to the development of polymer electrolyte membrane fuel cell technology, and thus to the overall DOE Hydrogen Program. Understanding the catalysts' ink composition and the required catalyst structure to achieve the highest platinum utilization is one of the key components in designing the MEA. Most project aspects are aligned with the Hydrogen Program and DOE RD&D objectives.
- The project seeks to address the cost and durability of proton exchange membrane fuel cells (PEMFC) by examining parameters associated with catalyst inks. Since catalyst inks have not been dismissed as irrelevant to commercial PEMFCs, this project is still relevant. However, DOE should carefully think about the extent to which a catalyst ink processing project will achieve results that meet commercialization targets. The results of this project will be incremental at best.

Question 2: Approach to performing the research and development

This project was rated **3.0** on its approach.

• The overall approach is very strong, and the area researched is very interesting with a lot of valuable information for the fuel cell community.

- The biggest weakness of this approach is the focus solely on decal LANL-type MEAs. Many companies are now also working on spray, die-coating type, and screen-printing type electrodes, and the reviewer wonders how transferable the findings here are.
- The team has taken a well-defined approach that provides good baseline systems for understanding correlations at the particular length scale of each technique, while enabling integration of the knowledge across broader length scales. The approach includes both baselining activities and experiments designed to test the theories that emerge from the initial studies. The approach does a great job of isolating individual effects (e.g., ionomer structure, catalysts, gradient structures) and their impacts to develop a complete understanding of the complex electrode structure. Electrode processing materials and methods are relevant for practical fuel cell systems, so that results from this fundamental research project should be readily transferred to more applied projects.
- Studying the effect of ionomer and solvent on performance is a valuable approach.
- Characterizing the ionomer properties is also valuable.
- More focus should be applied to studying the electrode pore structure and the structure of the ionomer within the electrode.
- Looking at degradation and changes in electrode properties over time/cycling is a positive approach.
- The industrial manufacturers have almost certainly optimized their electrode assemblies using the tools available to them. This project needs to emphasize the advanced instrumentation that can only be used at national labs, rather than repeating anything empirically.
- The approach developed for probing structural properties of MEAs is multifaceted and, if utilized effectively, could contribute significantly to overcoming technical barriers related to structural properties of ionomers. The authors used a variety of spectroscopic and structural techniques to probe the effect of solvents on physico-chemical properties of Nafion®. Hopefully in the future, equally successful probes will be developed to probe the stability of the catalyst layer itself. Therefore, the approach could be improved.
- The conclusions derived (especially about mobility and solvent interactions) could have been derived equally as well without resorting to the sophisticated methods employed.
- It is not clear as to what has prompted the choice of solvents.
- Many in the industry will expect that this project is too applied of an effort for government funding; in other words, it should be expected that MEA manufacturers will understand performance and durability differences that stem from processing. Polarizations and transmission electron microscopy (TEM) images that show very subtle differences based on solvent choice, confirm the suspicion that ink processing studies will result only in incremental improvements that ultimately do not address the commercial PEMFC targets.
- Despite the implications towards long-term targets, the researchers themselves excellently crafted a hypothesis and the means by which to test it. The hypothesis was that ionomer history would be preserved on a molecular scale, and that the effect of this would be realized in fuel cell testing. In this sense, the approach was simple and elegant. Perhaps more importantly, the approach was universal and can be applied for all ink processing.
- Results from the bilayer task were somewhat expected. More interesting results might be produced by looking at lower ionomer content in different parts of the catalyst layer, rather than higher.
- In my opinion, this is a weak part of the program. The success will be measured based on understanding the properties of the catalysts layer, rather than the ionomer itself. The authors should focus more on degradation of platinum catalysts including platinum bi/multi-metallic surfaces.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated **3.0** based on accomplishments.

- A lot of high-quality work has been done at this time with some very useful data and findings. However, more temperatures and relative humidities should be investigated to confirm/understand their effect.
- The project team has made significant progress in correlating processing solvent with electrode microstructure and validating emerging theories about impact of ionomer structure and mobility. Their experiments are well defined with appropriate interpretation at the relevant length scale. The team is beginning to combine information from several analytical techniques to develop a complete suite of ideal electrode features and the necessary processing materials and methods to achieve improved electrodes. This is a very challenging project that has already demonstrated that there should be approaches to improving both mass transport and kinetic performance.
- Significant progress has been made since last year.

- Performance results have been correlated with ionomer properties based on nuclear magnetic resonance, small angle X-ray scattering, and TEM/atomic force microscopy.
- The solvent type has been shown to affect both performance and durability.
- The value here would be to emphasize the application of advanced instrumentation; solvent effects are well known by the industry. Industry needs to be given detailed mechanisms here for this project to be more useful.
- The results obtained are ambiguous; however, more time should be provided to the team to work through the research objectives and tasks.
- Despite the concerns that the approach of this project is not suitable for government funding, it must be acknowledged that the actual project execution has improved tremendously from the past year.
- The researchers have done an excellent job in attempting to rationalize why certain solvents represent the changes that they see in different regions of the polarization curve, by exploiting NMR, small angle neutron scattering, and AFM. However, where inconsistencies exist (e.g., water), it would be interesting to find some deeper explanations. Are mobility and phase separation truly enough to explain all the data?

<u>Ouestion 4: Technology transfer/collaborations with industry, universities and other laboratories</u>

This project was rated 2.9 for technology transfer and collaboration.

- Collaboration at this time is limited but fruitful. Excellent characterization of MEAs is ongoing with one of their partners. The team may want to bring on-board an MEA fabricator to help the PI understand in more depth the industrial realities.
- The team leverages other national lab expertise in analytical characterization methods to interrogate relevant length scales over a broad range. The project goals could not be achieved without these interactions.
- Collaboration with ORNL provides opportunity for structural characterization.
- The project could benefit from collaboration with an MEA supplier.
- There needs to be much more industrial collaboration.
- The program is multifaceted and the PI successfully built a team of experts capable to deal with the projected challenges.
- Collaborations exist and are being leveraged.
- ORNL has been used in the past by this project, but this year's work does not obviously show where they contributed.
- The role of NIST is not entirely clear.
- The use of an industrial partner would seem to be an obvious step for this project.

Question 5: Approach to and relevance of proposed future research

This project was rated 2.7 for proposed future work.

- Proposed future work is okay, but it would be nice to see the expansion to different types of MEA fabrication techniques and more in-depth fuel cell studies such as temperature effects, RH effects, and durability.
- The team will build on recent work understanding ionomer structure, mobility relationships, and gradient electrodes by expanding the range of solvent systems, incorporating catalysts into the systems, and adding that layer of understanding.
- The proposed work on Nafion® interactions with catalysts will be very important.
- I would recommend not focusing on multi-layer/gradient structures in favor of the ionomer/carbon/catalyst interactions.
- The plan to look at different carbon dimensions should be interesting. I would like to see different carbon types also investigated.
- Again, emphasize the light sources, neutron sources, and the microscopy at ORNL.
- The proposed work is good, and if executed, may significantly improve the understanding of MEA interfaces.
- The proposed work seems to branch out into numerous directions, and a more focused approach using a single model system would perhaps yield more tractable results.
- There is no end to the parameters to consider in ink processing, but considering the effects of catalyst and temperature is a good start. Stir rate, fluidization dynamics, temperature ramps, and time involved in

temperature hold and drying are just a few more parameters that could be studied (or have been studied, but perhaps not with the rigor demonstrated by this past year's project performance). Unfortunately, the project is boxed into a situation where either a large number of parameters must be studied, or else the results are only relevant to a very particular ink processing scheme.

• It would be significantly better (if an ink processing project must be done) to take an industrial partner's experience and direction and combine that with LANL's analytical prowess (both in terms of instruments and scientific expertise) to begin blocking off whole regions of parameters that are undesirable. Then, begin attacking what the true issues are for processing. Is solvent choice truly something that Gore or DuPont is still agonizing over? It would be interesting to bring them into this and find out, but without allowing the industrial partner to take away the universality of the project.

Strengths and weaknesses

Strengths

- World-class fuel cell team investigating a very important fuel cell topic.
- Great fundamental research designed to provide relevant practical results/impact.
- There is a strong combination of thorough material characterization with fuel cell testing.
- The fundamental approach to understand the dynamic and structural properties over the range of relevant length scales is a strength.
- Builds on LANL's fuel cell expertise.
- This is a well-organized project with a clear goal to understand the MEA interface. However, the question of how much this will help in improving fuel cell performance still remains. The approach used in this work could contribute significantly to overcoming technical barriers related to structural properties of ionomers.
- This is a strong team.
- Analytical techniques have been used to draw simple and elegant conclusions regarding set hypotheses.
- There has been experimental execution.
- The results are interesting and thought-provoking.

Weaknesses

- Due to the inherent strength of the team, the reviewer wonders if the PI looks outside enough to see the changes in the fuel cell community.
- None.
- The focus has been on bulk ionomer properties. The ionomer properties of very thin films in an electrode are likely to be very different, and it would be great if the PI could make progress in better understanding the properties of the ionomer in the electrode.
- The team has spent too much time reinventing the wheel; there needs to be a higher level of science.
- The program should focus more on testing catalyst layers. Furthermore, the PI should focus more on science and less on testing; the latter should be done in collaboration with an R&D program of industrial partners.
- There is a lack of focus.
- The overall premise that this is the right work for government funding is questionable.
- Collaboration with parties who would have a lot to say on the topic is missing.
- There is a lack of confirmation that the parameters being studied are the ones that would have the most impact on cost and durability of PEMFCs.

Specific recommendations and additions or deletions to the work scope

- The reviewer would like to see the expansion to different types of MEA fabrication techniques, such as spray, die-coating, and screen-printing.
- More in-depth fuel cell studies need to be done, such as temperature effects, RH effects, durability, etc.
- More focus is necessary on the impact of process conditions such as drying temperature and rate.
- More focus is necessary on bulk electrode properties such as pore volume and sheet resistance.
- The team should correlate performance losses during voltage cycling with electrochemical surface area loss.
- More characterization is necessary (both ex situ & fuel cell testing) at lower RH.
- The team should emphasize using advanced instrumentation to really study this problem.

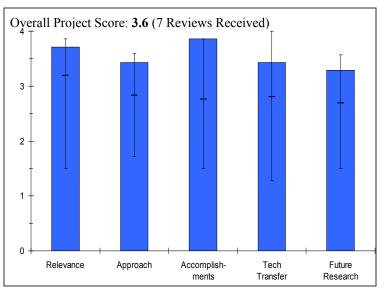
FY 2009 Merit Review and Peer Evaluation Report

- This is a very good team of people who should be permitted more time to study the issue; however, a more focused approach with fewer variables in terms of materials should be recommended.
- An industrial partner must be added.
- With recommendations from an industrial partner, the team should focus the project on the true issues in ink processing and figure out what parameters could make the greatest impact on cost and durability of PEMFCs.
- Perhaps the project could be changed entirely to look at new electrode structures for ultra-thin catalyst layers. Is it always true that a catalyst layer of 1 µm or less must be plagued by flooding at lower temperatures? That would be more interesting in a world where catalyst loading has significantly decreased. To what extent do large and small hydrophilic pores help or hurt water transport? Are hydrophobic pores necessary to avoid flooding?

Project # FC-17: Advanced Cathode Catalysts and Supports for PEM Fuel Cells *Mark K. Debe; 3M Company*

Brief Summary of Project

The overall objective is to develop a durable, low-cost, high-performance cathode electrode (catalyst and support), that is fully integrated into a fuel cell membrane electrode assembly with gas diffusion media, fabricated by high-volume capable processes and is able to meet the 2015 DOE target. The objectives of this project for the past year were to 1) define and implement multiple strategies for increasing nanostructured thin film (NSTF) support surface area, catalyst activity, and durability, with total loadings of <0.25 mg-Pt/cm²/membrane electrode assembly (MEA); 2) work closely with subcontractors to fabricate and screen new electrocatalysts using high throughput characterization



methods for activity and durability gains; 3) conduct fundamental studies of the NSTF catalyst activities for oxidation reduction reactions; 4) apply more severe accelerated tests to benchmark the NSTF/MEA durability; 5) define and implement multiple strategies to optimize the MEA water management; 6) advance the high-volume roll-good NSTF catalyst/membrane integration; and 7) work closely with system integrator to validate NSTF functional properties/issues.

Question 1: Relevance to overall DOE objectives

This project earned a score of **3.7** for its relevance to DOE objectives.

- This project is critical to the Hydrogen Program. The research addresses all major objectives of the program, and results are above the DOE targets on several technical barriers.
- The project is critical to the Hydrogen Program as it focuses on implementing DOE goals on development of new durable supports and highly active catalysts. It is highly relevant because it offers a new approach to MEA development and manufacturing.
- This project is extremely relevant to the DOE goals for reducing the cost and improving the performance and durability of polymer electrolyte fuel cell (PEFC) power systems. These are the critical barriers to implementation of PEFC power systems for a variety of applications.
- This program is forging ahead toward the metrics needed for fuel cell catalysts needed to transition an affordable and durable fuel cell vehicle. They have made outstanding progress on all fronts. The main problem with the program is that the DOE metrics might be somewhat irrelevant for this class of catalysts where the water management at high power is the major problem for transition. That is, they might be able to achieve the activity and durability metrics, but the catalyst morphology may not be inherently useful for vehicle applications. Mark Debe said, though, that they are moving toward more focus on water management issues and explained that they needed to work on the scale-up first before they could answer this problem meaningfully. With more time, hopefully the water management problem will be addressed.
- The 3M project is dead-on target to address the necessary targets that make fuel cells commercial, low cost, high performance, and of extended durability.
- Thanks to making improvements to MEA performance and especially durability its primary target, this project is very relevant to DOE objectives.

Question 2: Approach to performing the research and development

This project was rated **3.4** on its approach.

- The research is focused on technical barriers; my reservation pertains to the combinatorial design of the catalysts. Stability and surface segregation in these mixtures usually invalidate initial activity. Scientific support for selecting the compositions is desirable, in particular for binary catalysts.
- The project is well designed and addresses multiple aspects of the development of practical fuel cells.
- The team has taken a good approach, with considerable coordination with other research groups. It would be nice to see more corroboration with stack integrators.
- The approach leverages the higher durability and activity of bulk-like Pt catalysts, but achieves low Pt loadings by dispersing this catalyst structure as a thin film on a high surface area structured support.
- This 3M team has the intellectual and experimental horsepower to address the multiple complexities associated with the scale-up and commercialization of the 3M MEAs. They have a complex approach, which is needed to solve the problems.
- Dr. Debe has shown consistent excellent planning, thoughtful evaluation, and focused direction on a very complex, multidimensional technical problem.
- 3M has pursued the NSTF approach for many years by now. It remains promising, but significant challenges remain; they need to be addressed.

Ouestion 3: Technical accomplishments and progress toward project and DOE goals

This project was rated **3.9** based on accomplishments.

- With the exception of Pt mass activity, results are better than the DOE targets on several technical barriers.
- The project already met almost all DOE targets for 2015.
- The team has shown impressive effort, with combination of fundamentals and in-cell demonstration. The team is asking and answering some key questions about the correlation between ideal catalyst systems and practical MEAs.
- It is important to understand the value of exchange-current density at varying oxide states, allowing correlation between *ex situ* rotating disc electrodes and in-cell MEAs.
- The team exceeded DOE's 2015 inverse power density target for MEA.
- The team met the DOE activity target of 0.44 A/mg platinum group metal (PGM) in rotating disk electrode (RDE) experiments, but not in MEA.
- The team has made excellent progress in developing and improving the activity of MEA, and in meeting the durability targets.
- Tremendous progress has been made within the goals of the DOE metrics.
- Too many reviewers thought the DOE milestones were perhaps too aggressive, but they have been addressed and met, way ahead of schedule and under budget. This is just a success story!
- There was very good high-current response in fuel cell testing, but not so good at low currents, in which range there has been no improvement since 2007 (possibly caused by the lower catalyst loading though). Would higher cathode catalyst loading result in needed better low-current performance?
- It is not clear whether performance improvements distribute equally between the two fuel cell electrodes. Lowering catalyst loading on one electrode rather than both at the same time would provide better insight into the sources of observed improvement.
- What was the reason for using very high catalyst loadings in RDE testing? While obviously helping the RDE data appearance, this seems to be causing lots of confusion in the electrocatalysis community. Testing at lower loadings would be desirable.
- What was the outcome of GM testing? The "real-world gaps and issues" should have been spelled out in this year's presentation, rather than merely mentioned in the summary.
- In spite of previous declarations to the contrary (see responses to 2008 reviewers' comments), there has been little data and no emphasis on water management in the past year.

<u>Ouestion 4: Technology transfer/collaborations with industry, universities and other laboratories</u>

This project was rated **3.4** for technology transfer and collaboration.

- The collaboration with excellent national laboratories and university teams seems quite successful.
- There is close collaboration with universities, national labs, and industrial partners.
- There is very good corroboration and collaboration.
- This is an excellent team with varied and complementary expertise.
- It appears that the choice of catalyst composition is not based on RDE experiments, but on MEA tests, and also that the catalysts are treated differently for RDE and MEA tests (intrinsically acid-washed vs. not acid-washed), so what is the value of RDE experiments? It was also not clear if the post-fabrication processing of catalysts performed at ANL was just for the RDE experiments, or if it is being implemented in the catalysts that are fabricated into MEAs.
- It is not clear if the Dalhousie and Jet Propulsion Laboratory (JPL) work led to the identification of the best of class catalyst (PtM), or if it has guided the choice of catalyst compositions used in the present MEAs or in previously studied MEAs. In particular, the JPL results were not included in presented material.
- The 3M team is very big, but seems to be managed appropriately. The program recognizes how many problems need to be solved to commercialize the 3M membranes, and has the right team to solve the problems. The role of JPL was a bit unclear.
- The collaboration is outstanding, especially because the partners have very clearly defined and supporting roles. One understands that there is one project, and several excellent groups all singing on the same page, but not the same notes. This is another result of Dr. Debe's management style, building a well-functioning team.
- There has been very good collaboration between 3M and Argonne, but the roles of two other partners in the project are not well defined.
- The impact of Dalhousie's University combinatorial testing is unclear. In spite of a significant amount of the Dalhousie data in the presentation, the University seems to have played a rather limited role in the progress achieved.
- There has been little contribution from JPL to the project in the past year. The Laboratory's role should be either enhanced, or its participation re-considered.

<u>Ouestion 5: Approach to and relevance of proposed future research</u>

This project was rated **3.3** for proposed future work.

- The plans address some remaining obstacles to prototypes construction, including stack testing, durability, Pt mass activity, and water management.
- Future work is carefully planned and built on past progress.
- In light of program success, it is suggested that the team scale back or redirect to go after the remaining problems more aggressively, rather than staying on the current path.
- The biggest challenge with the NSTF-based MEAs appears to be water management; therefore, the future proposed work focused on gas diffusion layer development/optimization is on target.
- The 3M team should put less emphasis on the global DOE metrics for catalysts, and focus on the metrics that are specifically a problem for the 3M MEAs.
- Dr. Debe discussed the need to rethink the tail end of the project, being in the unique position of having pretty much crossed the finish line, well ahead of the pack. The next phases need some careful thinking.
- Focus on water management, including testing under "wet" conditions, is necessary. Results need to be summarized in next year's presentation, which has been long overdue.
- The effect of impurities on NSTF-based catalyst performance, especially at the cathode, should be studied.

Strengths and weaknesses

Strengths

- There are excellent teams at 3M, national laboratories, and the university.
- There are possibilities for large-scale catalyst production.

- The team executed good planning of critical research tasks.
- The team showed creativity in development of new catalysts.
- The team took a unique technical approach with good effort on fundamentals. Explaining the difference between model systems and MEAs is of primary value.
- The greatest strength of the project is the unique approach that combines the stability and area-specific activity of bulk catalysts with a unique support and dispersion technique that allows high dispersions (cm²/g catalyst). Another strength of the project is the rolled-goods approach to manufacturing.
- This is a very good team solving a complex problem.
- Dr. Debe has this wonderful combination of profound theory mixed with a very good pair of highly capable hands.
- The theory suggested new, complex nanostructures, and the hands worked to make those visions real. It was a team effort, and required the technical excellence of a company that made its fortune by coating material rolls of highly controlled uniformity. This success would have been very unlikely outside of the 3M corporate excellence, the people who began with sand paper, "Scotch Tape", and now NSTF electrodes.
- The team showed excellent MEA durability in 3M fuel cell testing.

Weaknesses

- There was a lack of characterization with atomic resolution.
- There are no weaknesses.
- I would like to see more third-party stack verification and characterization of mass-transport issues.
- The unique architecture that allows high dispersions on chemically and electrochemically stable supports also presents challenges in terms of removal of water from the electrode layer. 3M believes they can overcome this challenge with the correct design of the microporous layer (MPL) and gas diffusion layer (GDL). This next year will be critical to see if they can address these challenges.
- It's not clear if the water management problems associated with this class of MEAs can be solved. More research in the next few years should show whether this is possible.
- It is hard to find any weaknesses.
- There is an apparent further delay in addressing water management issues.

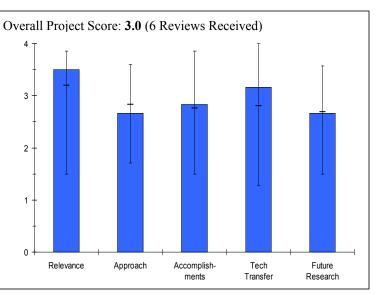
- See above.
- The project should focus more on durability issues.
- The reviewer recommends sharper focus on understanding what happens between *ex situ* and *in situ* testing.
- The project should more clearly present how the subcontractors are guiding the development of the catalysts and processing of the catalysts that are actually used in the MEA. For example, it appeared from the presentation that ANL is developing a catalyst treatment to improve the activity of the catalysts in the RDE experiments, but is this implemented in the preparation of catalysts incorporated into the MEAs? Why are the catalysts in the MEAs not acid-treated prior to incorporation into the MEA, when it was stated during the presentation that the majority of the non-noble metals easily leach from the catalysts in an acidic environment? If the catalysts are not acid-leached prior to incorporation into the MEA, then the non-noble metals are most likely being leached during MEA testing and may be poisoning the membrane.
- Funds need to be redirected for the next project phase. This reviewer suggests that tasks that support commercialization of the existing formulations, perhaps leading to simpler or less costly manufacture, higher durability, or other goals comprise the next phase. Some additions to the project scope are in order.
- After many years of development and continued DOE support, it's time for the NSTF-based MEAs to be independently verified in a broad range of operating conditions.
- The effect of common anode and cathode impurities needs to be addressed. This is especially important for NSTF-supported catalysts, not as well dispersed as other catalysts.
- The "rotating electrolyte" case needs theoretical treatment that would relate it to rotating disk geometry and help interpretation of oxygen reduction reaction (ORR) kinetic data from JPL.

Project # FC-18: Highly Dispersed Alloy Catalyst for Durability

Vivek S. Murthi; UTC Power

Brief Summary of Project

The objective of this project is to develop a structurally and compositionally advanced cathode catalyst that will meet the DOE 2010 targets for performance and durability. The impact of oxygen on Pt dissolution and structural stability for various core/shell systems has been qualified. A number of elemental and alloy cores have been evaluated; Pd₃Co and Ir cores lead to the highest improvement in oxygen reduction reaction (ORR). Various PtIrX alloys have been synthesized and tested to understand activity and durability trade-off.



<u>Question 1: Relevance to overall DOE</u> <u>objectives</u>

This project earned a score of **3.5** for its relevance to DOE objectives.

- The cathode catalysts development is of key importance for successful deployment of fuel cells. Therefore, this program is indeed relevant to the development of polymer electrolyte membrane fuel cell technology, and thus to the overall DOE Hydrogen Program.
- The project team took a very highly coordinated approach to lowering catalyst loading in fuel cells.
- The development of more active, less costly, and more durable cathode catalysts is very relevant to the DOE polymer electrolyte fuel cell (PEFC) objectives.
- High performance, excellent durability, and low cost in proton exchange membrane (PEM) electrocatalysts are primary DOE goals, and therefore appropriate.
- This project is relevant to DOE objectives, directly focusing on the cathode electrocatalysis challenge.

Question 2: Approach to performing the research and development

This project was rated 2.7 on its approach.

- The approach developed for probing activity and stability of catalysts for the ORR is, in general, *ex situ* which, by definition, is not sufficient to provide information required to understand surface processes at an atomic scale. The latter is the key for tailoring catalytic properties of catalysts.
- This project encompasses two approaches, Pt alloy catalysts and Pt shell-Pd alloy core catalysts. UTC Power is pursuing the Pt alloy approach, whereas BNL and Johnson Matthey Fuel Cells (JM) are pursuing the core-shell approach. It is not clear how the UTC Power and BNL approaches are integrated. It is also not clear how the core-shell approach pursued in this project differs from the core-shell approach pursued by BNL in the LANL-led catalyst project. Unfortunately, the UTC Power approach involves replacing a portion of the platinum with an even less abundant metal, iridium. It is also not clear how the modeling activity is impacting the choice of materials or explaining the experimental data for the Pt alloy activity. Are there any characterization results that show the calculated structures are those that are obtained experimentally?
- Feedback between modeling and experimentation could be more clearly reflected.
- Restructuring/dissolution of ternary catalyst during potential cycling/fuel cell operation remains a concern, and hence, it is not clear if alloying with less noble metals is the way to go.
- The materials science aspects of the program are fine, and there is a focus on barriers.

- The approach is not entirely clear. There is some "theory," but much more trial and error. The partners appear more as vendors. Indeed, there was no description of team interactions and assignments, although one assumes that JM makes the catalysts, etc.
- Comments were made that others had superior supports, although there was no description of how such supports would be built into the program.
- The project's heavy reliance on iridium, a metal approximately ten times less abundant than platinum, is a serious drawback. In reality, there is no path forward for the use of Ir in practical fuel cell catalysts.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated 2.8 based on accomplishments.

- The team has created structures with high-catalytic activity for the O-O bond making and bond breaking events. For the former, much more fundamental experimental work is required in order to demonstrate a true activity and stability of ternary alloys. For the latter, appropriate testing in the rotating disk electrode (RDE) configuration would be desirable in order to be able to confirm the observed increase in catalytic activity of the oxygen reduction reaction (ORR) on the Pt monolayer (shell) structure. Overall, significant progress has been made in overcoming barriers.
- The team has made steady progress, with good fundamental understanding.
- Progress was shown in replacing a significant portion of the iridium in the alloys with less expensive, more abundant metals (Co and Cr). The modeling activity shows that the "non-segregated" alloys are more stable against dissolution than pure Pt; however, are the Ir and Cr stable against dissolution if they are in the surface layer of the alloy?
- It is stated that the purpose of the iridium is to stabilize the Cr or Co against leaching from the alloy. The activity and stability of the PtCrIr and PtCoIr ternaries should be compared with their binary PtCr and PtCo counterparts rather than to Pt, as these binaries have been shown to have improved activity and durability compared to Pt in past studies (i.e., show the necessity/advantage of adding an expensive platinum group metal (PGM) to the binary).
- There have been issues with maintaining activity when scaling up core-shell catalysts for Pt on Pd₃Co.
- There has been good progress in terms of reproducible preparing and testing of the catalysts.
- I am skeptical if using chromium is a good idea given potential impact on membrane degradation. However, applicants should be allowed to demonstrate through long term tests that membrane degradation rates are not significantly altered.
- The data were not convincing, and results showed a large loss of performance which appears far from state-ofthe-art. Many would claim the lack of durability is disappointing.
- Improved performance of Ir-containing catalysts is interesting for better understanding of the ORR on platinum group metal (PGM) alloys, but of limited practical consequence (the use of iridium).
- Johnson Matthey's scale-up of the synthesis of two catalysts is a notable accomplishment.
- High angle annular dark field-scanning transmission electron microscopy (HAADF-STEM) data indicating the presence of a core-shell structure in as-synthesized Pd₃Co is convincing. The post-cycling data are somewhat ambiguous. Is there core-shell structure preserved after catalyst operation in the cathode?

<u>Ouestion 4: Technology transfer/collaborations with industry, universities and other laboratories</u>

This project was rated **3.2** for technology transfer and collaboration.

- The program is multifaceted and the PI successfully built a team which is well coordinated.
- This is a very strong team that works well between fundamental studies/modeling, catalyst synthesis, and cell testing.
- There is good coordination between the project participants in the core-shell activities. It is not evident that there is very extensive coordination in the alloys part of the project.
- The project team exhibits nice collaborations.
- Some roles seem poorly defined. There seemed to be more competition with BNL than cooperation.
- There has been good collaboration between four partner organizations, but no collaboration mentioned with partners outside the project.

<u>Question 5: Approach to and relevance of proposed future research</u>

This project was rated 2.7 for proposed future work.

- The proposed work should be more challenging. It seems that the authors are focusing on routine experiments, and unfortunately, with this approach, no progress will be accomplished.
- Proposed future work should focus on demonstrating the effect and necessity of Ir by benchmarking against binary alloys (ternary alloys minus the Ir component).
- The future work was not described clearly.
- Prospects for increasing mass activity of both dispersed and core-shell catalysts remain uncertain. Ir-containing catalysts should be abandoned.

Strengths and weaknesses

Strengths

- This is a team of highly experienced and very good scientists, especially in the field of fundamental understanding of the ORR. The team is multifaceted, and with appropriate focus may bring us closer in our quest to design better catalysts for the ORR.
- The project team had very good partners.
- There was a good mix of practical and fundamental work.
- There were attempts to scale-up BNL core-shell catalysts by a commercial catalyst manufacturer. There was also testing of core-shell catalysts in an MEA environment.
- It is a strong team that had reasonable focus in terms of materials studied.
- The team utilizes an excellent supply of chemical tools, and seems to have strong materials science excellence.
- Activity and stability modeling is interesting and represents this project's strength.

Weaknesses

- The correlation between theoretical and experimental results is defocused. There does not appear to be any relevance between the d-bend center position and catalytic activity and stability. The theoretical approach in resolving segregation of Pt alloys is not clear and does not contribute to understanding this important phenomenon. For the experimental part, the differences in catalytic activity between Pt and alloy surfaces is rather small (factor of 2) and, thus, very careful analysis is required in ordered to claim catalytic improvement, especially in the case of ternary alloys. The core-shell structures stability of surface atoms should be addressed more rigorously.
- It is still unclear as to what will be happening as core-shell structures age.
- There is a lack of coordination between core-shell and alloy activities. There is a lack of atomic level characterization of Pt alloys and benchmarking against binary analogs of Ir-containing ternaries.
- The dissolution and restructuring of less noble components over the long term may render the proposed system impractical.
- Although the "core shell" results from BNL were mentioned, the main consideration seemed to be to demonstrate that the "highly dispersed" materials were superior. Even so, there was no mention of experimental error, and the sets of data demonstrated disappointing durability. The UTC Power materials were somewhat more stable, but hardly good enough. Even so, the results presented were not convincing that there was any advantage.
- The presentation was poorly done. The graphics were difficult to read, especially the legends. This is probably some Microsoft problem; even so, from the second row while squinting, it was not easy to read.
- The use of Ir is a major weakness.
- Catalyst performance should refer to the total PGM content, not only to Pt, as used in most slides.

- From a practical viewpoint, there should be more focus on durability, since both catalyst and membrane as a resultant of catalyst dissolution is needed.
- The roles and tasks of the team partners need to be defined.

- There is no indication of error in measurements and repeatability, thus making it difficult to evaluate the utility of the results and conclusion.
- Although "fundamental" (in regards to approach) is thought to be an attribute, the need now is on commercial development.
- Testing of core-shell catalysts' durability in fuel cells is needed, not only in the RDE.
- Ir should be eliminated.

Project # FC-19: Development of Alternative and Durable High Performance Cathode Supports for PEM Fuel Cells

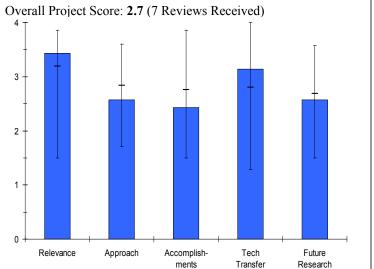
Yong Wang, Jun Liu, Vilayanur Viswanathan, Yuehe Lin, Rong Kou, Yuyan Shao, and Yuyan Shao; Pacific Northwest National Laboratory Sheng Dai; Oak Ridge National Laboratory Stephen Campbell; AFCC Jingguang Chen; University of Delaware Brian Willis; University of Connecticut

Brief Summary of Project

The overall object is to develop and evaluate new classes of alternative and durable high-performance cathode supports. The objectives for 2009 were to identify compositions with 2x better stability than carbon black-supported catalyst for cell demonstration and demonstrate durability under accelerated test protocols that meet DOE lifetime criteria.

<u>Question 1: Relevance to overall DOE</u> <u>objectives</u>

This project earned a score of **3.4** for its relevance to DOE objectives.



- The project addresses DOE targets for fuel cell durability and cathode supported catalyst performance.
- The project addresses DOE goals on development of more durable supports.
- The project supports goals identified as key to durability success for both automotive and stationary applications.
- This program is indeed relevant to the development of polymer electrolyte membrane fuel cell technology, and most project aspects are aligned with the Hydrogen Program and DOE RD&D objectives.
- The nature of the catalyst/support interaction is very important and critical to DOE's long-term goals.
- This is a good project that tries to characterize the fundamental nature of what happens at the catalyst/support interface. It is appropriate to have both modified carbons and metal supports.
- Catalyst support corrosion has been one of the problems identified as a barrier to proton exchange membrane fuel cell (PEMFC) durability. This is the only project that directly addresses catalyst supports. It is most certainly relevant to the DOE Hydrogen Program goals.

Question 2: Approach to performing the research and development

This project was rated **2.6** on its approach.

- There is a good mix of fundamental theory and experiment to guide approach. Significant emphasis on model systems should provide fundamental insight into cathode catalyst and support effects.
- The consistency and clarity of the approach are not obvious.
- The 2009 objective stated as "2x better stability than carbon black" is not specific enough.
- The approach is focused on durability only, and underestimates the influence of metal-support interaction on platinum electrocatalytic activity.
- Using modeling to guide the search is a good basis for approach, especially with experimental follow up.
- It is an interesting approach to decouple carbon from Pt corrosion mechanisms.
- How is electrode manufacturing related to this approach? Are there limitations to catalyst selection due to ink making problems?

- In general, combining experimental and theoretical methods in resolving catalytic and stability properties of electrochemical interfaces is the right way to go. Based on this, the authors are on the good track and they should proceed with the approach they developed. However, in order to overcome important barriers, the author should develop methodology on how to test the activity of catalysts.
- The team has taken a good approach that handles problems from a variety of perspectives, such as modeling, characterization and cell performance.
- Given the problems with carbon, it is at the least deflating to find that the project intention is to support the alternative supports on some form of carbon. Since this is the only support project in the portfolio, it would be preferred for this project to have begun by laying out support requirements, and the entire range of materials that could be considered.
- Some of the materials involved (ITO, SnO₂, TiO₂) have conventionally low surface area. It would be more interesting to see what could be done to make these materials at high surface area, both in terms of synthesis protocols and tradeoffs with conductivity. Then, if you have to support on carbon, you would make that decision after exploring every avenue to avoid it.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated 2.4 based on accomplishments.

- Many different experiments looked at individual aspects of the issue, and each approach made good progress in a niche area. The team has made piecemeal progress toward meeting the DOE targets. The path to bringing all the individual pieces of information together to develop a cathode catalyst to achieve the DOE targets is not clear. They have incorporated carbon nanotubes (CNT) into the mix, but no case has been made that this will be a cost-effective approach, and there has been no direct performance comparison to the other support materials under consideration.
- Reference points for improved durability are ill-defined.
- Published data on intrinsic properties of the substrate materials considered in the project are not taken into account.
- Progress has been made towards the identification of new stable supports.
- It is unclear whether the wt% of oxide on carbon support has been optimized.
- The graphene work is encouraging.
- The identification of potential supports looks good, but the PI should be able to reference DOE's catalyst kinetic targets too, since while durability is a key target, kinetics are ultimately important, too.
- Unfortunately, the approach resulted in very little useful information regarding relationships between stability of support and activity of catalysts. In particular, the presented activity of Pt is unacceptably low (a couple of orders of magnitude from the benchmarking values); therefore, before the PIs start focusing on the stability of the substrate, they must provide the evidence that activity of Pt on different supports is sufficiently high that any improvement in stability will be beneficial.
- There has been some good progress towards the goal, and towards understanding the nature.
- I would like to see a more relentless root-cause analysis to understand specifics/mechanisms of differences between the various support/catalyst combinations.
- Rotating disc electrode (RDE) evaluations appear to have been completed in sulfuric acid, which means that anionic interactions with the Pt surface may distort results.
- Experimental data that shows Pt/WC was more stable than WC was already established in prior years. Modeling that shows Pt/WC and Pt/VC should be more stable and active is interesting. Higher activity is shown for Pt/WC/ordered mesoporous carbon (OMC) with RDE, but what is the mass/specific activity at 0.9 V?
- The low degradation shown by TiO₂ is promising, but more material characteristics should be shown for TiO₂. Is it rutile or anatase? What is the conductivity? What is the surface area and particle size? Is the stability a function of any of these properties?
- It is strange that following a high voltage hold test on an MEA, TEMs would be shown of Pt particle size. Would SEMs of MEA cross-sections be preferable to observe layer thinning with support corrosion?

<u>Ouestion 4: Technology transfer/collaborations with industry, universities and other laboratories</u>

This project was rated **3.1** for technology transfer and collaboration.

- Strong coordination existed with partners that provide complimentary expertise and capabilities.
- It is not clear how interactive the team was.
- There was good collaboration with industry and national labs.
- They assembled a good team. It was not clear which of the team members contributed to specific work packages.
- Collaboration between different institutions is close and partners are fully participating.
- These are very good technical teams, with appropriate alignment.
- Some collaboration exists, but it is not entirely clear that ORNL and the University of Delaware have contributed anything more than delivering carbons, which is not the most interesting part of the project.
- Fuel cell testing at the Automotive Fuel Cell Cooperation has not yet yielded the results that are crucial to showing progress; those results (activity of Pt/WC/OMC and durability of Pt/TiO₂/Vulcan) have been shown with RDE.

Question 5: Approach to and relevance of proposed future research

This project was rated **2.6** for proposed future work.

- These really are two parallel projects, the model Pt/carbon system and the broad survey of other potential catalysts/supports. The PIs need to tie these together more closely and/or conduct some of the same fundamental studies on the newer systems to develop a broader understanding more quickly.
- There are quite a few reported studies on the topic of "Study C Degradation."
- Plans are to build in order to meet the 2x durability improvement goal.
- The team should incorporate electrode-making, i.e., ability to make an ink and electrode of good porosity should be made part of the process.
- Future work would require both more RDE measurements for the ORR on different supports, as well as a deeper understanding of relationships between the nature of support and catalytic activity of Pt.
- The reviewer would like to see more characterization to understand the nature of degradation, and whether relative importance of various failure modes changes among the supports.
- The future plans include further durability testing and material development on OMC and CNT, which is to be expected.
- Evaluating Pt/carbon (whether OMC, CNT, or other carbons) may be of little importance since these carbons' instability or cost makes their prospects of enabling PEMFC commercialization questionable.
- Future work should emphasize material properties much more so than it does. There is not just one form of TiO₂ or WC; we need to know more about the surface area and phase of these materials to relate these properties to activity and stability.

Strengths and weaknesses

Strengths

- The team has stable supports, but alternatives to carbon are needed.
- It is a model approach to development of new support.
- The PIs have performed careful microscopic characterization.
- The team has made good use of modeling and experimental verification to base studies.
- The team has identified some good potential candidates for stability.
- I like the idea of developing a new type of supports and the approach used to tackle this issue.
- There was a good focus on fundamentals of catalyst/support interactions.
- The research includes both ORR and catalyst stability.
- The PIs showed some progress with WC and TiO₂.
- The team has the ability to back up experimental results with some modeling capability.
- The team also has the ability to use a large array of analytical techniques.

Weaknesses

- The team has done lots of individual niche experiments without a clear path to developing the ideal cathode material. There are two separate projects for model systems and new catalysts/supports, the latter of which is highly exploratory without adequate scientific support for the broad range of materials (thus a lot of niche experiments that are not linked).
- The project is lacking a clear focus, and much is needed as it enters the final period.
- The quality of RDE data is poor and does not allow reaching a conclusion about higher activity of Pt/WC/C.
- The quality of polarization curves in membrane electrode assemblies (MEAs) is poor and does not meet current standards.
- The team should also include cost considerations for the various supports, for example, current cost at low volume and projected cost at high volume.
- The team should start to include kinetic data in selections, or show how you would improve kinetics.
- The activity of Pt shown is below the benchmark activity of Pt and this must be corrected.
- The authors must understand why Pt supported on oxides is more active than Pt supported on carbon.
- I see no reason for using the density functional theory calculation without trying to understand how this method may help in designing better supports.
- Scanning tunneling microscope micrographs would be more helpful if the Pt images are compared between different supports.
- A plot of the percent of degradation vs. the percent of carbon loss seems to have no mechanistic basis, and doesn't have a particularly good fit.
- The role of ionomers in mediating performance and degradation, and the role of catalyst ink formulation should be explained.
- The team needs to use proper RDE conditions and show validation of the technique.
- The overall premise of simply supporting materials on carbons is questionable towards meeting cost and durability targets.
- The execution has been slow in materials synthesis.
- There is a lack of materials characterization reporting, but more importantly, a lack of relating materials properties to activity and stability.

- The team should carefully characterize platinum-oxide interactions.
- The PIs should either include a kinetic/activity task, or a plan to increase this if a highly durable support is identified, but initial kinetic rates are lower than state-of-the-art or reference material.
- The project team needs to include relative cost of materials, near term (low volume) and longer term (high volume), using Vulcan XC-72 as a benchmark.
- The sensitivity of model results to assumptions about an electrode/electrolyte interface should be addressed.
- The PI should comment on whether catalyst degradation is occurring more on the carbon or platinum side of the interface.
- The contact resistances/electronic-phase resistance of MEA should be characterized.
- The project would be more useful with an intense focus on the novel support materials (ITO, SnO₂, TiO₂, SiO₂, WC). Information on carbons usually appears similar to what has already been studied. While actual performance would certainly be lower, disposing of the carbons might force this project to explore the novel materials even further, and then create more useful materials for later application.
- The project would benefit from laying out requirements for catalyst supports, even if it is only as a function of active species parameters.

Project # FC-20: Non-Platinum Bimetallic Cathode Electrocatalysts

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W.A. Goddard, III, B. Merinov, Y. Sha, and T. Yu; California Institute of Technology

J. Regalbuto, S. Ekambram, and H.-R. Cho; University of Illinois at Chicago

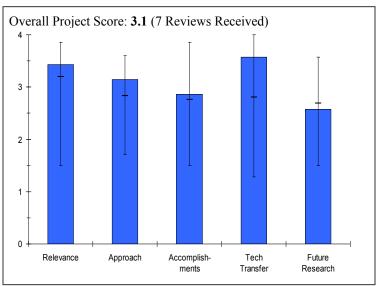
C. Heske, T. Hofmann, and Y. Zhang; University of Nevada, Las Vegas

K. More; Oak Ridge National Laboratory

P. Zelenay, F. Garzon, H. Chung, and G. Wu; Los Alamos National Laboratory

Brief Summary of Project

The overall objective is to develop a nonplatinum cathode electrocatalyst for polymer electrolyte fuel cells to meet DOE targets that 1) promotes the direct fourelectron oxygen reduction reaction (ORR) with high electrocatalytic activity; 2) is chemically compatible with the acidic electrolyte and resistant to dissolution; and 3) is low cost. The objectives for the past year were to 1) optimize ORR activity and stability of Pd-Cu nanoparticles, study the correlation between Pd-Cu electronic structure and activity, and perform membrane electrode assembly (MEA) tests; and 2) synthesize and evaluate the oxygen reduction activity and stability of nanoparticles of one palladium alloy system



and two rhodium alloy systems (Pd-Co, Rh-Co, and Rh-Fe).

Question 1: Relevance to overall DOE objectives

This project earned a score of **3.4** for its relevance to DOE objectives.

- The project addresses fuel cell targets for electrode performance, durability, and cost. Specific quantifiable targets for the program are listed in the brief, indicating a clear understanding of the basis for progress and success.
- Expanding the option for catalysts beyond platinum, to include other platinum group metals (PGMs), is okay.
- The project addresses three of the most critical barriers for MEAs, but is limited to only the cathode catalyst and cost reduction by reducing the PGM content.
- The project addresses durability, kinetics, and reduced cost via the core-shell approach and is highly relevant to achieving goals.
- Reducing catalyst PGM-loading is the highest priority for enabling automotive fuel cell commercialization.
- It is unclear if the proposed systems are practical from either the performance or (more importantly) the durability viewpoint.
- This project takes a rigorous and systematic analysis of non-platinum catalysts. The PIs focus on Pd-based materials that may be critical to next generation catalysts for proton exchange membrane fuel cells (PEMFC).

Question 2: Approach to performing the research and development

This project was rated **3.1** on its approach.

• There is a strong fundamental scientific basis for this approach and for bimetallic systems selected for initial studies. The team has used a strong iterative process to develop the theoretical methods to determine the DOS for various systems and to identify the most promising materials, experiments to validate the theory, and further theory and experiments to refine the approach.

- It is not clear how the theoretical/modeling work is guiding the experimental effort. Perhaps it should be vice versa.
- The approach is very theory-based, and is actually led by theory rather than the other way around. This is good, but may not be adequate to reveal the right path due to the myriad of factors that material processing can introduce that affect the real catalyst synthesis and performance.
- The team used a strong theoretical basis to making these materials.
- There was good coordination and explanation of team members' activities and contributions.
- The combination of modeling and experimental work will be helpful to enable optimal alloy and core-shell structures to be developed. The missing piece is the characterization aspect so the PIs know what their particle surface and near-surface atomic structures are.
- Also, the PI should be careful of replacing Pt with other PGMs (Pd and Rh).
- The team took a very good approach with combined theory and analysis. The only drawback might be that the theory is not able to predict the actual materials that will be stable at the cathodes of PEMFCs, after Pd and some of the other metals oxidize.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated 2.9 based on accomplishments.

- The team addressed several key concerns mentioned in the reviewer comments from the 2008 AMR review, specifically the basis for the overall approach and the validity of the aqueous treatment approach used to screen the Pd-Cu samples. The attempt to modify existing colloidal particles with Pd was not successful, but the PIs will continue to pursue other methods to fabricate the bimetallic systems. The team demonstrated good correlation between theory and experiments for Pd-Cu density of states. The team is making good progress on demonstrating the benefits of this combined theoretical/experimental approach.
- A large number of samples were prepared (and tested).
- The work done to-date is very impressive for its fundamental and theoretical contributions. However, the technical accomplishments so far have not demonstrated any catalyst systems that can approach the required activities or cost reductions needed to overcome the target barriers.
- The team has made good progress; the synthesis of core-shell catalysts presents unique challenges that may consume resources.
- The "best" candidate is still below the current state-of-the-art.
- ORR mass activities per PGM still have not shown improvement over Pt.
- Progress has been made by optimizing alloy content, and has a fundamental basis from d-band and X-ray photoelectron spectroscopy (XPS) studies.
- The molecular model was developed at California Institute of Technology, but still needs validation with experimental studies.
- It was difficult to decipher data as presented, and very few results are meaningful from an applications viewpoint; only one MEA test was seen and was not compared to one with a traditional Pt-based catalyst.
- Much more MEA testing is needed.
- The team has made a lot of progress toward probing the properties of Pd-based catalysts.

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated **3.6** for technology transfer and collaboration.

- This is a strong team with complementary expertise. There is good interaction between the team activities.
- Too many participants for effectively steering the program toward a common/unified goal.
- The project shows very good team strength compatibilities.
- The project has a strong government and university team. Perhaps one commercial partner or qualifier would help, especially with catalyst production.
- There is very good coordination and collaboration throughout a complex project covering theory and practice.
- This is an outstanding team with expertise in synthesis, characterization, modeling, and testing capabilities.
- This is a very broad, highly capable team.

<u>Question 5: Approach to and relevance of proposed future research</u>

This project was rated **2.6** for proposed future work.

- Proposed future work builds on prior results. It is highly dependent on the outcome of purely theoretical calculations, and would benefit in the screening process from including some additional literature research on the catalyst materials that are identified to see if they are really suitable for a practical fuel cell environment.
- The classes of sample catalysts have to be reduced.
- I suggest that the theoretical strengths be put more on improving the world's best Pt alloys, since they are much better than the pure Pt target of the current project already, and they probably have a better chance of reducing total Pt loading without a loss of performance.
- No d-band center alloy with Pd₃M approaches the Pt₃Co alloy's d-band center of 2.76 eV. The target of trying to just reach that of pure Pt, 2.47 eV, may not be adequate and, therefore, no Pd system can ever reach the performance or mass activity of the best Pt alloys.
- The future plan is acceptable, but the synthetic component should be increased.
- More focus should be put on making core-shell structures to increase mass activity.
- The plan should be expanded to include stability to voltage cycling and advanced characterization of alloy surface structures.
- More focus is needed, and more time needs to be spent, on meaningful test systems such as a single cell.
- Durability will remain an issue and must be aggressively addressed.

Strengths and weaknesses

Strengths

- The project team is collaborating with a lot of high-power institutions and researchers.
- There is a very strong fundamental understanding among the collaborators.
- There is a very strong theoretical basis to guide research, validated by extensive literature support.
- They have a strong team assembled.
- The team has modeling capabilities.
- The team also has a wide range of materials made and tested.
- This is a very good team with a multi-pronged approach to implementation of non-Pt catalysts.

Weaknesses

- There are too many high-power institutions and researchers.
- Sub-par reference RDE data is reported.
- This project could benefit from more materials synthesis and screening to help guide the modeling to demonstrate trends that the modeling can then try to explain.
- Synthetic approaches to build the designs dictated by theory may ultimately limit progress.
- There is a lack of evidence of alloy structure to validate models.
- The best mass activity is still below Pt.
- There is a lack of MEA test data.
- The team needs a more focused approach with respect to practically relevant goals.
- They may not be modeling the materials that are electrochemically stable at the cathode.

- At this stage, the project needs a very narrow focus.
- The team should apply the modeling and first principles to improving the activity of the very best Pt-based alloys known to be in practice or in the literature. This approach could have better payback in reducing the Pt or PGM loading without a loss of performance.
- Try to let more experimental measurements drive the modeling as well as the other way around.

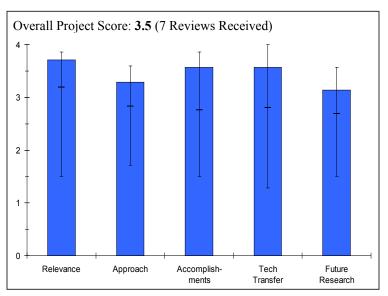
- A combinatorial style component to sort through some of the finer details of what is trying to get accomplished (such as changing ratios of the metals, sintering temperature, sintering gas such as hydrogen vs. Ar) may be needed. The team should use the theory to determine the boundary conditions for the combinational approach.
- More modeling in the presence of water and oxygen is needed in the computational studies to determine susceptibility to dissolution/oxidation.
- The PIs need to develop a better understanding of atomic layering on the core shell.
- The project should focus on appropriately characterizing the alloys to be able to validate the modeling work.
- More work on voltage cycling is recommended.

Project # FC-21: Advanced Cathode Catalysts

Radoslav Adzic; Brookhaven National Laboratory Paolina Atanassova; Cabot Superior MicroPowders Plamen Atanassov; University of New Mexico Karren More; Oak Ridge National Laboratory Debbie Myers; Argonne National Laboratory Andrzej Wieckowski; University of Illinois at Urbana-Champaign Yushan Yan; University of California, Riverside Piotr Zelenay; Los Alamos National Laboratory

Brief Summary of Project

The overall objective is to develop an oxygen reduction reaction (ORR) catalyst, alternative to pure platinum, capable of fulfilling cost, performance, and durability requirements established by the DOE for the polymer electrolyte fuel cell cathode. In the past year the project team 1) developed a number of catalysts with much reduced platinum content, ORR activity exceeding the DOE target, and very good rotating disk electrode cycling durability; 2) accomplished industrial scale-up of the first core-shell catalyst; and 3) demonstrated non-platinum group metal catalysts with volumetric ORR activity on track to meeting the DOE 2010 target.



Question 1: Relevance to overall DOE objectives

This project earned a score of 3.7 for its relevance to DOE objectives.

- The project addresses DOE targets for electrode performance, durability, and cost. Inclusion of the quantifiable targets in the brief indicates a clear understanding of the metrics for progress and success.
- Low Pt/platinum group metal (PGM) or PGM-free catalysts are critical.
- The project supports DOE goals on reduction of Pt loading and fabrication of non-precious metal catalysts.
- All aspects align with the Hydrogen Program objectives but, to this reviewer, not all are critical, because there are other more promising approaches already demonstrated. The nanostructured polymeric materials (NPM) catalysts are simply not necessary to enable a viable commercialized fuel cell business, given that existing internal combustion engine vehicles have the equivalent of 10 g of Pt in them.
- The inclusion of electrode structures places this program above typical catalyst-only projects.
- There are many excellent aspects to this program, for instance, the scale-up of the BNL materials. Some of the work seems somewhat irrelevant, but LANL is doing a pretty good job of ending approaches that do not work, thus keeping the program relevant.
- The most crucial area of study for meeting the DOE Hydrogen Program goals and objectives is novel oxygen reduction catalysts. This project studies exactly that, and is therefore extremely relevant to the objectives.

Question 2: Approach to performing the research and development

This project was rated **3.3** on its approach.

• There is a good balance of catalyst composition breadth while still conducting key experiments to evaluate viability of each approach (Pt-containing and non-Pt-containing), and specific materials sets within each approach.

- The approach is well designed.
- Very tough challenges are addressed by this project to meet the Pt equivalency (or better Pt alloys) with the non-precious metal approach. There is a very small chance of success if not fundamentally impossible for NPM catalysts to meet the required performance targets, despite the significant progress demonstrated by this project.
- The ultra-low Pt shell-core catalyst work is much more promising, but still suffers from the fundamental specific activity limitations of nanoparticles.
- They have made good use of the team's strengths to accomplish goals of project.
- The team has made great use of analysis to support and guide results.
- The approach is very good in that LANL is using multiple approaches to solve the complex problems associated with the development of new ORR catalysts. They are making good use of their team. The only downfall is that they are looking at too many catalyst systems, and they might make more progress if they narrowed their scope. They are down-selecting their catalyst systems, but probably not fast enough.
- The approach has been considerably improved this year. Catalysts that were not performing (chalcogenides) have been removed, while the remainder of the portfolio has been sharpened.
- Improvement could be found on the crucial aspects of the non-PGM catalyst work: narrowing the mechanistic possibilities for ORR, and identifying why durability does not yet exist.
- More direction should be given as to the intent with PtAu catalysts. Last year, high activity was shown in the context of a Ni core, while this year, the stability of PtAu (no Ni) was touted. The project needs to consistently show progression of activity and stability with the same series of PtAu catalysts and/or note when formulations are changed and why.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated **3.6** based on accomplishments.

- Performance of industrial scale-up of Pt/Pd/C systems was impressive. The team has made good progress in understanding fundamental science that contributes to the observed catalyst behavior, while making significant progress toward meeting the DOE quantifiable metrics.
- Excellent activities have been reported by BNL, LANL (non-PGM), and Cabot (scale-up).
- The project demonstrates steady progress towards DOE goals.
- Relative to past work in each technology approach, this team has made very good and impressive progress. However, that progress still falls short of demonstrating the potential to overcome the target barriers.
- The group provided an excellent demonstration of the potential of the Pt monolayer on the Pd/C system.
- The peroxide sensor in polymer electrolyte is a significant accomplishment.
- The stabilization of the Pd-based catalyst is exceptional.
- Scale-up to 5 g, while a benchmark, should really go to the 20-50 g range as first step, unless there is a precedent that 5 g in process can be consistently scaled to 500 g, for example.
- The LANL team is making a lot of progress on multiple catalyst systems.
- Progress this past year has been excellent, although not outstanding since the prospect of stability with higher activity core-shells is still questionable, and the prospect of durability with higher activity non-PGMs is perhaps 10x more questionable. That said, however, the higher activity is impressive.
- The 0.75 A/mg Pt on multiple-wall carbon nanotubes (MWCNT) is interesting. It would also be interesting to see if this can be done on shorter MWCNTs and how reproducible the result is.
- The silica-derived electrode structures appear to be making progress with smaller pores, but it is unclear how this will impact either PGM or non-PGM electrode design and why.

<u>Ouestion 4: Technology transfer/collaborations with industry, universities and other laboratories</u></u>

This project was rated **3.6** for technology transfer and collaboration.

- This is a strong team that includes collaborators outside of the DOE program.
- As with most/all national lab projects, participants work (here successfully) on their own.
- Cabot scale-up does not seem to have much in common process-wise with the BNL effort.
- The project demonstrates close collaboration with universities, national labs, and industrial partners.

- The project team exhibits strong and broad expertise.
- This is a massive effort with a large team. It is good to see an industrial partner, which has been deemed critical.
- The LANL team is large but talented, and seems to be well managed, as evidenced by their high productivity.
- What was formerly a weakness of this project has now turned into a strength. It is now possible to look at each partner in the project and point to how they are contributing (BNL: core-shell; ANL: non-PGM characterization; University of New Mexico (UNM): silica-derived materials and XPS; University of California, Riverside (UCR): nanotubes; Cabot: scale-up; ORNL: STEM).
- Praise must be given for exercising a no-go option on a collaborator that was not appreciably contributing University of Illinois at Urbana-Champaign (UIUC).
- There is still some work left in incorporating UNM's silica-derived materials better into the remainder of the project.

Question 5: Approach to and relevance of proposed future research

This project was rated **3.1** for proposed future work.

- Proposed future work builds on prior work for the most part. Expansion to include nanorod and nanowire structures was not explained. The project continues to include a very broad range of materials and approaches and should add to the fundamental understanding of these systems.
- Future work is built to overcome current technical barriers.
- The catalysts should be tested under more rigorous durability conditions, such as scanning from 0.6 to 1.2 V in actual fuel cells at elevated temperatures, to really judge their tolerance for Pt dissolution.
- The team should stop the nanostructured polymeric materials work and focus more on the core-shell catalyst.
- The majority of work focused on the catalyst; it would be nice to see more electrode work as part of the title objectives.
- The team has proposed very good future work. The team would benefit from selecting their top catalyst systems and focusing their resources on fewer systems.
- There are certain points in the future work that need further justification. For example, if smaller nanoparticles are less stable (a hypothesis that may need further validation), why make smaller nanoparticles? It is not clear that smaller nanoparticles will maintain activity.
- Will nanostructures for polyaniline (PANI)-based catalysts eliminate carbon and decrease layer thickness? If so, this approach makes sense, but the rationale is not clear.
- It would be good to take a look at Pt monolayer stability using conventional accelerated stress tests before investing a lot in fabricating more catalysts with Pt monolayers.
- At some point in the near future, the scaled-up batches of core-shells should be attacked with durability testing.

Strengths and weaknesses

Strengths

- The individual participants have good accomplishments.
- The team has made fast progress in the development of new materials.
- The team has made careful in situ characterization with a variety of spectroscopic techniques.
- The team members are excellent researchers.
- The collaborators have extensive experience.
- This is a highly productive team with a wide assortment of offshoots giving a greater chance of success.
- The team has a great portfolio of potential solutions to meet DOE goals.
- This complex team is very well managed.
- This is a large effective team trying to sort out the advantages of different fuel cell catalysts systems.
- The team has demonstrated higher activity for both PGM- and non-PGM-based catalysts.
- There is a considerable breadth of novelty.
- There has been better collaboration than in the past.
- There is a powerful range of analytical techniques available.

Weaknesses

- This is still a very broad project, and it is not clear what the ultimate goal/output of this project is at the end of the four year performance period. Will there be a further catalyst down-select recommendation to focus future efforts, or would the full scope of fundamentals to industrial scale-up continue in a follow-on effort? It is not clear that this effort wrapsup at the end of the performance period.
- The project has too many parts that are not related to each other.
- There are too many resources on approaches that appear to be fundamentally limited to ever overcome the target barriers, e.g., the NPM approaches.
- Scale-up level (5 g) seems still under a level that would be a significant first step to show feasibility.
- The team is spread too thin looking at too many catalyst systems.
- There is a tendency to drive towards a finished product before entirely exploring fundamentals (e.g., why PtAu is durable, why non-PGMs are not durable, whether or not scaled-up catalysts are durable).
- PGM catalysts still do not meet mass activity targets on a per mass of PGM basis.
- There are still some aspects of the project that need to tie-in better to the remainder.

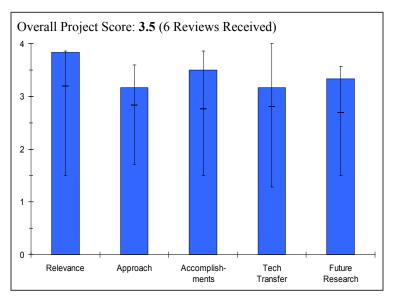
- The UNM effort does not seem to be related to the project, and it is not clear what kind of contribution can be made for the duration of the project.
- The team needs to extend scale-up synthesis to quantities higher than grams.
- They need to refocus the NPM work on the best core-shell and non-carbon support combinations that can exceed the DOE barriers in order to facilitate moving the fuel cell technology into reality in the nearer term.
- The team needs to boost up electrode structure work.
- The PIs should scale-up the synthesis task to 20-50 g, minimum.
- There needs to be greater emphasis on non-PGM durability.
- There should also be more emphasis on the durability and uniformity of scaled-up core-shell nanoparticles.
- Fundamental studies on the durability of Pt/Pd nanotubes from UCR are needed.

Project # FC-22: Effects of Fuel and Air Impurities on PEM Fuel Cell Performance

Fernando Garzon, Rod Borup, Eric Brosha, John Davey, Fernando Garzon, Mark Nelson, Tommy Rockward, Josemari Sansiñena, Tom Springer, and Francisco Uribe; Los Alamos National Laboratory Brian Kienitz and Thomas Zawodzinski; Case Western Reserve University Idoia Urdampilleta; Cidetec, Spain Thiago Lopes; University of So Paulo, Brazil

Brief Summary of Project

The overall objective of this project is to contribute to the scientific understanding of the effects of fuel and air impurities on fuel cell performance and how it affects DOE fuel cell cost and performance targets. The specific objectives are to 1) understand the effects of fuel cell operation with less than pure fuel and air, i.e. simulate "real world" operation; 2) understand how impurities affect DOE fuel cell cost and performance targets; 3) contribute to the scientific understanding of impurity-fuel cell component interactions and performance inhibition mechanisms; 4) develop sciencebased models of impurity interactions upon fuel cell performance; 5) perform experimental validation of models; and 6) develop mitigation strategies and methods.



Question 1: Relevance to overall DOE objectives

This project earned a score of **3.8** for its relevance to DOE objectives.

- Understanding fuel cell degradation mechanisms due to fuel and air impurities is one of the key remaining barriers for commercial applications of fuel cells. Understanding degradation mechanisms will allow fuel cell developers to design more reliable systems at reduced cost since impurities affect some of the most costly components of the system (e.g., Pt).
- Membrane electrode assembly (MEA) materials' robustness with real world usage profile is technically critical for fuel cell variability.
- The effects of impurities in air and fuel are important for developing fuel standards and determining lifetime. The team needs to concentrate on fuel impurities for the fuel standards timeline.
- Air side contamination work is needed. It would make far more sense to test the air side with representative air quality of, say, Los Angeles.
- This project is excellent and very well delivered. It is of real-world relevance and critical to RD&D objectives. The project is science-based, methodical, and useful.
- Much work has been done using ultra-pure fuels. The understanding of fuel impurities for real application is of utmost importance.
- The most relevant impurities were chosen for the investigations.
- Long-term tests of up to 100 hrs were addressed.
- DOE cost and performance targets are addressed through understanding of contamination mechanisms. Incipient mitigation strategies are developed.
- At this stage, the investigations meet the critical issues and DOE targets fully. A broad range of impurities is considered. In the next stage (for future projects), it is recommended to include impurities originating from pipeline systems.

Question 2: Approach to performing the research and development

This project was rated **3.2** on its approach.

- The PI investigated the biggest contributors to fuel cell poisoning; thorough testing allowed the PI to develop models of the contamination effects.
- Model development/validation is necessary for H₂S and NO_x degradation mechanisms. Molecular dynamics can be applied. Metal cation analysis properly uses modeling and empirical approaches.
- The project is well designed and focuses on important impurities. Testing appears to be all on Pt commercial fuel cells/vehicles that are likely to utilize Pt alloys to get needed activity. Work on these higher activity alloys, modeling, or other activities to relate Pt results to Pt alloys is needed.
- There is pressure to develop a fuel quality standard. Fuel impurity data is needed for this, and a focus on fuel impurities versus air impurities would help this effort.
- This approach would make more sense if gas mixtures were used. Single constituents have been tested by a number of institutions.
- Again, there were very clear explanations of the methodical approach to single-gas effects and testing protocols. The team gave solid explanations of plausible mechanisms of degradation and possible reversal of effects, in some cases.
- Elucidation of mixed-gas effects (if any) was not presented. Effects of aromatic contamination were not discussed.
- The approach is scientifically solid and appropriately considers the technical challenges, like long-term stability and air contaminations like SO₂; however, more work will be needed in the future. The current program is very well focused on the technical challenges, and the effort fully justifies the budget assigned to it.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated **3.5** based on accomplishments.

- The PI addressed the biggest original equipment manufacturer (OEM) suggestion from the 2008 AMR, that the PI should begin developing degradation models.
- It was not clear if the model was validated with real world operation and experience. The model is clearly based on testing (important), but will it correlate well to future designs? Time will tell.
- Coefficients/constants should be provided in the model to guide developers.
- The project had well-identified H₂S, NO_x, and cation poisoning.
- Measurements on H₂S, along with methods to measure S in the C support, and drive cycle testing effects of 10 ppb H₂S are important work. Ammonia and hydrocarbon work is useful for hydrogen fuel quality standards.
- Testing mixtures would be more relevant as the effects are not additive.
- There is good progress shown, and the team gave excellent explanations of cation effects.
- An H₂S crossover measurement method was developed, and crossover rates were measured. NO_x was investigated as a poison, and the interaction of humidification and NO_x poisoning was noticed, though it is not fully understood. Ammonia and cations were addressed as well. The investigations were backed by modeling in case of the cations, to identify the blocking mechanism. These investigations are ongoing activities.
- The results will help to overcome barriers.

<u>Ouestion 4: Technology transfer/collaborations with industry, universities and other laboratories</u>

This project was rated **3.2** for technology transfer and collaboration.

- LANL is a well-recognized team in fuel cell research; they collaborate well with the industry and other academic institutions.
- For fuel contaminations, it is recommended that they work with the hydrogen storage technology team to identify possible NH₃ contamination levels.
- The team exhibited good collaboration with other national labs and universities.
- A wide range of partners was selected for the modeling effort.

- The team demonstrated good collaborations, but the role of The Canadian National Research Council (NRC) Institute for Fuel Cell Innovation is unclear.
- The work was shared between LANL and Case Western Reserve University for modeling, Berkeley National Laboratory for modeling, and NRC for fuel cell impurities, as well as two further partners. The partners mentioned are internationally renowned. The work share is based on competencies, and the partners share vital parts of the activity, thus, they are full participants and well coordinated.

Question 5: Approach to and relevance of proposed future research

This project was rated **3.3** for proposed future work.

- The team should continue with model development; results should be published with general guidance provided for constants and general behavior.
- Knowledge transfer to other/novel gas diffusion layer designs in various operating conditions should be addressed.
- This project is ending.
- Future work should include some work to determine effects on alloys that are likely to be used in commercial fuel cells.
- Future work as outlined was quite shallow and could use more depth.
- The team had good conclusions on possible non-uniformity challenges, but specific experiments (or analytical methods) to investigate such inhomogeneities should be addressed.
- The team has good future plans for cationic effects.
- This is a very good and relevant project that is very well conducted.

Strengths and weaknesses

Strengths

- The PI is very receptive to OEM feedback.
- The PIs have performed well-controlled testing to evaluate poisoning effectiveness.
- There is much analytical expertise present in this project and understanding of the fuel cell catalysts.
- Air side contaminant effects have been needing study for some time. This particular project seems to have a path, rather than the infinite loop of past investigations.
- This was a clear presentation that was very methodical with mechanistic/modeling explanations. They took solid single-gas approaches.
- This team has conducted rock-solid scientific investigations on a broad range of contaminants.

Weaknesses

- There is not much modeling capability of H_2S and NO_x poisoning.
- The team needs more mixed gas experiments. They need to look more at chlorides (and their associated cations).

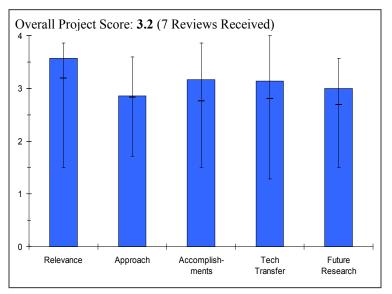
- The PIs need publications to make valuable data available.
- I recommend some initial work with high activity alloys such as PtMnCo (3M) and core-shell catalysts to see if effects are significantly different.
- The team should explore more cyclic effects with simulated diesel or gasoline exhaust as inputs on the air-side.
- Contaminants of the hydrogen distribution chain should be identified, and their impact should be investigated using the same approach. This is not meant to be added to the project, but would represent a new project. The same holds true for further gases, particularly exhaust gases of internal combustion engines.
- A way to seek out mal-distribution effects, i.e., some impurities cause areal inhomogeneities over surface leading to current density variations and hence, spotty degradations over a membrane surface could be explored.

Project # FC-23: Effects of Impurities on Fuel Cell Performance and Durability

J.G. Goodwin, Jr., Jack Zhang, L. Hongsirikarn, and Michael Martinez; Clemson University Hector Colon-Mercado and Scott Greenway; Savannah River National Laboratory Peter Finamoore; John Deere, Advanced Energy Systems Division

Brief Summary of Project

The overall objectives of this project are to 1) investigate in detail the effects of impurities in the hydrogen fuel and oxygen streams on the operation and durability of fuel cells (CO, CO₂, NH₃, H₂O, HCs, O₂, inert gases, and H₂S); 2) determine mechanisms of impurity effects; and 3) suggest ways to overcome impurity effects. Objectives for 2008-2009 were to: 1) complete the investigation in detail of carbon monoxide poisoning of platinum as well as the effect of NH_3 poisoning; 2) complete the study of NH₃ poisoning of the Nafion® membrane as a function of impurity level, relative humidity (RH), and temperature; 3) finalize the study of the minimal effect of carbon monoxide on



Nafion® conductivity; 4) investigate the effect of a Cl-containing hydrocarbon (PCE); 5) carry out long term study of effect of NH_3 poisoning per DOE request; and 6) start correlation of fundamental and fuel cell performance results for NH_3 poisoning.

Question 1: Relevance to overall DOE objectives

This project earned a score of **3.6** for its relevance to DOE objectives.

- Understanding effects of impurities is important to the objectives of the DOE Fuel Cell Technical Team (FCTT) with respect to improving fuel cell durability and reducing cost due to Pt requirements and catalyst poisoning. Some of the impurities the PI has selected are questionable in the sense that they have already been extensively tested (CO) or may not be a significant poison in real world operation (chlorinated HCs).
- The project directly responds to the need of understanding the effects of contaminants on fuel cell performance and durability, and aims at developing mitigation strategies for these effects. The project targets a significant amount of individual contaminants.
- The effect of impurities is critical for real work usage profile. Fuel impurities can affect hydrogen fuel cost and availability.
- Effects of impurities are a key aspect of fuel cell durability.
- The project is tracking more closely to the industry needs for data to support the International Organization for Standardization (ISO) fuel specification activity. Impurities effects studies are divided among working group members to provide input to the ISO hydrogen fuel quality specification process. Clemson is studying the effects on fuel cell performance of perchloroethylene, CO₂, ethane, and ethylene.
- Determining hydrogen fuel impurity effects is a high priority to guide not only fuel cell development, but also production and storage development.
- The study of impurities and their effect on the performance of proton exchange membrane fuel cells (PEMFC) is very important and the project supports DOE RD&D objectives. The two major impurities discussed, CO and NH₃, are important impurities to understand their impact on performance.

Question 2: Approach to performing the research and development

This project was rated **2.9** on its approach.

- The PI continues D₂-H₂ testing despite the recommendations of the FCTT to use simpler, more cost effective techniques.
- The project combines experimental studies to understand results. Modeling would additionally be beneficial to understand the poisoning mechanisms. Modeling results should be used in addition to experimental results to develop mitigation strategies.
- Milestones address the study of a large number of impurities.
- Milestones do not address the development of mitigation strategies proposed in the technical approach.
- If the modeling approach is combined with a phenomenological measurement approach, it would be more effective to determine mechanisms of impurity effects.
- It is necessary to clarify how to distinguish multiple mechanisms of impurity effects in fuel cell performance analysis.
- The combination of phenomenological and fuel cell experiments is an excellent approach.
- The Clemson project is focusing on contaminants of interest such as NH₃ and perchloroethylene. Longer-term testing is underway, and lower impurity levels are being tested that are more aligned with the proposed ISO fuel standard.
- The team has matured this year, and their technical approach has improved. However, impurities studied to date are replowing old ground.
- The approach to CO poisoning confirmed information that was in the literature, but it did not necessarily add a new level of understanding. The use of H₂-D₂ is interesting, but it was not clear how this would improve our understanding of CO poisoning.

<u>Ouestion 3: Technical accomplishments and progress toward project and DOE goals</u></u>

This project was rated **3.2** based on accomplishments.

- PI has thoroughly researched these materials.
- Contaminant concentrations that are closer to the suggested values for fuel quality guidelines should be investigated. The CO concentration tested was 50x above the 0.2 ppm SAE value, and the NH₃ concentration was 20 times above the comparable 0.1 ppm value.
- Little progress was reported on durability aspects of fuel cell contamination.
- No progress was reported on the development of mitigation strategies.
- There was interesting phenomena of hydrogen spillover. It was good to quantifiably identify CO poisoning on Pt/C.
- Much progress has been made in characterizing effects of CO, NH₃, and PCE.
- Progress appears to be good, and the Clemson results can be compared with those from other organizations as the round robin testing has been completed and results are comparable at any of the locations.
- There was a concern raised last year about the reliability of the impedance spectroscopy measurements. The presentation did not address this concern. The study of hydrogen spillover from the Pt catalyst onto the carbon support is not really germane to the impurities discussion. Further work in this area should be de-emphasized, as automakers have devised operating strategies to deal with CO poisoning.
- Progress continues to be slow, though the fuel cell testing seems to be coming up to speed. This project is halfway through in time and money, with little added to date to overall understanding.
- The claim of surface restructuring of the platinum catalyst did not appear to be corroborated by atomic force microscopy or some other method. It is not clear how the authors justified this claim. Did the electrochemical surface area (ECSA) change as a result of addition and removal of CO? The ammonia data did not appear to provide any new information. "A higher impurity tolerance and PEMFC performance would be expected at higher humidity." Is this true for all impurities, or just for impurities in the membrane? This statement needs justification. The mechanism for perchloroethylene poisoning should be addressed.

<u>Ouestion 4: Technology transfer/collaborations with industry, universities and other laboratories</u>

This project was rated **3.1** for technology transfer and collaboration.

- The PI does not seem to be collaborating with LANL impurity research efforts. LANL studies are generally regarded as practical and useful to the FCTT. The FCTT recommended PI establish a relationship with LANL in the 2008 Annual Merit Review.
- The type of collaboration between project contributors and ANL for modeling efforts is unknown. Such an exchange may significantly support the project's goal to "suggest ways to overcome impurity effects."
- It would be good to work with the Hydrogen Storage Technology Team to identify possible levels of NH₃ in the hydrogen fuel from the hydrogen storage system.
- There has been excellent collaboration between Clemson and SRNL.
- Clemson participates in the DOE Hydrogen Fuel Quality Working Group activities and collaborates with other organizations to avoid duplication of effort. The results are shared amongst the members and with the representatives to the ISO technical standards committee.
- Reported collaboration and coordination is good, though this set of projects has a DOE funded activity to ensure coordination, so it is not clear how much of this is due to this PI and team.
- They are good collaboration partners. It is not clear what the contribution of John Deere is to the program. The advice of John Deere should be provided.

<u>Question 5: Approach to and relevance of proposed future research</u>

This project was rated **3.0** for proposed future work.

- I would recommend that the PI drop the CO work (plenty of literature exists for this).
- The PI should really investigate what the real world exposure of a fuel cell system (FCS) to chlorinated hydrocarbons is.
- The future work does not include the development of mitigation strategies.
- The future work is addressed at the key issues.
- For the 2009-2010 timeframe, Clemson plans to study the effects on fuel cell performance of perchloroethylene, CO₂, ethane, and ethylene. Lower levels of impurities are consistent with recommendations of the DOE Hydrogen Fuel Quality Working Group.
- Some of the future work appears to duplicate effort already or nearly completed elsewhere, e.g., H₂S, and coordination activity needs to work hard to make this set of projects accomplish as much as possible.
- The project team is finishing up program, but with no explanation of deliverables. Will models and/or mechanisms be defined or developed for effects of PCE, CO, ethane, or ethylene impurities? After testing 1,000 hours with 0.1 NH₃, what will be done with the data? Most future work is studies, but the deliverable should be described.

Strengths and weaknesses

Strengths

- New techniques were successfully applied to the study of the effects of contaminants in fuel cells.
- The project addresses a significant number of relevant fuel cell impurities.
- The project demonstrates that it successfully contributes to the general understanding of the effects of fuel cell impurities.
- The team has conducted well-controlled testing to measure the effectiveness of impurities.
- The PIs have taken an excellent approach for evaluating, understanding, and mitigating effects of impurities on fuel cell degradation.
- The collaborations are good.
- The PIs have used a lot of equipment.

Weaknesses

- Up-to-date experiments addressed contaminant concentrations that were significantly higher than the expected concentrations in hydrogen fuel.
- It is unclear if and how modeling is contributing to reaching the project's goal.
- Up-to-date development of mitigation strategies is not addressed.
- There was no mention of the impedance spectroscopy issue raised in last year's review or its resolution. Neither was there a lot of evidence shown that Clemson has a thorough understanding of the relatively vast literature on impurities effects in fuel cells.
- The team is still learning fuelcell-relevant conditions. Progress has been slow (but appears to be improving).
- For a university and national laboratory, the RD&D did not appear to be very focused, and seemed to be a little undergraduate in nature. Everyone knows CO and NH₃ poison PEM fuel cells. What are the mechanisms? What are the catalyst crystal faces that are poisoned? Is one face more selective than others? What if the membrane was poisoned with NH₂D? Would this provide some fundamental understanding of the poisoning mechanism? What happens to anode catalysts when oxidizing PCE off the surface? The researchers do not appear to have a structured mechanistic approach and are conducting Edisonian R&D.

- More emphasis should be placed on mitigation strategies. Less emphasis on CO and on the H₂-D₂ reaction is recommended; they should use cyclic voltammetry instead. These activities do not relate directly to the task at hand, that is to provide data that can be used to set fuel quality specifications. Other membrane materials should be considered.
- The set of impurities to be studied in the remainder of project should be revisited, in coordination with related projects and DOE.
- The team should refocus this project. The DOE should take a strong hand to guide the program and assure that new and pertinent information will be obtained.

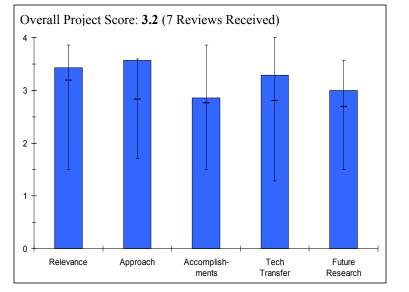
Project # FC-24: The Effects of Impurities on Fuel Cell Performance and Durability

Trent M. Molter, Ph.D.; University of Connecticut

Brief Summary of Project

The overall objective of this project is to develop an understanding of the effects of various contaminants on fuel cell performance and durability. The specific focus for the past year has included 1) the screening of hydrocarbon impurities per standard test protocols to identify impurities of concern; 2) the quantification of the effects on fuel cell performance; 3) the effects of cations on membrane properties; and 4) the development of fundamental models based on experimental findings.

<u>**Ouestion 1: Relevance to overall DOE**</u> <u>objectives</u>



This project earned a score of **3.4** for its relevance to DOE objectives.

- Understanding fuel cell poisoning effects is critical towards designing optimal fuel cell systems and meeting DOE targets.
- The project directly responds to the need of identifying fuel cell contaminants and identifying fuels purity standards for hydrogen fuel. The project is in contact to groups that define International Organization for Standardization (ISO) standards for hydrogen fuels purity for fuel cell vehicles. These standards are essential in moving forward towards hydrogen-based transportation.
- In general, the effects of impurities are critical for the viability of fuel cell systems. Hydrocarbon-related contamination is more relevant to stationary applications and less important for automotive applications.
- Understanding impurity effects on membrane electrode assemblies (MEAs) is a very important aspect of fuel cell system durability.
- The University of Connecticut (UC) is a member of the Hydrogen Fuel Quality Working Group and regularly participates in group meetings and teleconferences. The group is dividing the impurities of interest according to each member's interest and capabilities. The selected impurities and overall objectives are relevant to the DOE Fuel Cell Technologies Program.
- Effects of impurities in the hydrogen fuel and air are of high relevance to the department's program. Understanding will help guide not only fuel cell development, but also production and storage development.
- The determination of the effects of fuel impurities on the performance of proton exchange membrane fuel cells (PEMFC) is of critical importance to the advancement of fuel cell systems. Foreign cation impurities can significantly reduce the efficiency of PEMFCs.

Question 2: Approach to performing the research and development

This project was rated **3.6** on its approach.

- Prioritize the species to be tested: do the experiments in order of what is most contaminating to fuel cells.
- The team has taken a very systematic and straight-forward approach that focuses on the objectives of the project, and has thoroughly considered the details of the approach to ensure valid results.
- In addition to an empirical modeling approach, a first principle modeling approach would be effective.
- The PIs took a well-structured and thorough approach.

- The approach is very good and includes a literature search, experimental studies, and contaminant modeling. UConn and the other impurities projects should consider using state-of-the-art MEAs with lower catalyst loadings.
- Test cell break-in on different test stands must be done carefully to avoid introducing experimental variables other than the impurity. Cleaning of "wetted" components between tests is a commendable practice, and shows the team strives for quality testing. They need to resolve MEA performance issues and move to lower Pt loadings.
- The approach focuses on technical barriers identified by DOE and builds on existing databases. This approach should minimize repetitive research reported by others. The development of empirical models should assist others in predicting the effects of impurities on PEM fuel cell performance.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated **2.9** based on accomplishments.

- The PI prioritized (as per OEM request) halogenated hydrocarbons as a more important contaminant to study.
- The project team did consider material sets; it is hard to tell if there was an effect or not.
- The project team completed a study of a known fuel cell poison so the project can show it can measure contaminant effects in line with others' data.
- Some difficulties in experimental equipment were successfully overcome.
- Researchers may consider using the existing gas analysis equipment to test for reactions of the contaminants in the cell. This information would add significant value to the results.
- The testing conditions (impurities level) should be explained.
- The team needs to clarify the rationale of impurities assumptions.
- Formic acid has been identified as an impurity with a potential deleterious effect on MEA performance.
- Among other accomplishments, UConn demonstrated the importance of fully characterizing the initial state of the MEA. This is a necessary step toward specifying a commercial MEA that is stable under these test conditions.
- Characterization data showed variation within and between MEA lots. UConn is working with the manufacturer and other labs to identify lots that show more consistent performance and has spawned an interlab effort to specify generic, stable MEAs. This effort is critical to ensure the reliability of the impurities effects data.
- No work has been done yet on halogenated compounds in spite of slide titles. The PIs have not yet started looking at effect mitigation. The sharing of raw data with modelers is an improvement this year.
- The concentrations used in the experiments were too high to provide critical information regarding those impurities that affect performance, e.g., 50 ppm formic acid. It is recommended that after initially observing impurity poisoning, the concentrations be reduced to levels consistent with fuel cell experience, e.g., <5 ppm. The data on ammonia impurities is beneficial; however, ammonia is a well-known impurity and testing at lower concentrations is necessary. Testing at 25 ppm does not appear to be productive. The recovery from ammonia poisoning is also well documented. Something new is needed, and other laboratories need to be involved.

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated **3.3** for technology transfer and collaboration.

- There is a significant amount of collaboration and exchange among the work groups and other institutions.
- There is effective collaboration.
- Collaborations are in place to address issues of testing standardization and MEA variability.
- Collaboration is very good within the Hydrogen Quality Working Group. Data is being fed to the modeling efforts in an attempt to provide a solid argument for impurity limits in the ISO fuel specification effort.
- Addition of Fuel Cell Energy to the team is an improvement. ORNL helped train a student in MEA sectioning for transmission electron microscopy. It is not clear that Hamilton Sundstrand (electrolysis background) adds much. DOE funds a coordination activity for this group of projects.
- Collaboration is high and should productively help the program.

<u>Ouestion 5: Approach to and relevance of proposed future research</u>

This project was rated **3.0** for proposed future work.

- While the fuel specifications are critical in the near term, there are also impurities that could come from fuel cell system materials, e.g., plasticizers. Someone should eventually account for this in the overall impurities project.
- There should be a continuation of the systematic approach for future work.
- This experimental procedure was expected to be tuned for impurities that show performance effects.
- A systematic approach for development of mitigation strategy for contamination was not presented.
- There should be more specifics as to what hydrocarbons and cations will be examined in the future.
- Contaminant studies should be extended to ensure that all relevant species are studied and models validated against the experimental data. The need for a commercial source of stable MEAs with state-of-the-art material sets has become an important issue in establishing the reliability of the data output from this project, as well as for the other impurities projects.
- The project team needs to work on halogenated compounds typical of those found in operating environments.
- There has been good experimental activity, but the deliverable from the future work should be explained.

Strengths and weaknesses

Strengths

- The project team uses a very systematic approach.
- This project is highly focused to respond to immediate needs.
- This is a strong team with versatile capabilities.
- There is high exchange with other institutions and organizations.
- The PIs have a well-controlled experiment capability.
- The project is relevant and well structured. Significant results have been obtained in a timely fashion.
- The PIs have taken a good approach with literature search, experimental effort, modeling, and model validation.
- There is a good mix of experimental science and modeling effort. The team seems to have matured this year and is positioned to make more of a contribution.
- There is good collaboration in the program and an important collection of experimental methods and equipment.

Weaknesses

- The request for peer-reviewed journal publications has not yet addressed.
- Possible reactions/conversions of impurity in operating cells have not been considered.
- The MEA variability is a concern. Perhaps a "standard" MEA should be employed.
- Results to-date may be with MEAs configuration that may distort the true behavior that might be expected with state-of-the-art material sets.
- Impurities tested to-date are of minor interest. Issues with their commercial MEAs need to be resolved and the PIs need to move quickly to lower Pt loadings.
- The project should focus on the relevant concentration of impurities.

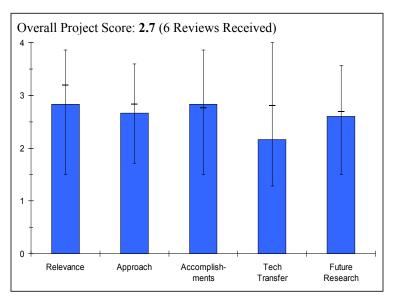
- Of the remaining species, the halogenated hydrocarbons may be most important.
- The project team should consider material sets; it is hard to tell if there was an effect or not.
- Do a study of a known fuel cell poison so the project can show that it can measure contaminant effects in line with others' data.
- With respect to the project's cation level studies:
 - The conductivity tests are being conducted at extremely high ion-exchange levels (which are conditions under which a fuel cell would not perform well anyway).
 - \circ Perform the tests at lower concentrations and show conductivity data.
 - Consider developing a standard impurity testing protocol.
- The PIs should continue the project, with careful coordination with similar projects to maximize learning from available effort.

Project # FC-25: Development and Demonstration of a New-Generation High Efficiency 1-10kW Stationary PEM Fuel Cell System

Durai Swamy, Ph.D.; Intelligent Energy

Brief Summary of Project

The overall objective of this project is to develop and demonstrate a proton exchange membrane fuel cell (PEMFC)-based stationary power system that provides a foundation for commercial, mass produced units that address identified technical barriers. The technical objectives are 1) 40% electrical efficiency (fuel-to-electric energy conversion); 2) 70% overall efficiency (fuel-to-electric energy plus usable waste heat energy conversion); 3) the potential for 40,000-hour life; and 4) the potential for \$450/kW. Intelligent Energy (IE) will engage international partners and demonstrate phase in an International Partnership for the Hydrogen Economy (IPHE) country other than the United States.



Question 1: Relevance to overall DOE objectives

This project earned a score of 2.8 for its relevance to DOE objectives.

- Design and demonstration of a small adsorption-enhanced fuel-processor-based combined heat and power (CHP) unit is consistent with DOE broad stationary fuel cell system goals.
- The project supports the DOE fuel cell program objectives to develop, demonstrate, and introduce fuel cell systems into the stationary marketplace.
- The aspect of international cooperation is appropriate. The technical and economic targets are laudable, but what markets are truly served at this power level? Has there been a detailed market analysis or is this simply a technology push?
- Refocusing of the DOE program to nearer-term applications makes this project even more relevant. CHP is a challenging market for a low-temperature polymer electrolyte membrane fuel cell, but it is important to determine how applicable the technology can be.
- The project addresses the construction of a fuel cell system that includes a reformer system. The focus of the project is continuous operation. Critical fuel cell data, e.g., decay, were not presented. The efficiency target was not adequately discussed since it was not identified if the target was beginning-of-life or end-of-life. The end-of-life target should lose about 5%. The presentation was too high-level for the maturity of the audience.

Question 2: Approach to performing the research and development

This project was rated **2.7** on its approach.

- The approach is methodical and follows normal steps of design analysis, sub-scale testing, and scale-up.
- Actually, answers given during the Q&A session led me to the conclusion that the overall system concept is not finally developed. For instance, questions about efficiency were answered, from my point-of-view, very optimistically.
- Developing a low-temperature PEM CHP system may not yield a system that has the potential to meet the project and DOE technical targets, because the temperature of the waste-heat stream is quite low. Absorption-enhanced reforming has been proposed by others and does not appear to have been widely adopted because of the process complexity it introduces. In fact, from the presentation, it is not clear if the reforming options

mentioned in last year's presentation have been abandoned in favor of the current concept. The approach to increasing the fuel cell, reformer, and power conditioning efficiency, and reducing parasitic power losses is generally sound.

- Having a flow chart as an approach chart is novel and elegant (given that, in my view, this is a system engineering demonstration). Such system-level demonstrations are truly appropriate, especially if DOE is moving toward technology transition programs (as opposed to its traditional role of simply demonstrating science frontiers).
- The integrated systems approach, where thermal sources are appropriately utilized to support parasitic loads, is good; however, caution must be exercised because component optimization may often lead to system sub-optimization see comment in the next section.
- The team continues to work on absorption enhanced reforming, but has shifted the project baseline to steam methane reforming with QuestAir pressure swing absorption for clean-up, which seems appropriate for this project. The team passed the August 2008 go/no-go point. They are now pursuing coated stainless steel (SS) plates (coating may be gold).
- The approach appears to be to assemble the components. No discussion was had on the design, construction, and performance parameters of the system. The team achieved >69% thermal efficiency, but they did not discuss how they achieved this efficiency. Variation in heat recovery was discussed and ranges given for cathode off gas, etc; however the electrical output was shown as a constant. The range for electrical efficiency would be 33% to 52% and the high value is probably incorrect.

Ouestion 3: Technical accomplishments and progress toward project and DOE goals

This project was rated 2.8 based on accomplishments.

- The project seems to be on schedule.
- On slide 18, it is impossible to gauge fuel cell performance without cell size, number of cells, temperature, pressure, fuel composition, catalyst loading, etc. It is difficult to assess fuel cell performance improvement without a baseline.
- The absorption enhanced reformer (AER) may need more R&D to improve natural gas conversion and thermal efficiency.
- More or less state-of-the-art components are going to be integrated together inside the final application.
- Progress during the last year appears substantial; however, the paucity of data in the presentation makes it difficult to assess the project's true technical progress. The hydrogen production data shown does not indicate the fuel type. Hydrogen composition into the fuel cell is not shown. The short run times for the major system components do not inspire confidence that the project durability target can be met. No cost projections are presented. Balance of plant issues appear to be surfacing, which will negatively affect system durability.
- AER systems are best used in continuous operations. So, what happens to overall system efficiency when the system is turned down? The team needs to better explore transitions and turn-down ratio effects on overall system efficiency.
- Sub-system results are clearly explained, but need more experiments at different output levels.
- They have completed the system design. They have achieved more than 2,000 h of testing on stack, 180,000 cycles, and 150,000 cumulative on cells during development. System efficiency projected was high, but not demonstrated; depends in part on using cathode exhaust for absorber purge (unproven). They claim very high efficiency on the stack (60% at 60% power). The cost was reduced 30%. The stack has 192 cells, 200 cm², and operates at 68°C.
- Progress toward operating an integrated system was demonstrated. The discussion on the CHP System Design was more of an advertisement listing properties or future properties. There was no information regarding decay in performance or stability of balance-of-plant (BOP) subsystem. The failures were all associated with BOP failures. Data showing system performance and stack performance as a function of time would have been helpful.

<u>Ouestion 4: Technology transfer/collaborations with industry, universities and other laboratories</u>

This project was rated **2.2** for technology transfer and collaboration.

- Participation of BOP vendors is not explicit in terms of minimizing cost, weight, or volume.
- Collaborators are indicated in the presentation, but there is no indication of the extent or significance of their contribution.
- The use of CE standards at the component level was great, and so is the certification strategy.
- However, the project team needs better, clearer definition of work related to grid-interconnections (beyond the single slide.)
- Collaboration seems limited to working with subcomponent developers. Coordination with the utility to host the integrated test seems adequate.
- Partners are identified; but no information on contributions from the University of South Carolina (USC), California State Polytechnic University, Pomona, or SNL.

<u>Ouestion 5: Approach to and relevance of proposed future research</u>

This project was rated **2.6** for proposed future work.

- IE is marching along the schedule and following the logical sequence of tasks.
- Fuel processor start time of 1 hour needs to be shortened.
- The future work plan is consistent with the project objectives to demonstrate a PEM-based CHP system.
- More details are needed on future work and the team needs a clearer definition or identification of critical barriers/road blocks.
- Necessary steps for an integrated consumer appliance and representative integrated testing all appear to be appropriate and underway.
- Future activities are identified. Is Phase 4 the same as Task 4? If not, there was no discussion on Task 4. If they are the same, then change the terminology to be consistent with the Gantt chart.

Strengths and weaknesses

Strengths

- Fuel cell stack performance appears good. Operating on high-purity hydrogen should enhance durability.
- This is a well-articulated approach and systematic testing of components/sub-systems.
- The team took a solid approach to system design, development, and testing, which may well facilitate early commercial entry and market transformation.
- The main project strength is that they got the system to work for a brief period of time.

Weaknesses

- Seeking certification for an as-yet-to-be-tested complete CHP system may be premature.
- They need to work on turn-down challenges with comparisons to incumbent/legacy systems used in this market space.
- The efficiency projected may be hard to achieve.
- There was very poor discussion of the technology and benefits of fuel cell systems. The following were unclear: the durability of the pressure swing adsorption unit (PSA); the concentrations of impurities exiting the PSA; the life of the adsorbants in the PSA; and the durability of the fuel cell. The project does not give adequate information; even information that would be very general in nature is not provided.

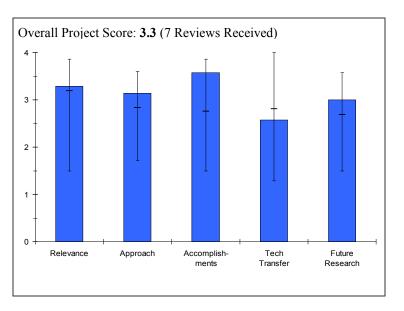
- Emphasis going forward should focus on durability issues and confirming performance projections.
- The project team needs to elaborate on future plans.
- They need to continue to completion.
- The reviewer recommends that the program be terminated unless more information is provided by IE. The information provided was more of a press release. The presentation was too high-level for a review.

Project # FC-26: Stationary PEM Fuel Cell Power Plant Verification

Eric Strayer; UTC Power

Brief Summary of Project

The objectives of this project are to 1) evaluate the operation of a 150 kW natural gas-fueled proton exchange membrane fuel cell (PEMFC); 2) assess the market and opportunity for utilization of waste heat from a PEM fuel cell; 3) verify the durability and reliability of low-cost PEM fuel cell stack components; 4) design and validate an advanced 5 kW PEM system; 5) conduct demonstrations of PEM technology with various fueling scenarios; and 6) evaluate the interconnection of the demonstration 5 kW power plants with the electric grid.



Question 1: Relevance to overall DOE objectives

This project earned a score of 3.3 for its relevance to DOE objectives.

- Small stationary fuel cell units are consistent with DOE's broad goals. Durability and cost are being addressed.
- This project focuses on system and performance optimization of a practical stationary PEM fuel cell system, and is very relevant to the goals and objectives of the Hydrogen and Fuel Cell Program.
- The project clearly meets and fully supports DOE objectives. The project advances the technology and prepares the technology to eventually enter marketplace.
- The project addresses major barriers for commercialization of cost and reliability.
- The project is relevant to the DOE Fuel Cell Program objectives. If the system appears viable, it could be selected for early deployments.
- The project serves objectives A, B, and field robustness.
- The coverage of this project is very broad and comprehensive. UTC fulfills the expectations fully. The integrated approach from basics to engineering is considered to be contributing notably to the success.
- However, there is one point which might be considered a weakness: as of now there is no PEM membrane material available which has been proven to fulfill the lifetime requirements of 40,000 hrs. Existing materials are good for about 10% to 30% of the required lifetime. A strategy should be outlined for how to overcome this potential barrier. Long-term testing of different materials may be necessary. It is not required to demonstrate the ultimately required longevity, yet the potential of a material should be validated.
- With DOE program refocusing to nearer-term applications, the project has increased in relevance this year.

Question 2: Approach to performing the research and development

This project was rated **3.1** on its approach.

- UTC is applying accepted design and engineering methods to this project.
- The durability and reliability of cell/stack components are being verified in parallel, as well as cost.
- The approach is based on implementing incremental improvements in system design and performance for stationary applications. The approach is clearly structured and appropriate.
- The project is sound and it's easily believable that UTC will perform well, but there should have been a greater discussion of barriers and challenges. The presentation discussed water management issues, but what other barriers and challenges make this a difficult project?

- The UTC project is very effective and contributes to overcoming boundaries, but an expansion of the challenges would have made this project stand out. What is truly difficult that others are not facing?
- Durability testing including start-stops is important. It is not clear what load cycle was utilized for the durability testing or how it relates to expected real world operation. Including multiple units in the tests provides some confidence in field durability data. It is not clear that the current platform (5 kW-33 cell stack) is an appropriate size to utilize for lab tests for an eventual 150 kW system.
- UTC displays an understanding of requirements for commercial viability in the back-up power market. Reduced cost is absolutely required, as is operability and durability that matches or exceeds conventional technology.
- The technical approach is professional and scientifically sound. The system's approach, which has been taken, is strictly oriented to overcome the barrier of commercialization through addressing power density, stack cost, and degradation. See the potential barrier above.
- The approach is solid, as expected from a long-term successful commercial system developer. Stack cell components are evolving from demonstrated UTC PEMFC stacks. The project appears on track for meeting their internal metrics and advancing progress toward DOE targets.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated 3.6 based on accomplishments.

- Power density has been quadrupled.
- Grid connection issues are being addressed.
- Cost has been reduced by 30%.
- Several early units are installed in the field and operating very well.
- Significant progress has been reported in improving system design and performance, while lowering cost based on a total system perspective (both fuel cell stack and balance of plant).
- The project is clearly working towards goals and yields a great deal of product and data. Program metrics indicate that work is completed on those areas where significant barriers could exist, and that remaining work most likely has limited barrier threats.
- The team has increased the packing factor by ~45% and increased power density to ~28 kW/m³ for a 5 kW system. It has developed water management strategies that allow for <30 second start-up time for fuel cells; the team achieved >3,500 h operation and >450 starts on the system. The team achieved good system efficiency (45%), exceeding its target. It appears to be behind schedule; 60% complete after 4½ years on a 5 year project.
- Considerable progress has been made in the past year. The UTC advanced system is 30% less costly than the baseline system. The power density matches that of engine generator sets. Costs, as has been the case throughout this project, are not presented, and neither are cost targets.
- A low-cost stack has successfully been developed. Degradation was investigated, yet the time of 100 hrs is not sufficient to address the required longevity for a stationary application. The power density of the UTC system performed well when benchmarked against other commercial fuel cell systems. The 5 kW systems performed well with 42% efficiency and 99.6% availability.
- The program is very focused, straight-forward, and designed to overcome the main barriers. As mentioned above, the barrier of limited longevity of PEM stacks is not addressed appropriately. The rating is kept on outstanding, since in all other aspects the program falls into this category.
- It appears that considerable progress was made this year on durability, power system volumetric size/packaging, cost reduction, and system integration.

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated **2.6** for technology transfer and collaboration.

- The team is well-rounded, including testing services and power electronics/grid entities.
- Appropriate collaborations are reported that augment the expertise of UTC Power. Clearly the collaborators have made significant contributions to the impressive results reported.
- Partners' roles exist, but this project seems close to being solely a UTC affair, especially as Houston Advanced Research Center (HARC), U.S. Hybrid, TDI, and Avalence are non-cost share suppliers rather than equal collaborators and partners.

- The project appears to most closely resemble the statement that most of the work is done at UTC with little outside collaboration, especially given the large scope of the project, almost \$11.4 million from DOE.
- The presentation makes clear that the role of partners is non-cost share, but there remains little definition of their roles. Their roles seem miniscule compared to the effort of UTC, almost as if their greatest and sole role is to be listed as partners for the project.
- The project team is collaborating with HARC, and others.
- The development efforts are concentrated at UTC and its suppliers. Numerous locations have been identified as demonstration sites which could provide the information necessary to verify commercial viability.
- There is a limited role of cooperation partners. Since UTC has a broad in-house base in fuel cell technology and systems technology, collaboration is more critical and this might not be regarded negatively.
- System-development collaboration seems limited to working with component developers and testing at the HARC. Coordination with a number of test locations seems on track.

Question 5: Approach to and relevance of proposed future research

This project was rated **3.0** for proposed future work.

- Future work is a logical progression of the project. It looks as if the project will need to be extended.
- Adequate plans for completion of this project were described.
- Work to date appears to have been significant and supports future completion of the project as well as possible transitioning of the product to market.
- Future work is carrying out field demonstrations. Bringing the field test results back into the reliability modeling to get feedback in to the loop would be very beneficial.
- Not much time is left in the project. It may be too short to provide sufficient information to determine commercial viability.
- The project appears to be a well-planned, commercially focused effort with multiple test locations and fuels. It should result in a near-commercial system suitable to a variety of special applications.

Strengths and weaknesses

Strengths

- There are strong collaborators.
- UTC is a capable company that clearly is a leader in advancing the hydrogen economy.
- The main strength is the high and comprehensive competency of UTC. The project is designed to that strength and is well-conducted.
- The team is an experienced developer executing and planning well. Internal metrics add valuable commercial focus to DOE system-level targets.

Weaknesses

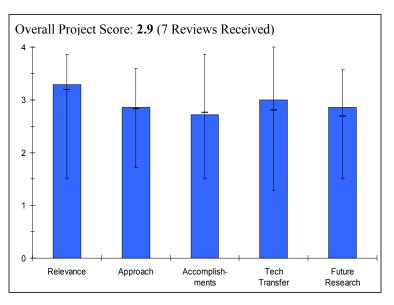
- There is very little collaboration with other organizations.
- There is a lack of cost targets and any indication of how close this system is to meeting those targets.
- There is a limited longevity of PEM membranes.

- The project team should consider making the system freeze-capable.
- None are noted at this time.
- Extending the demonstration period should be considered so that sufficient data can be gathered to assess the commercial viability of the system.
- The project team should include investigations as to whether, with novel membranes, the 40 khr goal can potentially be achieved.
- Continue to conclusion.

Project # FC-27: Intergovernmental Stationary Fuel Cell System Demonstration *Richard Chartrand; Plug Power*

Brief Summary of Project

The objective of this project is to design and produce an advanced prototype proton exchange membrane fuel cell (PEMFC) system with the following features: 1) 5 kW net electrical output; 2) flex-fuel capable (liquefied petroleum gas, natural gas, ethanol); 3) reduce material and production cost and increase durability; 4) increase electrical efficiency over the current alpha design; and 5) increase total efficiency by incorporating combined heat and power (CHP). Plug Power will also show a path to meet long-term DOE objectives, including 1) 40% system electrical efficiency: 2) 40,000-hour system/fuel cell stack life; 3) \$750/kW integrated system cost (with reformer); and 4) \$400/kW fuel cell stack cost (direct hydrogen).



Question 1: Relevance to overall DOE objectives

This project earned a score of **3.3** for its relevance to DOE objectives.

• Relevance would have gotten an outstanding rating if one of the fuels for this system was hydrogen. The team claims to show a path to \$400/kW fuel cell stack cost operating on direct hydrogen. The PI does not test direct hydrogen based on a relevance chart, not to mention that this was a high-temperature system until chart 13. Is it a high-temperature system, and what is Ballard's function with a high-temperature system?

Question 2: Approach to performing the research and development

This project was rated 2.9 on its approach.

- The approach is to follow accepted engineering principles to design, build, and install the prototype demonstration unit.
- The unit will be installed at Construction Engineering Research Laboratory (CERL) to provide CHP for an existing building.
- The team has conducted demonstrations of a low temperature unit at CERL and a high-temperature unit at Union college, both reformate-based and providing both power and heat. The low temperature unit will have 32% efficiency.
- Great identification of tough barriers and challenges including system efficiency, system and fuel cell stack direct material cost, and system and fuel cell stack durability. These are barriers that if only partial progress was achieved, it would still be a significant accomplishment.
- The work is highly relevant towards meeting DOE goals and could yield benefits throughout industry.
- The approach is sound. Plug Power is focused on cost reduction and system simplification. The decision was made to purchase fuel cell stacks from Ballard for integration into the Plug Power system. This decision conserves Plug Power resources and provides a developed fuel cell stack for integration into the system.
- The project seems to be more system design and integration rather than component development or improvement, with a focus on grid interconnection testing. They selected a Ballard stack and have developed GenSys targets to supplement DOE stationary targets.
- The approach chart was a list of the activities from a Gantt chart and did not provide information on what the technical problem to be solved was and how the approach would lead to a solution.

Ouestion 3: Technical accomplishments and progress toward project and DOE goals

This project was rated 2.7 based on accomplishments.

- The project appears to be on schedule and making tangible progress. Site installation is imminent.
- Concept development and system definition is 100% complete. The system integration part of the project is 40% complete, and the field demo task is 10%. Have passed design review with DOE. System integration began for both steady state and transient operation. The team claimed to achieve system material cost reduction of 53% (in production quantity).
- There was great identification of tough barriers and challenges including system efficiency, system and fuel cell stack direct material cost, and system and fuel cell stack durability. These are barriers that if only partial progress was achieved, it would still be a significant accomplishment.
- The team has made clear progress compared to last year's presentation.
- The prototype system has been designed. Plug Power indicated that they had achieved material cost reductions of about 53% compared to the system as defined in the previous year. The reduction assumes production quantities of 10,000 units per year; however, the presentation did not indicate how close Plug Power had approached the DOE cost target.
- The prototype system achieved an electrical efficiency of 32%. Achieving the 40% target could be difficult.
- The team passed DOE go/no-go decisions for concept development and system definition. Efficiency is projected at 32%, far below the DOE target of 40%. They have a creative definition of "appropriate performance," that being components that demonstrate their "specified performance."
- The technical accomplishments provide information that progress is being made, but do not discuss the benefits of the accomplishments. There was no information on performance and durability of the system. Was this proven previously? The criteria for passing a go/no-go decision point were not fully identified. It is not clear if this is polybenzimidazole (PBI) or a perfluorinated sulfonic acid system. These are two very different fuel cell systems with different performance targets.

<u>Ouestion 4: Technology transfer/collaborations with industry, universities and other laboratories</u>

This project was rated **3.0** for technology transfer and collaboration.

- CERL has extensive experience with fuel cell installations.
- Ballard is a respected fuel cell supplier.
- National Grid (utility) provides grid connection expertise.
- Both CERL and Union College are just demonstration sites. They have done good work with National Grid to get installed at Union College.
- Plug Power appeared to avoid resume-building that listed team members whose sole role was to be listed as a partner on a presentation. Instead, Plug Power appeared to have teamed with strong active partners. Though few in number (three partners), the partners appeared to be true partners in the project.
- They were well-coordinated with CERL in the role of customer activity. CERL is providing requirements that Plug Power is working to meet. This aspect will be crucial to making the product saleable in the marketplace.
- Strong partners are involved!
- The major collaboration is with Ballard Power Systems that brings world-class expertise in fuel cell technology to the project. The system will be demonstrated at the U.S. Army CERL site. A high-temperature system will be demonstrated at Union College. National Grid will participate in defining and specifying the interconnections between that system and the existing electricity grid.
- Ballard is supplying stacks. There is coordination with U.S. Army's CERL and National Grid for testing.
- It is not clear why collaboration with Ballard on system integration of a high-temperature stack is beneficial. Maybe a definition of high temperature is needed. Is this a PBI-phosphoric acid system, a silicon carbidephosphoric acid system, or a perfluorinated sulfonic acid system?

Question 5: Approach to and relevance of proposed future research

This project was rated **2.9** for proposed future work.

- Future work is straightforward for this demonstration project.
- The team will install a unit at CERL in the 3rd quarter of 2009 for winter heat. Union College is awaiting installation. They will complete field tests and post test analysis and close out in 2010.
- Work plans are clearly built on past success and when work plans are completed, the work path will lead to well-thought next steps. Current efforts appear to be part of a coordinated plan so that current work can be built on with future work just as current work was built on past work.
- The project plans are to complete installation and shakedown testing of the units in 2009 and commence longerterm testing in 2010.
- No path to improve efficiency was suggested. This project will demonstrate grid-connected operation (which has been demonstrated before), and does not seem to advance the state-of-the-art.
- What is the prototype system to be commissioned at CERL? Is it the same high-temperature system for Union College? What are the criteria for the commissioning of the system at CERL? Not enough information was provided.

Strengths and weaknesses

Strengths

- The project team put on a grid at Union College; a good example of working with a utility.
- This is a well-coordinated project in all aspects.
- The team took a good approach and good collaboration was apparent from the presentation.
- The team has done well with system integration and packaging.
- Plug Power has extensive 5-kW system building and testing of PEM.

Weaknesses

- There is some question that it will be possible to complete the project on time. Only two units will not prove out durability and show potential for cost reduction, as is claimed. Very short term testing is to be done (less than one year).
- The presentation did not convey any information concerning the cost of the systems. The presentation did not provide an indication of the overall efficiency expected from these systems, or any details concerning the technology employed in the high-temperature system.
- Nothing in the project seems to advance technology toward DOE targets.
- It was not clear what the fuel cell system was, because data were not made available.

- The team should add in more units to prove out durability and cost reduction.
- No recommendations are noted.
- Future presentations need to be more informative and provide a better description of the technology.
- The remaining project is primarily system testing, which should probably be completed at this point.
- The team needed to define the system to the reviewer.

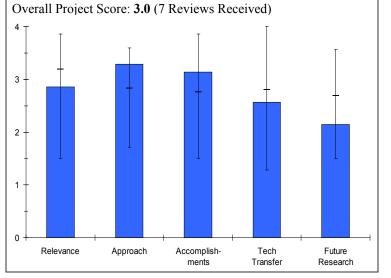
Project # FC-28: Development of a Low Cost 3-10kW Tubular SOFC Power System

Norman Bessette; Acumentrics Corporation

Brief Summary of Project

Acumentrics creates battery base uninterruptible power supplies for harsh environments. The overall objectives for this project are to 1) improve cell power and stability; 2) cost reduce cell manufacturing; 3) increase stack and system efficiency, 4) prototype test meeting system efficiency and stability goals; and 5) integrate to a micro combined heat and power (mCHP) platform.

<u>Question 1: Relevance to overall DOE</u> <u>objectives</u>



This project earned a score of **2.9** for its relevance to DOE objectives.

- The project is ultimately aimed at mCHP units, consistent with DOE goals.
- This project is very relevant to the Fuel Cells subprogram since responsibility for solid oxide fuel cell (SOFC) stationary systems were added to the subprogram portfolio.
- Project goals are to reduce SOFC cost, increase power density, increase efficiency to >40% lower heating value (LHV), increase durability to meet a 40,000 hr lifetime for stationary power applications, and CHP.
- There was some description of relevance to DOE goals, but not very clear.
- The mCHP appliance could be an important early market for high-temperature fuel cells. With the DOE refocus to nearer term applications, this project is very relevant.
- The project does not fully address the program goals of the Hydrogen Program. The 1-kW home appliance is better suited for Europe or Japan than North America. The program does not appear to address the trade-off of electric power which is costly, and thermal energy which is inexpensive.

Question 2: Approach to performing the research and development

This project was rated **3.3** on its approach.

- The list of necessary improvements is listed, but details of how the improvements will be achieved are vague.
- The proposed approach to systematically improve system design and performance is appropriate and sound.
- This work started as a Solid State Energy Conversion Alliance (SECA) project and has been funded through this program since April of 2008. The approach is to perfect the system components, then integrate them into a system. The system will be a mCHP prototype with 90% energy efficiency. The mCHP will have 10%-25% lower primary energy consumption, 10%-25% lower CO₂ emissions, and 10%-25% lower cost. It is intended to use line natural gas for fuel; a 1 kW system for residential.
- The barriers being addressed are key to improvements.
- There is good focus on overcoming relevant barriers and a good approach to attacking each problem.
- The project demonstrates a systematic approach to improving required performance, cost, and durability. Internal targets have been developed, and progress toward those targets assessed and used to guide further development activities. They have an understanding of real-world heat to electricity ratios (residential maybe 3:1) and implications for system design and operation are apparent.
- The "Acumentrics Approach" slide states that they were going to make things better, but does not provide information on the pathway to improve the power and stability or stack integrity. Better explanations are needed.

Ouestion 3: Technical accomplishments and progress toward project and DOE goals

This project was rated **3.1** based on accomplishments.

- Several of the progress graphics only show data through 2007. What progress has been made in the last 1.5 years?
- Most of the data are for single cells. Stack improvements can only be inferred from the single-cell data and from the diminishing stack volume.
- There are insufficient data on the uniformity of fabricated cells in terms of initial performance and degradation rate.
- Very significant progress was reported in system design and performance. Advances in size, weight, and volume were also reported.
- The project is 25% complete. Because the project has been funded for many years through SECA funding, it is difficult to determine what has been accomplished explicitly using Energy Efficiency and Renewable Energy (EERE) funding. Apparent progress has been made in manufacturing and moving to isostatic pressing; elimination of one braze joint; decrease in tube wall thickness by 45%; improved (decreased) cell degradation rate to approximately 1% per 1,000 hr. They have also apparently been able to run the system without a purge. Progress has also been made in comparing catalytic partial oxidation (CPOX) with steam reforming. Steam reforming gives better thermal balance. Also, decrease cells in the stack from 126 to 36, although this probably started under SECA funding.
- Good improvements in cell degradation rate have been made.
- Manufacturing process improvements contribute to cost reduction.
- The project team has made good durability progress.
- CPOX and steam methane reforming capabilities are good for multiple applications.
- Heat recuperator weight and volume reductions are excellent.
- Good progress was demonstrated on improving performance and durability. More attention to projected costs would be good.
- Some (much?) of the progress reported seems to have been under the SECA program, but technology progress is nonetheless impressive. Progress that can be specifically tied to this project, such as lower-cost, higher performance tube manufacturing is also impressive. Electrical efficiency is high-(46%-48%); heat utilization further improves fuel conversion to useful products.
- Acumentrics data shows improvement in the cell power and the degradation process. How were these improvements achieved? In Chart 11, what is Method 1? Progress is shown, but explanations are not given. If "equivalent performance" was achieved with a reduction in wall thickness, what was the benefit? Was Acumentrics seeking improved performance with a reduction in wall thickness? What is the average layer voltage?

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated **2.6** for technology transfer and collaboration.

- The list of strategic partners is impressive, but their roles are not elucidated.
- There was no discussion of collaborations. It is assumed that all of the work was done in-house. Some interactions with European energy providers were discussed. It is suggested that collaborations with U.S. energy companies be sought in order to maximize the projected benefits to U.S. taxpayers.
- There were no real collaborations, but they were demonstrating a residential system in Europe with utilities.
- The team is complimentary.
- European members have good experience
- The collaboration seems excellent. Coordination of European tests (which must utilize "waste" heat) seems good.
- The "Strategic Partners" list does not mean collaboration and coordination with other institutions. A better explanation is needed.

<u>Ouestion 5: Approach to and relevance of proposed future research</u>

This project was rated 2.1 for proposed future work.

- There are no "Future Work" slides.
- The future plan appears to be adequate to complete this project in an orderly and timely fashion.
- They need to finish units and test home units and get data. Future plans are not well-defined.
- The plan seems to be adequate.
- Additional pathways to improve current density will be more productive.
- Additional information would be helpful.
- Future plans have not been clearly addressed. Apparently, future plans are to continue the current work.
- This project seems on track to advance the state-of-the-art, perhaps significantly.
- There is no proposed "Future Work" chart.

Strengths and weaknesses

Strengths

- The CHP application is positive. They have demonstration of residential units in a willing market (Europe).
- The technology based on an anode-supported design has shown maximum advantages.
- The team has a good technology base.
- The team has an experienced developer and a strong approach, with measurement of metrics and redirection as required.
- Acumentrics is experienced in the development of SOFC tubular stacks and cell components. They have made improvements, but it is not clear they are reaching their business targets.

Weaknesses

- The project shows very low power density for cells, <0.3W/cm². This will make it difficult to commercialize. They only will demonstrate in Europe.
- SOFC technology is not as mature as other fuel cell technologies, and will likely not be market-ready soon.
- Data on cell stack life was not presented. Does the cell stack last five years in order to fulfill the needs for CHP application? Little or no information was provided on methods of improvement. The application is not consistent with the Hydrogen Program.

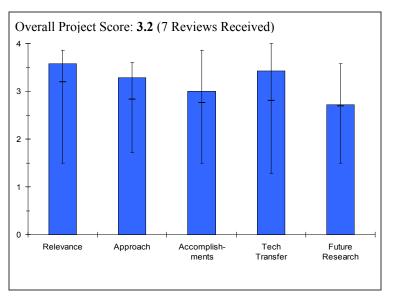
- The project team should seek U.S. collaborations to define system requirements applicable to U.S. stationary power deployments.
- The team needs to provide system cost analysis, and work to demonstrate in the U.S.
- Efficiency data should be based on electrical AC output.
- Continue to conclusion.
- Acumentrics should define their targets better so a judgment on progress can be made.

Project # FC-29: Fuel Cell Systems Analysis

R.K. Ahluwalia, X. Wang, K. Tajiri, and R. Kumar; Argonne National Laboratory

Brief Summary of Project

The objective of this project is to develop a validated system model and use it to assess design-point, part-load and dynamic performance of automotive fuel cell systems. This project includes supporting the DOE in setting technical targets and directing component development as well as establishing metrics for gauging progress of research and development projects. Argonne National Laboratory will 1) develop, document, and make available versatile system design and analysis tools; 2) validate the models against data obtained in the laboratory and at Argonne's Fuel Cell Test Facility; and 3) apply the model to issues of current interest.



Question 1: Relevance to overall DOE objectives

This project earned a score of **3.6** for its relevance to DOE objectives.

- The project to develop and validate fuel cell component and system level models is critical to the success of the DOE Hydrogen Program and addresses many of the key targets for performance, system thermal and water management, air management, start-up and shut-down time, transient operation, and cost.
- This project is developing a sophisticated fuel cell system model that provides very relevant input to the Fuel Cells subprogram.
- Having a model to provide fuel cell system analysis is highly desirable; however, so much of the technology that really drives major portions of the system definition is still on fairly steep development curves. Furthermore, the details of system architectures are generally among the most tightly guarded secrets with the original equipment manufacturers (OEMs), since these are generally the areas where competitive advantage is key. It is important that this effort be focused in areas that are more generalized whenever possible.
- The project could extend systems expertise to all fuel cell applications.
- There is reference to this work in the Directed Technologies, Inc. (DTI) cost analysis work presentation, but no linkage explicitly explained in this talk; integration of efforts should be highlighted.
- This project is fully relevant and supports program targets and goals. It provides necessary input to cost studies, but the program is not absolutely critical to the success and progress of the technology, i.e., the results of this program do not directly "raise the bar."
- The technical program supports the DOE program and FreedomCAR technical teams by providing critical modeling and analysis for the DOE of industry and university performance/durability data. The project evaluates the complete system and provides baseline analysis of balance-of-plant (BOP) components. It developed a baseline design for fuel cell systems and established interaction of BOP components in the system.

Question 2: Approach to performing the research and development

This project was rated **3.3** on its approach.

• The approach is a good balance between component- and systems-level considerations in optimizing fuel cell systems. The clearly identified baseline fuel cell system design and specific components provides good starting points against which to compare other components and system trades. The approach provides significant

flexibility to consider other components and designs. The project took a strong approach to provide a widely available modeling capability, rather than an overly proprietary model that cannot be broadly built upon.

- The approach involves continuous improvement of the comprehensive, complex analytical model and validation of the model with the latest fuel cell experimental performance data. The results of this model couples with a companion cost model to provide valuable planning for the Fuel Cells subprogram.
- The project is too limited on air machinery and thermal management system. It is not clear that stack model is realistic enough; there was no collaboration with an appropriate organization like an OEM.
- The project is very focused, maybe a little too much so; three major factors are highlighted.
- The approach could be broadened.
- Evidence of more parties from the industry tuning into this work would be valuable.
- The approach is appropriate for the stated goals.
- The approach is well-organized and based on experimental data. A potential weakness is the dependence on data from industry without the ability to crosscheck the data.

<u>Ouestion 3: Technical accomplishments and progress toward project and DOE goals</u></u>

This project was rated **3.0** based on accomplishments.

- The project has been very flexible and agile in evaluating key issues during the past performance year.
- Substantial progress has been made during the past year in model development and improvement. The model has been used to explore system design configuration and allows the subprogram to make informed and validated decisions regarding programmatic directions, performance target definition, and research investment opportunities.
- Subfreezing start-up simulations are not likely to be very helpful since they lack specific details of the stack and membrane electrode assemblies (MEA). It is not clear that the issue of ice formation in the electrodes is accounted for.
- The work on system pressurization and freeze start is excellent.
- Attention to duty cycles and integrated efficiencies seems lacking.
- What about the battery or energy buffer? It is missing! This needs attention as a key (potential) powerplant component, especially hybridization, electrical issues, and battery performance decay.
- There was little consideration of aging effects overall.
- For a year's worth of effort dedicated to analysis, results seem a little light.
- Modeling expertise is very solid but needs to be applied to more critical areas, or at least where the effort can contribute to advancing the state-of-the-art (impurity, freeze, water management modeling, and validation).
- The technical accomplishments working with 3M and Honeywell provide the background validation of the two emerging technologies. The team identified efficiency issues for the compressor/expander module. The discrepancies in the Hawaii Natural Energy Institute (HNEI) CO data and the simulation were presented in additional data, but it was not fully discussed why the discrepancies occurred. The data analysis on the 3M materials needs a much better explanation than was presented at the AMR. The test appears to be at constant efficiency (50%) with a strong variation in the Pt content with temperature and relative humidity (RH). A 5°C temperature difference (90°-95°C) greatly changed the Pt content, e.g., at 60% RH. A 5°C change is very common within a cell, so this would suggest the system is working on a knife edge. There was no discussion or explanation which was disappointing.

<u>Ouestion 4: Technology transfer/collaborations with industry, universities and other laboratories</u>

This project was rated **3.4** for technology transfer and collaboration.

- Results indicate very close collaboration/interaction with the full spectrum of component and system developers to develop and validate the models. These interactions provide confidence in the model outputs.
- This project has extensive collaborations ranging from those providing performance inputs for model validation to those who use the tool for guidance and direction.
- The level of collaboration was good, given the collaborators chosen.
- The project could be extended to a broader field of stakeholders, e.g., Vairex should have been consulted regarding the compressor motor expending unit, in addition to Honeywell.

- Interactions outside the U.S outside the US should be included if they exist.
- The team has a good working relationship with 3M, the Hydrogen Fuel Quality Workgroup, and Honeywell.
- The team needs more collaboration with other DOE impurity/contaminant programs and freeze and water management programs. These areas can greatly benefit from detailed modeling support.
- Efforts with 3M, Honeywell, HNEI, etc. are all very good. The Hydrogen Program establishes ANL as the lab to develop models and simulations for much of the R&D in other projects. It would be important to validate the quality of the ANL simulations and modeling with the input from 3M, HNEI, etc.

<u>Question 5: Approach to and relevance of proposed future research</u>

This project was rated 2.7 for proposed future work.

- The approach to future work builds on prior results. It would be nice to see when this project is anticipated to move beyond model validation and begin to impact some of the technical projects.
- The proposed future work is logical and sensible and continues to meet the analytical needs of the Fuel Cells subprogram.
- The project team needs to extend the model to non-automotive applications.
- I would like to see a high-temperature case exploiting high power density (allowing efficiency relaxation) across a range of driving cycles to really understand heat rejection issues and possible thermal management strategies; the radiator question needs to be revisited.
- A fundamental analysis of the trade-off of stack pressure drops and cell pitch and aspect ratios should be added to the pressure analysis.
- The project team should validate freeze modeling with Nuvera's freeze program.
- The team needs to increase effort on impurity and contaminant modeling (cathode air borne impurities as well as anode).
- They should consider a joint effort with LBNL, LANL, and NIST to elucidate water transport in the MEA.
- The future work is a shopping list of activities with no real statement of what would be delivered.

Strengths and weaknesses

Strengths

- The team has a solid technical staff generating good system models.
- The system tool is VERY powerful and broadly applicable.
- The PI is dynamic and has component modeling expertise.
- The project has access to a large amount of data generated by other research groups in the Hydrogen Program, and has applied simulation models to increase the understanding of the fuel cell processes. ANL is a collection point for many of the BOP data and simulations, which is a necessary function for the Hydrogen Program.

Weaknesses

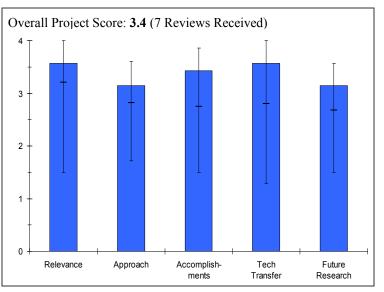
- The team could do a better job clarifying what is purely modeling, what is modeling using experimentally provided parameters, and what has been validated experimentally. This project covers a lot of things, and each requires a somewhat different modeling approach depending on the type of data available and what is possible from a purely theoretical standpoint. They could do a better job making the iterative process more clear (i.e., whether they started with a model, then saw how it fit the data, whether the model has been modified based on newer data, and whether new experiments were done to validate the model outcomes).
- The relevance and impact of this modeling effort is hampered by the lack of direct interaction with stack and system designers.
- The results seem a little lean for the funding level and timeframe.
- Duty cycle considerations are needed.
- There is too much emphasis on system optimization (this is the realm of the OEMs).
- The plots of the stack data appear to have "data points" and simulation curves. If a stack was operated, the plots should show its size/rating. If not, the project team should take the data points out of the plots since it gives the impression of real data. The PI needs to identify firm deliverables, e.g., how they will validate JARI and U.S. data and whether there is some absolute model that validates the data.

- It would perhaps make more sense to place less emphasis on these system-level activities in the future, because of the inherent issues associated with a national lab being able to get the most relevant technical input.
- There should be less focus on system optimization, and less effort on well-understood thermal management.
- The team needs to increase the focus on impurity modeling, freeze validation, and water transport through all layers of the MEA. They should validate their models using resources from the other DOE Hydrogen Program projects.
- There should be more effort on validating other DOE Hydrogen Program materials and claims.
- Is the Argonne reference 2009 data consistent with all vehicle fuel cell manufacturers or just one? With the program moving toward pre-automotive fuel cell systems, changes to simulation models and fuel cell system design data should be explained.
- It would be good to see more evaluation of systems used in other DOE-sponsored programs. It would also be good to see inclusion of other possible components for the air machinery and thermal management subsystems.

Project # FC-30: Mass-Production Cost Estimation of Automotive Fuel Cell Systems *Brian D. James and Jeffrev A. Kalinoski; Directed Technologies, Inc.*

Brief Summary of Project

The objectives of this project are to 1) identify the lowest system design and manufacturing methods for an 80-kWe direct H₂ automotive proton exchange membrane fuel cell (PEMFC) system based on three technology levels (2008 status technology, 2010 projected technology, 2015 projected technology); 2) determine costs for these three technology level systems at five production rates (1,000; 30,000; 80,000; 130,000; and 500,000 vehicles per year); and 3) analyze, quantify, and document the impact of system performance on cost. Some costs were not included (warranty, building costs, sales tax, and non-recurring engineering costs).



Question 1: Relevance to overall DOE objectives

This project earned a score of **3.6** for its relevance to DOE objectives.

- A reliable, detailed manufacturing cost estimate is essential to gauging progress and determining the relative importance of technology areas for the allocation of resources. Manufacturing cost is an important metric for original equipment manufacturers (OEMs) to make a go/no-go decision for the hydrogen fuel cell vehicle production decision.
- Cost analysis is imperative to measure technology status and important input for R&D direction.
- The program is relevant and in support of the objectives of the Hydrogen Program; however, assumptions regarding vehicle volume ramp-up rate are probably over optimistic.
- The analysis establishes a baseline for the cost of materials and manufacturing of proton exchange membrane fuel cell (PEMFC) systems at production rates approaching automotive needs.
- This project has an important role for the program to ensure that fuel cell vehicles are economically feasible at future high-volume production rates, ensuring there are no show-stoppers.

Question 2: Approach to performing the research and development

This project was rated **3.1** on its approach.

- The extensive use of detailed Design for Manufacturing and Assembly (DFMA®) analysis for stack and system components provides a solid basis for the system costing. Representative component designs were used where actual configurations were not available. The system model is derived from input derived from individual component suppliers and not thermodynamically integrated.
- The stack technology assumption is good, except 2010 Pt loading. Why it is higher than 2008 status?
- Fuel cell system architecture and its evolution should be analyzed to lower the total fuel cell system cost before technology assumption is fixed. There should be some trade-offs between operating conditions and cost sensitivities of each component, e.g., if humidification cost sensitivity is small, the system doesn't have to eliminate external humidifiers.
- The barriers as described will not be significantly impacted by the approach. Manufacturing costs will be driven by vehicle volumes, and this assumption has already been addressed as over optimistic. Platinum group metal (PGM) costs will be out of the control of any manufacturer and projecting these costs is very difficult.

- The approach uses DFMA, innovation, and practicality, and grounds the results in realistic components and costs.
- The team took a solid approach, building on previous successful years of cost projections.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated **3.4** based on accomplishments.

- Since the Directed Technologies, Inc. (DTI) 2007 cost analysis report, nearly every component cost has been updated or refined (some costs increased and some decreased) from both a design and analysis basis, which resulted in a net substantial system cost reduction. Further, new component technology and designs were analyzed and the cost was estimated for various system components.
- Progress in system cost analyses of this type is difficult, as many of the subsystems under consideration are in a constant state of flux. Without close involvement of OEMs and Tier 1 suppliers, true costs are difficult to pinpoint.
- Analyses and results are systematically developed and demonstrate a firm technology/cost base for projecting the cost of an automotive PEM fuel cell system. Some of the costs developed by DTI appear to be aggressive based on present industry practice. It was not clear there was adequate technical justification for the Treadstone coating work.
- The team gave an outstanding explanation of what has changed (specifically) since the 2007 analysis, and what impact that had on the overall fuel cell system cost (\$/kW net).
- The team made good use of detailed process analysis for things like stamping metal bipolar plates and membrane electrode assembly (MEA) frame gaskets.
- It is fortunate that Pt cost dropped precipitously due to the recession (by a factor of 2x), or the "current" evaluated costs of the fuel cell system could be significantly off.

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated **3.6** for technology transfer and collaboration.

- The detailed analysis of various new and improved components indicates substantial collaboration with component developers and suppliers.
- The team did not provide enough detail regarding collaborations.
- DTI works closely with industry to meet the goals of the cost analysis and provide a practical base for the data.
- Good collaborations are apparent with companies like Honeywell.
- The project team should discuss whether interactions have occurred with TIAX cost study, or are they totally independent?
- Would be useful for both TIAX and DTI to have one slide highlighting the major differences between the two studies.

Question 5: Approach to and relevance of proposed future research

This project was rated **3.1** for proposed future work.

- A plan and time schedule is presented in detail that includes NSTF, and low pressure fuel cell system analyses that are among the most fruitful areas for cost reduction.
- As mentioned at the "Approach" section, the cost analysis approach should be improved.
- Proposed future work plows no new ground and refines only what those analysis already performed.
- The future work discussion was lacking in detail, and appeared to be more of a schedule than a statement of deliverables. Future work should include the polybenzimidazole (PBI)-phosphoric acid (or equivalent fuel cell system) analysis.
- The 2009 updates look interesting.
- How will range-extended EVs (such as the Volt) be factored into potential sizing reductions for the system? Specifically, how much more (\$/kW) would a 40 kW fuel cell system cost than the 80 kW system?

Strengths and weaknesses

Strengths

- The team conducted fair detailed work with a good synergetic view of actually all cost influencing parameters/technologies.
- All major and some minor stack and system components have had detailed DFMA analysis performed, including updates for recent advances. The number of components included is extensive and representative of a complete Bill of Materials (BOM) assuring that the calculated cost is realistic.
- Cost modeling development was good.
- The team is well-grounded in the principles for conducting cost analyses. The program is well-organized and structured.
- The team gave an excellent presentation with clear explanation at each step of the process.
- They provided detailed results of what changed in the updates and what the impact on costs were.
- Reduction of labor cost was appropriate given the current labor market conditions.

Weaknesses

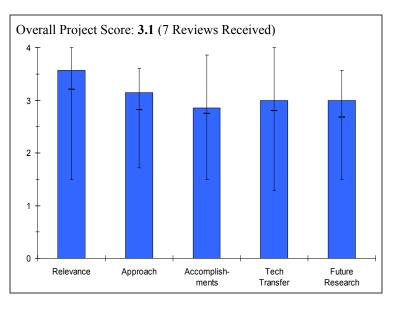
- The system model was based on component vendor input rather than thermodynamics, which can lead to incorrect performance/cost trade-offs and erroneous system efficiency.
- The vehicle volume projections are over optimistic.
- A broader range of information sources including European and Asian fuel cell manufacturers could improve the data.
- The PIs need to include the impact of handling freeze on cost.
- While the Monte Carlo analysis was performed, it would be nice to see the results presented.

- The presentation is kind of lost in details, and the slides are by far too busy and almost impossible to read/understand.
- A comprehensive summary with the most important findings is recommended.
- In addition to the extant plan, the team should increase the 2009 scope so that DTI can incorporate a thermodynamically correct model equivalent to that developed by ANL and use it to make the cost/performance trade-offs required to attain the lowest system costs. Further, multi-variable sensitivity cost studies should be added.
- The team should expand the effort to include PBI-phosphoric acid, silicon-carbide-phosphoric-acid, and other high-temperature (HT) membrane fuel cell systems. Do a comparison of these HT fuel cell systems to PEM.
- With such a high sensitivity to Pt cost, they need to have a plan of how to have year-to-year comparisons (and yet still a relevant projection) if Pt cost goes back up to where it was at its peak and stays there.
- Analysis of lower pressure systems (which was mentioned) is critical because of multiple OEMs heading in that direction.

Project # FC-31: Direct Hydrogen PEMFC Manufacturing Cost Estimation for Automotive Applications Jayanti Sinha, Stephen Lasher, and Yong Yang; TIAX LLC

Brief Summary of Project

The overall objective of this project is a bottom-up manufacturing cost assessment of an 80 kW direct H₂ proton exchange membrane fuel cell (PEMFC) system for automotive applications. The objectives for 2008 were to perform 1) a high-volume (500,000 units/year) cost projection of the Argonne National Laboratory 2008 PEMFC system configuration assuming a nanostructured thin film catalyst-based membrane electrode assembly (MEA) and a 30 µm perfluorosulfonic acid membrane; 2) bottom-up manufacturing cost analysis of both stack and balance of plant components; 3) sensitivity analyses on stack and system parameters; and 4) independent peer review of cost analysis methodology and results.



Question 1: Relevance to overall DOE objectives

This project earned a score of **3.6** for its relevance to DOE objectives.

- A reliable detailed manufacturing cost estimate is essential to gauging progress and determining relative importance of technology areas for allocation of resources. Manufacturing cost is an important metric for original equipment manufacturers (OEMs) to make a "go/no-go" decision for the Hydrogen Fuel Cell Program.
- An independent assessment of fuel cell system cost is directly relevant to the DOE Hydrogen Program objectives, and thus supports and is a necessary component of the program.
- None.
- The projection of cost based on present technology, present manufacturing capability, and future production provides a metric to judge the progress of the Hydrogen Program.
- Projecting fuel cell system cost is very important to show the glide pathway toward commercial viability in light-duty automotive applications.

Question 2: Approach to performing the research and development

This project was rated **3.1** on its approach.

- The utilization of the integrated system model developed by ANL gives additional credibility to the selection and sizing of components. This selection is critical to the determination of overall system efficiency, which in turn impacts system cost.
- Various types of fuel cell system architecture should be studied to lower the total system cost. Trade-offs between operating conditions and components cost sensitivities should be studied. Fuel cell systems for this cost study are not optimized to lower the cost.
- Overall model refinement should include some form of risk analysis in the approach description.
- The assumption of complete OEM control of the stack is unrealistic and should be changed to include some estimation of markup from tier 1 suppliers.
- A systematic approach was used that is based on inputs from the DOE HFCIT Program management, the Fuel Cell Technology Team, and the ANL system model. Critical Bill-of-Material was identified and used to specify manufacturing equipment and materials. The bottom-up approach provides practicality and realism to cost analysis. Interaction with industry builds confidence in the approach.

- The approach is solid, using a bottom-up approach to determining the high-volume manufacturing cost.
- There was good involvement of industry for vetting the assumptions and results; it keeps projects bounded by the inputs of experts.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated 2.9 based on accomplishments.

- Major progress has been made in stack cost reduction as a result of lower catalyst loading and increased power density of the nanostructured thin film catalyst (NSTFC)-based MEA. The balance-of-plant (BOP) components do not appear to be updated and have not had any cost reductions compared to the 2007 cost study report.
- Cost analysis on 3M's NSTF catalyst MEA is valuable. It is a new catalyst concept and different from Pt/C.
- The program has accomplished their stated objectives in a competent manner, and overall results are reasonable and believable.
- I do not give it a higher rating since the program cannot, by its objectives, actually move the technology forward as it just assesses this progress.
- The whole project seems to have a seat-of-the-pants feel.
- The project systematically forecasts the cost of the cell components, cell stack, and BOP. The values are consistent, but in some cases optimistic, with industry inputs. The project maintains checks and balances through its interaction with DOE, the fuel cell technical team, and industry.
- This year's update looks like it has made incremental improvements to respond to any weaknesses from previous years.
- Excellent detail provided of the key costs of each of the major parts of the systems.

<u>Ouestion 4: Technology transfer/collaborations with industry, universities and other laboratories</u>

This project was rated **3.0** for technology transfer and collaboration.

- Collaboration with ANL has been important in establishing a valid system model. Only limited collaboration with non-stack component suppliers is indicated even though these components contribute 50% of the cost.
- Interactions with the fuel cell technical team and an independent review panel are key steps that have been taken.
- However, it may benefit from earlier screenings of the system and assumptions with system developers.
- It is not clear as to the degree of collaboration between investigators.
- Collaboration with industry, ANL, and DOE is high and should be maintained. Fuel cell system models other than the ANL model should be considered.
- It is not clear how coordinated this is with the work of Directed Technologies, Inc. (DTI) (perhaps it is not supposed to be so that they are two totally independent/objective evaluations).
- I'm not sure if redundancies with DTI work are intended or accidental.

<u>Question 5: Approach to and relevance of proposed future research</u>

This project was rated **3.0** for proposed future work.

- Generic discussion is provided for proposed future work, but specific plans and focus areas are not available for review. It is anticipated that the substantial differences in the ANL 2009 system configuration would require a major rework in the costing.
- The cost study approach of the fuel cell system architecture assumption should be modified and include a system optimization process to lower the total cost.
- The modest goal of updating the stack and fuel cell system cost to align with current performance status, in this option year, are in line with the modest funding and appropriate for what is required at this time.
- The reviewer recommends removing the anode humidifier as developers have demonstrated they can do without (for example, see mechanization in SAE 2008-01-0420).
- I recommend using thinner membrane for improved performance and reduced cost (no greater than 25 microns).

- None.
- The future work will build on 2008 results for a final report.
- I look forward to knowing whether the preliminary 2009 estimates hold at \$24-33/kW.
- The team also needs to be evaluating smaller fuel cell systems to account for likely hybrid scenarios, including the much smaller size that might be used in a range-extended electric vehicle, such as the Volt.
- Back-up slides provide important information; see if some of those details can be worked into future review presentations.

Strengths and weaknesses

Strengths

- The presentation had clear graphics and introductory illustrative flow sheets in the presentation.
- Literally all aspects for cost were covered.
- The Design for Manufacturing and Assembly (DFMA®) bottoms-up analysis for unique fuel cell systems, internal technology-based cost models, and off-the-shelf costing for commercially available components is a good use of resources. Reliance on ANL system models provides a sound technical basis. Single and multi-variable cost sensitivity studies are a plus.
- The team performed a risk analysis of overall cost.
- They have an experienced team at TIAX and ANL. The bottom-up approach is believed to be the proper approach. Monte-Carlo methods are beneficial but need better explanation.
- Really like the Monte Carlo analysis to show the sensitivity of cost to changes in input parameters; it makes the result more believable than a simple single-point analysis.
- This project builds on a strong baseline from several years ago, with future updates providing meaningful and timely insights.

Weaknesses

- Not enough effort was devoted to non-stack system/component costs and the trade-off between the performance and cost of individual components.
- The whole analysis has a seat-of-the-pants feel, meaning that the level or depth of analysis seems rather shallow.
- The cost of membrane materials may be underestimated since high volume (for chemical industry) will not be achieved at 500,000 vehicles per year.
- The project team needs to clarify the role relative to DTI; compare methodologies, whether the same industry experts are consulted, etc.

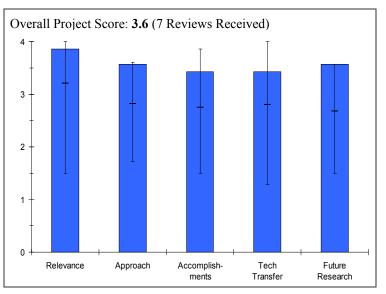
- A comprehensive summary would improve the presentation.
- The team should incorporate the latest system/component performance and design results from the 2009 AMR into the 2009 cost analysis study. They need to perform more DFMA studies of unique fuel cell components, and evaluate the trade-off between system performance and cost to develop the lowest system cost.
- The team should consider replacing the 30 micron membrane with a thinner membrane, likely 25 microns or less for commercial automotive fuel cell systems.
- The cost of \$16/m² for the membrane seems a bit too high. The team needs to compare this cost to projections from GM (Mathias et al., "Two Fuel Cells in Every Garage," The Electrochemical Society Interface, Fall 2005).
- An area utilization of 85% of the plates seems too high. If feasible, the project team should confirm with the Graftech DOE plate project.
- The project needs more depth and increased involvement of collaborators.
- The team should continue effort and expand industry contacts to Europe and Asia.
- No major changes required; project is on a good course.

Project # FC-32: Microstructural Characterization of PEM Fuel Cell Materials

Karren L. More, Larry Allard, Harry Meyer, and Shawn Reeves; Oak Ridge National Laboratory

Brief Summary of Project

The overall objectives of this project are to 1) identify high resolution imaging and compositional/chemical analysis techniques for the characterization of the material constituents comprising proton exchange membrane fuel cell (PEMFC) membrane electrode assemblies (MEAs); 2) apply these analytical and imaging techniques for the evaluation of microstructural and microchemical changes that determine fuel cell stability; and 3) elucidate microstructure-related degradation mechanisms contributing to PEM fuel cell performance loss. Collaboration with industry, academia, and national laboratories will be conducted to make these techniques (and expertise) available to



correlate structure and composition with MEA processing and/or life-testing studies.

Question 1: Relevance to overall DOE objectives

This project earned a score of **3.9** for its relevance to DOE objectives.

- These techniques are tremendously valuable to various aspects of materials development and failure analysis. It is important that enough time/effort can be effectively channeled to application of these methods to a wide array of materials.
- It is an outstanding and unique tool for understanding electrode structures before and after testing.
- Understanding the catalyst distribution and morphology, and the chemical composition of the MEA with time is key to understanding the degradation mechanisms of the fuel cell and is then key to improving the durability.
- This project has great possibilities to investigate catalyst particles with various methods.
- This project provides a unique and very useful capability to the fuel cell research community for materials characterization and development.
- The PI has developed several novel techniques for MEA and other fuel cell materials analyses.

Question 2: Approach to performing the research and development

This project was rated **3.6** on its approach.

- The potential for these techniques to provide valuable insight is clear. The ability to image electrode materials at conditions more appropriate to fuel cell operating conditions is extremely valuable. My only concern with the approach is that Dr. More's lab seems to get inundated with many samples from a wide range of studies at other labs. For microscopy analysis of this caliber to be truly successful in identifying fundamental information about electrode materials structures and durability, it is essential that efforts can be focused on a well-thought-out set of samples. Typically, this requires more time than perhaps the collaborating parties are willing to invest.
- It is not clear if DOE is footing the whole bill for this work. The assumption is that this capability would have application in a range of nanotech areas. My only comment is whether there could be synergies with other applications to accelerate progress in developing techniques.

- This effort focuses on development of a user facility providing state-of-the-art facilities for users to study the composition of MEAs at various stages of degradation. This excellent/optimal approach leverages the expertise of the microscopy experts with the fuel cell MEA expertise of the users/collaborators of the facility.
- Established know-how is used and adapted to current topics of interest.
- The project applies state-of-the-art electron microscopy techniques (including sampling preparation, mounting, and handling) to very high resolution (to Å scales) for materials imaging and compositional analyses.
- To address special issues and user needs, the project develops specialized approaches, such as microtomy to obtain depth profiles, and low-angle sectioning to determine variations in even very thin films and samples.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated 3.4 based on accomplishments.

- There are many fronts on which excellent progress has been made including the Å-level resolution of imaging and chemical analysis (with the Si-drift detector), *in situ* analysis of catalysts in liquid, 3-D tomography, and the ultra-low-angle microtomy method to perform through-plane chemical analysis via X-ray photoelectron spectroscopy.
- There are a lot of delays, which is understandable with such specialized equipment, but the presentation did a great job of highlighting progress.
- New tools have been added and existing capabilities have been improved.
 - Can study the chemical composition of MEAs to understand degradation;
 - Can look at the 3D distribution of the catalyst nanoparticle;
 - Can look in detail at the Å-level at the composition of the catalyst nanoparticle; and
 - Can study *in situ* the behavior of catalysts in a liquid electrolyte environment.

All of these are important accomplishments to help guide the community towards an understanding of the fundamental degradation mechanisms in the fuel cell.

- Large progress was made compared the last year report.
- This project is continuing to develop innovative techniques to provide useful data on MEAs and other fuel cell components.
- They are now able to provide Å-scale image resolution by aberration-corrected scanning transmission electron microscopy (STEM), which can be used to study core-shell nanoparticles, for example.
- They have built a liquid-flow cell for *in situ* electron microscopy at the nanometer scale.
- They are using electron tomography for 3-D analyses and imaging.
- They have developed ultra low angle microtomy to obtain as many as 19 30-µm "spots" across a 100-µm-thick MEA to characterize composition across the MEA.

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated **3.4** for technology transfer and collaboration.

- Clearly, this resource is being broadly used by many other institutions.
- Lots of collaborators; however, there is a lack of connectivity to any specific problem being addressed or solved. The audience is left to imagine utilization of the techniques for their own purposes. For example, there have been a lot of questions about electrode optimization:
 - o How uniformly dispersed is the catalyst in commercial products?
 - Why can 50% electrochemical surface area (be lost and performance unchanged?
- It would be good to show beginning-of-life vs. end-of-life with technical interpretation to fully bring home the value of these techniques.
- As an open-user facility, this project provides the best opportunities for technology transfer. The project has a good set of collaborations; still it seems there could be a significantly greater base of collaborations/users that could be developed.
- This project collaborates extensively with many of the organizations conducting fuel cell R&D.
- ORNL is also collaborating with several universities under the Shared Research Equipment Program, which provides access by other organizations to this project's specialized equipment and techniques.

<u>Ouestion 5: Approach to and relevance of proposed future research</u>

This project was rated **3.6** for proposed future work.

- Continued refinement and application of these powerful methods will be greatly beneficial to fundamental understanding of electrode materials.
- Development of the techniques is core.
- My suggestion is to place more emphasis on application of the techniques to solving specific user/customer questions/problems. This approach will help a bigger audience appreciate the value, and undoubtedly induce more solicitations for use.
- The impact of methods on temperature (heating) and/or electrification of samples may need further characterization.
- Future work is guided towards providing the state-of-the-art capabilities for fuel cell microscopy in support of the DOE program. The team must continue to develop collaborations to enhance the work performed at the facility.
- Due to good cooperation with different partners, the established methods are further developed in the right direction.
- Their plans call for developing the various techniques still further by adding other capabilities, such as electrical contacts to the samples in the liquid flow cell for *in situ* analyses.

Strengths and weaknesses

Strengths

- The project exhibits the excellent technical skills of the PI and world-class instruments. There are seemingly strong support staff and facilities at ORNL. The "user" nature of the lab to allow ready access to these techniques by other organizations is good.
- They are a talented research team with state-of-the-art equipment, and the user facility gives everyone access.
- The instrumentation and techniques developed in this project provide unique insights into MEAs, which gives insight of great value in understanding materials degradation over time and as a function of the operating environment and operating history of the MEA.

Weaknesses

- The team has the potential to get bogged down in too much technique development and somewhat diffuse analysis of a wide range of samples. It is important that these tools are focused on a couple of carefully planned sets of samples to get at a more systematic analysis of electrode materials properties and degradation modes.
- The team is a little biased toward the techniques and the "wow factor" (which IS definitely impressive!) than bona fide problem solving.

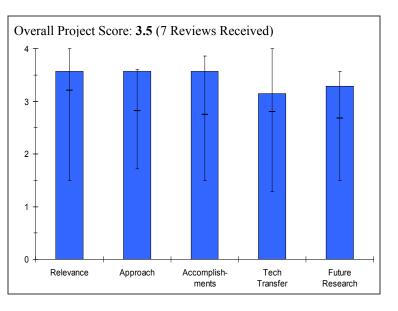
- A thought on a study that could be broadly beneficial: Analyze several commercial catalysts in powder form, as a new electrode film, and as an aged electrode (run for a few hundred hours) to identify general features, such as:
 - carbon and catalyst particle size/morphology;
 - interaction of catalyst-support among these 3 types (how well each adheres);
 - o carbon-ionomer interaction in the electrodes.
- Balance heavy lab/academia portfolio of collaborators with commercial/industrial collaborators, especially stack users with durability issues arising in real system applications.
- The planned future work described in the presentation should be executed.

Project # FC-33: Platinum Group Metal Recycling Technology Development

Lawrence Shore; BASF Catalysts LLC

Brief Summary of Project

The objectives of this project are to 1) achieve a platinum recovery rate of 98% to lower the effective cost of platinum used in a fuel cell membrane electrode assembly (MEA); 2) simplify the process so that platinum recovery is achieved using a single leach to reduce the cost of platinum recovery by increasing throughput; and 3) determine chemistry and reaction conditions to optimize platinum leaching to reduce reagent usage, reducing process cost, and to reduce cost of construction for the reactor vessel by identifying the most appropriate reactor liner. This project has achieved the objective of 98% platinum recovery, identified room-temperature alternatives, and reduced reagent usage for platinum leaching.



Question 1: Relevance to overall DOE objectives

This project earned a score of **3.6** for its relevance to DOE objectives.

- This project to evaluate Pt group recycling technology directly addresses DOE targets for overall cost and for stack material and manufacturing cost.
- Platinum is the single largest material cost component of the stack and system. Any reduction in this cost through recycling would move fuel cell stack costs closer to reaching the system cost targets.
- This is a great program to recover platinum and therefore reduce its cost as well as the cost of downstream products.
- Outstanding platinum recovery rates offer a method to minimize platinum costs and improve re-utilization of older systems.
- Due the fact that Pt loading is one of the main cost drivers in 2010 and 2015 stack cost analysis, the recycling becomes more and more relevant; therefore, this project has a high relevance.
- This project is developing simple, low-cost processes for recycling Pt. There is a significant concern, however, that this technology is not yet mature, and may change substantially between now and the time of commercialization.
- Pt recycling is a significant positive factor in stack life-cycle cost and PM supply, thus is of significant importance to the DOE Hydrogen Program.
- Recovery of the platinum from fuel cell electrodes is very important to the viability of fuel cell systems. This BASF Catalysts LLC project shows a relatively straightforward and cost-effective means to do so.

Question 2: Approach to performing the research and development

This project was rated **3.6** on its approach.

• This is a strong approach that is integrating prior work to develop a final system-level capability and analysis and focus on remaining primary challenges. The approach addresses both current and emerging polybenzimidazole (PBI) membrane MEA technologies. There is a good range of Pt recovery approaches evaluated, while keeping adequate focus on the overall goals/targets.

- The overall approach of exploration, validation, and process flow development has yielded positive results and attainment of project objectives of 98% or greater Pt recovery.
- Solid, steady progress has been made on a variety of well-identified challenges.
- The team has done very good work to overcome technical barriers and reduce costs of platinum recovery. The project was well-designed, feasible given the payback received, and fits well into overall DOE goals to make fuel cells affordable to the consumer.
- Their approach has been to select processes that are not specific to the platinum matrix, verify that the processes work with MEAs and other fuel cell components, develop a process flowsheet, and validate and seek process improvements.
- The PI has taken a methodical and comprehensive approach to the program and appears to have successfully met objectives, though it is unclear as to the potential impact of ultra low loaded and alternative electrodes which may be required to meet program commercialization (cost) objectives.
- The approach for this program is "outstanding" because they effectively accomplished their goals, and even expanded their effort to the BASF Celtec membranes. They made an effort to look at spent membranes that would be similar to what would be returned for platinum reclamation. This research is not very exciting, but is very good.

<u>Ouestion 3: Technical accomplishments and progress toward project and DOE goals</u></u>

This project was rated 3.6 based on accomplishments.

- Significant progress has been made in achieving the DOE targets and in identifying key issues/solutions for practical systems ranging from the Pt recovery processes to processing equipment corrosion impacts, and approaches to mitigate those issues. The team demonstrated a method for leach process quality control/analysis and made significant progress in simplifying the Pt recovery process (i.e., single vessel leaching). The team provided a good estimate of cost impacts for increasing Pt recovery by 1% from 98% to 99% based on their recovery experimental results.
- Process parameters appear to have been optimized and only details remain to be wrapped-up in a technology commercialization phase. The basic oxidizing acidic solution approach with aqua regia, HCl, H₂O₂, etc., had been identified in earlier patents by others.
- I wouldn't mind awarding BASF a score "5" for this area.
- Recovery processes offer real promise to lower platinum costs through the reduction of a number of in-use materials.
- It appears that BASF was willing to try, change, and adjust processes that meet goals, rather than finding a goal that meets the existing process.
- By developing a simplified leaching process, good progress was made since the last DOE report.
- A key accomplishment has been to achieve 98% Pt recovery without forming and releasing any hydrofluoric acid (HF).
- Another significant accomplishment has been the development of a one-step, one-vessel process (including vessel material validation).
- An added benefit of the process is that it avoids cryogenic milling using liquefied nitrogen cooling.
- The performance of the process has been verified with new and aged MEAs.
- The PI has taken a methodical and comprehensive approach to the program and appears to have successfully met objectives.
- It looks like they finished the job and are just waiting on 10,000 fuel cell cars now.

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated **3.1** for technology transfer and collaboration.

- The team had strong collaborations with partners that provide complementary expertise and facilities/capabilities.
- Collaboration has occurred with potential suppliers of processing equipment and chemicals.

- I recognize that BASF is only working with one collaborator now, which shows that the project has progressed from requiring a number of partners and collaborators to a project near its end-state. It is not worth punishing success, as BASF worked itself into a position to close-out collaborator support.
- Several important partners are involved in these activities.
- They have worked with several organizations from industry, suppliers, and consultants.
- The team may benefit from interactions with developers of novel electrodes (NSTF, core-shell) unless the PI can state assurance that the process will be applicable to these.
- BASF did a good job getting MEAs from different vendors; however, they might have expanded their effort more to some of the alternative catalysts being developed by other collaborators.

Question 5: Approach to and relevance of proposed future research

This project was rated **3.3** for proposed future work.

- The project is wrapping up. Proposed future work will complete key outstanding experiments and compile the results and analysis into a final report.
- Further process optimization/simplification is planned, but specific plans are not available for review.
- It is very nice to have a project completed as planned.
- This project has demonstrated outstanding year-to-year progress during the life of the project.
- The project has well-thought plans for the future work site floor plan.
- They will primarily be wrapping up some final points (effects of sonication to promote leaching, optimize process temperature and pressure, etc.) in the project that is already 98% complete.
- The program is near completion, but I'd like to see the following:
 - An estimate of yield and cost benefit/impact of lower Pt loaded electrodes (0.025-0.05 mg/cm² anode, 0.05-0.1-0.2 mg/cm² cathode) as well as alternate structured electrodes (NSTF, core-shell); and
 - An estimate of overall cost benefit (Pt yield vs. process cost) to assist DOE in assessing life-cycle Pt cost.
- The program ends this year. BASF has the opportunity now to build a plant once fuel cell vehicles become commercialized.

Strengths and weaknesses

Strengths

- The project clearly demonstrated that >98% recovery could be achieved with a simplified process using lower acid concentrations with reduced environmental load.
- The team did an outstanding overall job.
- They have an industrially strong team of collaborators.
- The team has the expertise of the PI in precious metal recycling, and took a solid, methodical approach.
- The project team solved the problem.

Weaknesses

• The project was relatively low-risk compared to others in the fuel cell portfolio since it was basic process optimization/simplification and did not move the Pt reclamation technology forward dramatically.

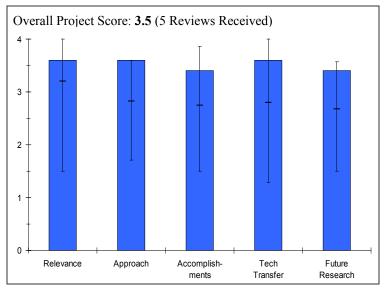
- The project team should wrap-up the program with a detailed report so that industry can benefit from results.
- The project is already 98% complete. There are no significant recommendations to offer.

Project # FC-34: Neutron Imaging Study of the Water Transport in Operating Fuel Cells

David Jacobson, Daniel Hussey, Eli Baltic, and Muhammad Arif; National Institute of Standards and Technology

Brief Summary of Project

This project aims to develop and employ an effective neutron imaging-based, nondestructive diagnostics tool to characterize water transport in proton exchange membrane fuel cells (PEMFCs). The objectives of this project are to 1) form collaborations with industry, national laboratories, and academic researchers; 2) provide research and testing infrastructure to enable the fuel cell/hydrogen storage industry to design, test, and optimize prototype to commercial grade fuel cells and hydrogen storage devices; 3) make research data available for beneficial use by the fuel cell community; 4) provide a secure facility for proprietary research by industry; 5) transfer data interpretation and analysis



algorithms techniques to industry to enable them to use research information more effectively and independently; and 6) continually develop methods and technology to accommodate rapidly changing industry/academia need.

Question 1: Relevance to overall DOE objectives

This project earned a score of **3.6** for its relevance to DOE objectives.

- Strong *in situ* analytical tools for measuring water conditions in active/running fuel cells are of paramount importance to developers in understanding and designing their systems. Water management is one of the most important aspects of fuel cell performance and durability. Any tool to help developers with water management will play a significant roll in helping DOE meet objectives of the program.
- One of the very few ways of seeing inside the "black box," this project is tremendously valuable for reconciling models and empirical results with respect to water management.
- The project helps to address fuel cell performance issues.
- It is not clear how any of this addresses the #1 key issue of fuel cell cost.

Question 2: Approach to performing the research and development

This project was rated **3.6** on its approach.

- The PI is using one of the inherent advantages of neutron images (having a larger cross section of H compared to other methods like X-ray that don't see H well) to help the objectives of the team. Recently, the PI has worked to improve the resolution of the equipment to visualize through plane water profiles, which is very important. The PI has also worked to compliment the water imaging by correlating with current and temperature profiles of the same systems. This combination of data (*in situ*) is very useful for developers.
- The project team has shown good focus on utility and application of the method to real problems.
- The capabilities are well-deployed, but it is not clearly presented what the exact challenges are to achieving higher resolutions and scan rates. The progress with LANL is excellent, although future membranes may be as thin as ~8-10 μ m; suggesting an ultimate resolution of ~2 μ m (4x higher than now) may be desirable. Is it possible and what will it take to get there?
- It is not clear if scanning slit option is available. A detector with a high aspect ratio (instead of square) over which a cell is moved, may provide more economy.
- I see a need for a high-resolution detection scheme that has a height equal to an actual fuel cell.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated 3.4 based on accomplishments.

- The PI has heeded the recommendations of the Fuel Cell Technical Team and original equipment manufacturers (OEMs) by completing the upgrade to higher resolution systems, correlating work with temperature and current density profiles. He has also worked to develop an improved understanding of the model discrepancies with real world testing.
- High-resolution work is excellent; keep going!
- Experiments at low temperature are extremely impressive!
- The work on H₂ storage was interesting, but could have been more succinct.

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated **3.6** for technology transfer and collaboration.

- NIST is teamed with the appropriate end users of the technology such as GM and Ford, and some of the best fuel cell research labs such as LANL. The combination of these partners provides NIST with the expertise and resources needed to build a successful program.
- The project has a very impressive portfolio of users!
- The technique is well-established, and technical publicizing has been extremely effective.

<u>Question 5: Approach to and relevance of proposed future research</u>

This project was rated 3.4 for proposed future work.

- Any further increase in spatial resolution (up to 1 µm) to visualize through-plane behavior of membranes would be appreciated, since membranes are becoming increasingly thinner as the technology progresses.
- In addition to listing collaborators, it would be considerably more compelling to have a matrix showing what type of study was done with that user; this activity is strongly encouraged for next year.
- The focus seems to be on developing new instrumentation and better capabilities, rather than working with major stack developers and helping them solve their problems.

Strengths and weaknesses

Strengths

- NIST is one of the few labs in the world that can conduct this work.
- They make a very expensive tool available to the research community at a cost-effective price.
- NIST is a unique facility with world-class staff and equipment; the users are obviously deriving high value.

Weaknesses

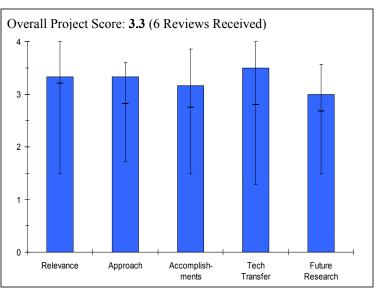
- Evidence of a user-voiced specification for what detection is necessary.
- The team needs high resolution over more realistic dimensions (~0.25 µm height).

Project # FC-35: Water Transport Exploratory Studies

Rod Borup; Los Alamos National Laboratory

Brief Summary of Project

The overall objective of this project is to develop an understanding of water transport in proton exchange membrane fuel cells (PEMFCs). The specific objectives are to 1) evaluate structural and surface properties of materials affecting water transport and performance; 2) develop (enable) new components and operating methods; 3) accurately model water transport within the fuel cell; 4) develop a better understanding of the effects of freeze/thaw cycles and operation; 5) develop models which accurately predict cell water content and water distributions; 6) work with developers to better the state-of-art; and 7) present and publish results.



Question 1: Relevance to overall DOE objectives

This project earned a score of 3.3 for its relevance to DOE objectives.

- Understanding water management is critical to optimal design of fuel cell systems and thus to meeting DOE objectives.
- This study developed experimental methods to look at water transport. Of particular interest (to me) were the neutron scattering pictures. Presumably the sort of techniques presented here will prove important to analyzing fuel cells for many years into the future.
- The focus of project work could be better.
- The issue of water management in PEMFCs is clearly important to understanding and addressing the key technical barriers for fuel cells, including optimizing performance and cost. The project approach based on detailed experimental characterization and modeling of water transport seems very relevant to the overall objectives, provided the approach continues to move toward clear recommendations. The non design-specific approach of the program makes it a little more difficult to move to specific recommendations.
- Water transport impacts numerous areas of major importance to the success of the hydrogen fuel cell effort: performance, durability, freeze survivability, and start. Thus, it is an important area for continued DOE funding.
- Serves objectives B, C, start-up energy consumption, and freeze start operation.
- The project team has designed an independent approach focusing on water concentration in MEAs. The project addresses cost and performance targets of the DOE, and involves the relevant industry. Water transport is of utmost importance for PEM technology. The program is critical to the Hydrogen Program of the DOE, and fully supports the objectives.

Question 2: Approach to performing the research and development

This project was rated **3.3** on its approach.

- The direction of effort is not clear.
- The project timelines, deliverables and go/no-go points need to be addressed. How will the data feed into a model?
- The PI generally did a better job this year of clearly specifying fuel cell operation conditions.

- Some methods seemed good, but others less-so. There are too many groups; they each do okay work, but each seemed to be going its own way.
- The "Characterization Approach" seems to be well thought-out and scientifically sound, taking into account industry approaches and current materials, while keeping the approach non design-specific as much as possible. The project's approach needs to continue towards making clear recommendations in the area of developing or enabling new materials and operating methods.
- The project team has taken a good approach to integrate the diagnostic effort with LBNL's modeling expertise.
- However, the program appears to be too wide-ranging and lacking focus. What are the primary objectives and expected outcomes? Perhaps it would be better to pick two or three areas. For example, developing a quantitative understanding of water transport through the electrode, membrane, and gas diffusion layers (GDL) by combining diagnostics such as NIST neutron imaging experiments with modeling efforts.
- Cutting edge *in situ* measurements of membrane water are being carried out. Water profiles for different membrane geometries were investigated, and the results were published. In the presentation, specific reference to published results was given. The water content vs. time was measured for wetting and drying modes. This is a case in point for the technical focus of the program. The same holds true for investigations on freezing. The x-ray tomography delivered impressive results. The modeling activities support the investigations. Modeling might gain additional importance as the project proceeds.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated **3.2** based on accomplishments.

- Experimental methods shown seemed good. Other work seemed less well developed. It was hard to pin down exactly what was accomplished beyond visualization.
- The technical accomplishments of understanding in the water transport and behavior are good, and the project needs to continue towards making recommendations.
- The project team has done good diagnostic work with many interesting observations, but little in the way of conclusions.
- The research raises a lot of questions (such as the actual lambda of membrane vs. relative humidity (RH) and temperature slide 7), but again, it is not clear as to the answers. Is membrane lambda vs. RH and temperature considered still controversial? Is this real or an artifact of signal/noise ratio?
- The high-resolution measurement quotes lambda to one decimal, but the measurement of thickness in a water-filled channel varies by over 30%; error seems significant (slide 7, center figure).
- On slides 10 and 11 (wetting/drying transients), is time scale actually due to GDL properties as suggested, or just due to airflow saturation (i.e., was the longer dry out time scale after down-transient due to reduced capacity of reduced airflow to hold water, or did I misunderstand and airflow was held constant)? It is not clear how wetting transient analysis is being used in the overall project.
- What size channels are being used for freeze durability experiments? Is the cell purged at shut-down? The degradation shown is not observed in application hardware with paper GDLs.
- The technical results are outstanding in that freeze properties can now be monitored. Fundamental characterization of the GDL was performed, including the introduction of the 3D x-ray tomography.
- A table of many accomplishments is included in the presentation.
- The progress made is outstanding in terms of quantity and quality.

<u>Ouestion 4: Technology transfer/collaborations with industry, universities and other laboratories</u>

This project was rated **3.5** for technology transfer and collaboration.

- The project team has demonstrated good collaboration with industry, national labs, and academia.
- If the PI is being used primarily as a data resource for other groups, then he should indicate it. The PI is conducting a tremendous amount of work on many fields, but has no specific end goal in mind.
- There are too many groups. They each do okay work, but each seemed to be going its own way.
- The project has an extensive list of collaborators, which appear to be actively involved and contributing to the program.
- The team demonstrated excellent interaction with NIST and the modeling effort.

FY 2009 Merit Review and Peer Evaluation Report

- It is less clear what the Nuvera interactions were. Can LANL provide insight into the observations and results from the Nuvera freeze study?
- There are six institutional partners involved and four companies. All of them are renowned, or at least well known. The program looks very well-organized.

Question 5: Approach to and relevance of proposed future research

This project was rated **3.0** for proposed future work.

- The PI proposes a large amount of work. The PI should reduce his scope and work on topics that may not overlap with other projects.
- Future goals, methods, and milestones seemed vague.
- The plans address key areas of further understanding of the behavior and changes in the GDL. It is important to focus this understanding on improvements and recommendations to address the key barriers of performance optimization.
- I support the modeling proposals.
- I would like to see more interaction with the Nuvera freeze project.
- The plan for how all these experiments are going to tie together is not clear. It seems that many fundamental issues have been highlighted, but does LANL have the resources to dig into each one?
- The focus on the 3D tomography is appreciated, as well as the increasing importance of modeling.

Strengths and weaknesses

Strengths

- Nice visualization methods are shown.
- The project brings together an excellent team with clear focus on understanding the fundamental behavior of water transport in the PEM. The project makes use of state-of-the-art scientific methods to develop an understanding of the fundamental characteristics that affect some key performance barriers in PEM fuel cells.
- The project has generally solid, broad-based experimental studies with lots of key fuel cell partners.
- The team has an excellent analytical technique portfolio and analysis capabilities.
- The broad scientific input through institutes and the technical input from the industrial cooperation partners are strengths of the project team.

Weaknesses

- There is a tremendous amount of data presented in this presentation. The PI does not do a good job of tying it together or describing the relevance to the overall objectives. It is unclear whether the PI is focusing on, cold performance, modeling, durability effects, or material effects.
- Beyond visualization, the project seemed to wander, and has a lack of focus, with no clear goals for future work.
- The project has a non design-specific approach, which may be a weakness in moving to clear recommendations to address the barriers. The project should try to make clear the recommendations for materials and operating profiles to address these issues, at least within the generalizations of a non design-specific cell configuration.
- It would be nice to come to recommendations from all these excellent measurements on how to come to improved performance via operating parameters and/or novel materials.
- There is some lack of program focus.
- There are no notable weaknesses.

- The PI does not tell me why his results are important, or how they relate to the bigger picture. The objectives are extremely vague and do not help tell the story either.
- The team needs to weed out collaborators. The PIs should focus work on targeted, defined goals.
- The team needs to continue to look at materials and operating profiles to move to recommendations for cell performance optimization.

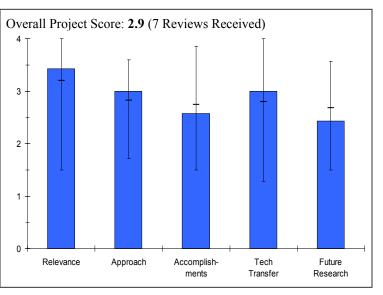
- I would like to see more interaction with the Nuvera freeze program.
- I am concerned about the use of serpentine flow fields in material degradation studies, as these flow fields are well-known to accumulate water in the U-bends. During freezing, water "slugs" can expand and damage the unitized electrode assembly (UEA). A non-serpentine flow field is recommended. Without U-bends, such a rig is more relevant to application hardware used by most or all automotive OEMs.

Project # FC-36: Water Transport in PEM Fuel Cells: Advanced Modeling, Material Selection, Testing, and Design Optimization

J. Vernon Cole and Ashok Gidwani; CFD Research Corporation

Brief Summary of Project

The overall objectives of this project are to 1) develop advanced physical models and conduct material and cell characterization experiments; 2) improve understanding of the effect of various cell component properties and structure on the gas and water transport in a proton exchange membrane fuel cell (PEMFC); 3) demonstrate improvement in water management in cells and short stacks; and 4) encapsulate the developed models in a commercial modeling and analysis tool. The fiscal year 2008 and 2009 objectives were to 1) complete baseline characterization for gas diffusion layer (GDL) materials; 2) gather experimental data under controlled conditions, test and apply models for water



transport in GDLs, channels, and across interfaces; and 3) evaluate performance and water management sensitivity in operational cells, evaluate cell-scale water transport models on a component level, and integrate with electrochemistry and test.

Question 1: Relevance to overall DOE objectives

This project earned a score of **3.4** for its relevance to DOE objectives.

- This project aims to improve the understanding of water transport in automotive fuel cells, issues of freeze/thaw cycle tolerance and cold start-up.
- Understanding water transport within PEM fuel cells is important for optimizing fuel cell performance, cost and durability
- Start-up of a fuel-cell car requires that frozen water in the FC can be purged; operation requires that water can be removed in operation. They found that these effects are strongly temperature dependent, but do most of their work at 35C, and study mostly the GDL. 35C operation may be a good average value to study, but it hardly constitutes the major operation conditions. Also, is water transport in the GDL the main water transport issue?
- Project addresses barriers D, E, and G primarily under task 4, develop gas diffusion layers.
- The project uses modeling and experimental characterization with the ultimate goal of improved components and fuel cell operating concepts. Current devices have power density limitations and durability concerns due to water transport. While this project addresses power density limitations, it has not as yet addressed any durability concerns. Water transport, while important, is not the most critical aspect limiting fuel cell commercialization.

Question 2: Approach to performing the research and development

This project was rated **3.0** on its approach.

- The project combines theoretical and experimental investigations of water transport in various components of PEM fuel cells.
- Characterization of materials feeding properties to modeling is a good approach to future developments.
- They do a good job of visualizing the flows, and have put them into multi-physics form. I'm sorry to say, but these models hardly include the effect of temperature, and seem to be based on constant low-temperature operation. My sense is that a fuel cell that operates at 65°C or 110°C will have very different behaviors than

shown here. My sense, also, is that higher temperatures are more relevant to the auto industry, so that there should not be as much plug formation as shown here. There seemed to be no formal way to integrate experiments with models.

- The team uses extensive characterization and modeling to understand water transport. The results are used for subsequent optimization.
- Combining modeling and experimental characterization is a reasonable approach to addressing key issues relevant to water transport in fuel cell systems. The project suggests the ultimate goal is improved components or operating concepts, but has shown no example how these will be achieved, or examples of how they are being currently addressed (at best this is not clear from the presentation). It is unclear how many of the experimental results are being tied to modeling studies.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated **2.6** based on accomplishments.

- At the midway point, the project is still in the phase of collecting data and formulating models. To date, the project has not produced results to demonstrate a clear path to improved understanding. Hopefully, this will happen soon.
- The team provided good materials characterization of GDLs.
- There seems to be minimal performance measurements in actual operating fuel cells.
- Laser scans of GDL structure and variation with polytetrafluoroethylene (PTFE) loading are interesting.
- They do a good job visualizing the flows, and have put them into multi-physics form. I'm sorry to say, but these models hardly include the effect of temperature. It is not clear how hard it would be to add temperature better. Whetting angle, viscosity, and vapor-liquid equilibrium will be much different at 80°C, for example. Similarly, ice behaves differently than water. We need models that help with the important issues of membrane electrode assembly (MEA) operation. There was some experimental data, but there seemed to be no formal way to integrate experiments with models.
- The team extensively characterized GDL properties. They had a model developed, although comparison to experimental data presented to validate the model was unconvincing. It also appears that the model is limited by the coarseness of the grid used, and is not yet applicable to varying flow field channel designs.
- The project has presented significant experimental studies including base materials characterization. The models being applied are not presented in full enough detail to assess shortcoming/limitations, and show poor agreement with experimental data under many conditions (much worse than other reported studies). The value of these models and the ability to be further refined for increased value is unclear. To date, it is not clear how the experimental studies are helping material design or operating strategies. It is also unclear how relevant self-humidified studies are and how applicable the reported results are to long-term operation where wetting characteristics of materials are known to change.

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated **3.0** for technology transfer and collaboration.

- The project has assembled a credible team.
- The team demonstrated good interactions with an appropriate set of partners.
- The team had a good selection of partners, but the presentation did not differentiate what work was done by which partners, or what benefits were gained from distributing the project. To the extent that experiment and theory work was done in different locations, there seemed to be poor integration.
- There was a good mix of partners with complimentary skills. If Ballard is involved, why does the team need to initiate technology transfer through the University of South Carolina?
- There are several strong partners with relevant skills. The level of coordination between partners is unclear in several areas, and it is unclear how experimental studies are feeding modeling work (slide 19 on). There was very little from the project publicly presented, with only a "Transactions" paper listed in the current literature. Although a paper and second "Transaction" paper are listed as accepted, this lack of data in the literature makes supplemental information about the project harder to evaluate.

<u>Ouestion 5: Approach to and relevance of proposed future research</u>

This project was rated 2.4 for proposed future work.

- The future plans appear logical, but there is no evidence that the project will produce models that can actually be useful in optimizing the structure of fuel cell components or cell performance.
- The objective of the project is to demonstrate improvements in water management in cells and short stacks; however, this seems to be missing from the future work plans.
- There is no particularly strong plan to cover the weaknesses presented. Future work goals and milestones were fuzzy.
- The team will complete the characterization and modeling of the GDL. It is essential that the effect of temperature gradients and electrochemistry be explored on both.
- It is not possible to evaluate whether or not the proposed future work will lead to enough modeling improvements to make the models useful in a predictive fashion. Current models show relatively poor agreement with experimental results and adding aspects heat transfer and phase change may help, but it's unclear they will be enough to resolve all issues. Without a validated model, exploring optimization strategies doesn't make sense.

Strengths and weaknesses

Strengths

- This is a good team.
- They team had good combined modeling and experimental studies.
- Coupling of material characterization and modeling is important for good developments.
- The team had nice pictures (multi-physics can be powerful).
- The team was sharply focused on the real problems in GDLs, and aiming for optimization of manufacturable complements.
- There was a good mix of team strengths, with modelers and experimentalists well-represented. There was significant materials characterization at least within a specific window (slide 6, for example).

Weaknesses

- There were no breakthrough results.
- There were no plans to produce data, or models that will address issues of start-up and shut-down, start-up from subfreezing temperatures, or freeze/thaw tolerance.
- The use of numerically generated GDL microstructure is not an accurate representation of GDL materials.
- The data presented look-like analysis, and was at unlikely operation temperatures; temperature effects remain largely unstudied. There was also poor integration between experiment and theory. At this point, water transport analysis seems unlikely to aid in fuel cell design and operation.
- There was a lack of integration of electrochemistry and the effect of temperature.
- Results to-date are not compelling, and there is no reason to believe future efforts will necessarily lead to significant improvements. The wide team seems to be taking on multiple aspects of water transport (at different levels) without addressing any of them particularly well.

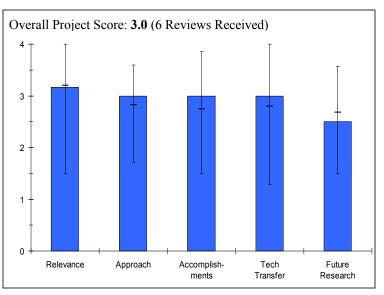
- The team needs major correction by looking at other (higher) operation temperatures. They need to integrate theory with experiment in terms of design/operation models. What happens when flow is in "up" direction?
- More electrochemical engineering and characterization of temperature is needed.
- The team should focus on a single aspect of water transport; for example, flow in the GDL or in the flow channel, rather than several aspects such as flow in the GDL, in the channel, and the transition between the GDL and flow channel. It is better to have a reasonably good picture of one of these aspects, than inaccurate representations of many.

Project # FC-37: Visualization of Fuel Cell Water Transport and Performance Characterization Under Freezing Conditions

Satish Kandlikar and Zijie Lu; Rochester Institute of Technology Thomas Trabold, Jerry Gagliardo, and Jon Owejan; General Motors Jeffrey Allen and Reza Shahbazian-Yassar; Michigan Technological University

Brief Summary of Project

The overall objectives of this project are to 1) gain a fundamental understanding of the water transport processes in the proton exchange membrane fuel cell (PEMFC) stack components; 2) minimize fuel cell water accumulation while suppressing regions of dehumidification by an optimized combination of new gas diffusion layer (GDL) material and design, new bipolar plate design and surface treatment, and anode/cathode flow conditions; and 3) meet U.S. DOE targets for 80 kWe transportation stacks. The goal for 2008 was to implement changes to the baseline system and assess the performance of 1) ex situ combinatorial performance; 2) in situ combinatorial performance: 3) water distribution and



current density distribution; and 4) microscopic study and models for water transport in GDLs and parallel channels.

Question 1: Relevance to overall DOE objectives

This project earned a score of **3.2** for its relevance to DOE objectives.

- Understanding water flow distribution is essential to building better fuel cells. Understanding misdistribution effects will help significantly reduce water purge energy, etc.
- The start-up of a fuel-cell car requires that frozen water in the fuel cell can be purged; operation requires that water can be removed in operation. They found that these effects are strongly temperature dependent, but do most of their work at 35°C, and study mostly the GDL. 35°C operation may be a good average value to study, but it hardly constitutes the major operation conditions. Also, is water transport in the GDL the main water transport issue?
- The project's approach to understand water management and address the effects under normal and freezing conditions clearly addresses some of the key technical barriers to fuel cell performance and adoption.
- This is a very effective visualization tool to qualitatively analyze what happens in the course of a purge.
- However, this doesn't seem to be set-up specifically to close a technical gap. This falls more under the purview of basic research and development, rather than a means to close the gap related to energy expenditure under a cold start.
- The project serves objectives C, D, and E.
- Relevant materials are investigated.

Question 2: Approach to performing the research and development

This project was rated **3.0** on its approach.

• The PI did a good job understanding how undesirable plug flow develops - high contact angles caused by hydrophobic GDL materials. This will present developers with a tradeoff situation of designing GDLs that don't induce plugs (hydrophilic materials) yet need to prevent flooding at high current density (hydrophobic

materials). Work is thoroughly well correlated to fuel cell operating conditions (temperature, humidity, stoichiometry, etc.).

- Results should lead to some kind of model development.
- The project team does a good job visualizing the flows, and taking the important step of making relevant models that look like they'd be easy to use and relevant. Unfortunately, these models are all based on data at 35°C. A fuel cell that operates at 65°C or 110°C will probably have very different behaviors. These higher temperatures seem more relevant to the auto industry than 35°C. Interestingly, the power data shown was taken at 80°C. The majority of data should have been taken at about this temperature, not at 35°C. Also, since transport in the GDL was very pore-structure dependent, a variety of pores should have been studied, or the effort should have been made to pick an optimal pore.
- The overall approach seems to address characterizing the water movement and accumulation in the fuel cell both by developing a clear understanding of the baseline conditions and a parametric study of the components. The approach to optimize the GDL and bipolar plate designs, as well as the operating conditions to provide improvements and recommendations, is important to addressing the key barriers of water management and control especially for freezing conditions.
- There is significant technical content here, as well as Parametric Studies followed by *ex situ* studies, *in situ* studies, and *in situ* performance in combinatorial studies.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated 3.0 based on accomplishments.

- The PI addressed many of the original equipment manufacturer (OEM) concerns by investigating effects of GDL intrusion. The results were somewhat intuitive though: increased intrusion equals increased pressure drop. What effect does that have on water formation?
- The technical collaboration to date is impressive.
- GDL properties are broadly covered. A capillary flow model was developed.
- The presentation is very descriptive and draws on the work done. Little information is given about lessons learned, rendering a lower score.

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated **3.0** for technology transfer and collaboration.

- The collaboration has generally been good. The project team could be working with LANL as well (LANL is working heavily in this field).
- The project team made a good selection of partners, and the partners have done good work. Given that RIT has developed the high-temperature fuel cells, they should be expected to contribute such membranes not the traditional low-temperature membranes.
- The project has sufficient technical collaboration and it seems to be well coordinated for the program.
- The degree of collaboration and the comprehensive approach towards characterization are impressive.
- Through GM, there is an industrial partner with a strong fuel cell background in the consortium.

Question 5: Approach to and relevance of proposed future research

This project was rated 2.5 for proposed future work.

- The project team should continue the study on effects of thermal conductivity and the important yet under appreciated characteristic of GDLs.
- The project team should plan is to vary flow channels and do more observations. The project team did not present any particularly strong plan to cover the weaknesses. The problem may be the lack of future funding and the impending bankruptcy of GM.
- The planned activities address the materials and measurements to target overcoming the barriers with materials and the operating parameters to address the purge and freezing behavior.
- The project team should provide a future plan with quantifiable goals.

FY 2009 Merit Review and Peer Evaluation Report

Strengths and weaknesses

Strengths

- This project provides a thorough study of material characteristics on GDL water management behavior.
- The project team produced usable analysis of water transport.
- The project has an appropriate team and is addressing both the characterization and the optimization materials to address the key barriers associated with the water management and shut-down behavior for freezing situations.
- The project team has good focus on the fundamentals of an interesting mix of characterization, modeling, and analysis. This will help to develop a comprehensive understanding of water content and water removal rates.
- There is a strong focus on GDL, combinatorial studies, and two phase flow studies.

Weaknesses

- The project team has a lot of topics to work on in a condensed time frame. The PI should try to aggregate results into a meaningful model or recommendations for GDL design.
- Testing conditions seem more relevant to the ease of testing than to actual operating conditions. The team should expect different water channel behaviors at 60°C to 100°C.

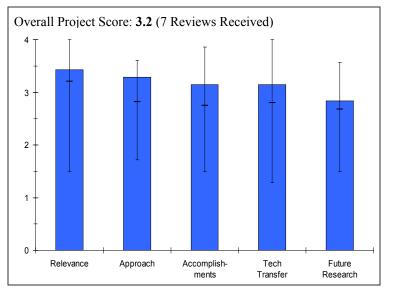
- The project team should perform work at higher temperatures. The team should try polybenzimidazole (PBI) membranes instead of Nafion®. On start-up, the project team should assume shut-down from idle (low power draw) at a low temperature. This tends to produce a worst-case water-plugging scenario.
- The project team has presented interesting and important findings; however, the translation of these findings into real improvements of performance is not clear.

Project # FC-38: Subfreezing Start/Stop Protocol for an Advanced Metallic Open-Flowfield Fuel Cell Stack *Amedeo Conti; Nuvera Fuel Cells, Inc.*

Brief Summary of Project

The overall objective of this project is to demonstrate a proton exchange membrane fuel cell (PEMFC) stack meeting the DOE 2010 cold start targets. The goals for fiscal year 2008 were to 1) achieve the -20°C cold start target respecting the energy budget; and 2) identify electrochemical material freeze cycle aging modes. The goals for FY 2009 were to: 1) provide reliability and durability of the -20°C start-up procedure, and 2) achieve the -40°C cold start target, enabled by new stack technology.

<u>**Ouestion 1: Relevance to overall DOE**</u> <u>**objectives**</u>



This project earned a score of **3.4** for its relevance to DOE objectives.

- The project addresses the issues of start-up and shut-down time and energy for a unique flow field design.
- The ability of a fuel cell to withstand freezing is absolutely critical to it being usable in the sorts of remote and mobile applications where it adds customer value.
- The program is focused on the key barriers of water management and the effect/optimization of start and stop protocols for fuel cells. Their program seems to maintain focus both on the energy requirement effects of the start and stop cycles, as well as the implications for the durability and reliability of the materials.
- The project addresses barriers D and G through Task 11, and has developed innovative concepts for fuel cell systems.
- The team has made a product development effort, which most of industry is addressing.
- Subfreezing effects, principally start-up and shut-down are critical to RD&D objectives, and are the primary focus of this task. The project itself is very Nuvera design-specific, and many of the details regarding how targets can be met or how the community in general can benefit from the lessons learned in this project limit the relevance of this project.

Question 2: Approach to performing the research and development

This project was rated **3.3** on its approach.

- The project has taken an experimental approach to determine the important parameters that affect the start-up time and energy and material durability.
- The approach seemed to be to develop new Nuvera fuel cells that start well from low temperatures, down to -40°C, and then to take data on these cells. There were no particularly general findings. For example, the effect of different start-up processes is not studied in a formal way.
- The program's approach seems to be following an overall sound scientific and product-development approach to understanding and addressing the barriers. Improvements in the approach to the measurements and testing of the effects of freezing conditions are good for ensuring relevance to the real world tests, as well as the increased collaboration to ensure the effects of freeze/thaw conditions on durability are taken into account fully.
- The set-up this year using an environmental chamber is a huge improvement on last year's freezer approach. There was good use of partners' skills in being able to diagnose failures due to freeze/thaw cycles.
- The project team needs to identify failure modes, root causes, and corrective actions to mitigate failures.

• The approach of the project has been effective at resulting in designs and data that meet DOE targets. The focus on lowering thermal mass is clear and open flow fields as part of the approach is mentioned for the andromeda stack design. Still, it is not clear whether or not the design/materials used and the lessons learned from this project are broadly applicable due to the lack of specific data that is likely considered proprietary. Information relating to the specific lessons learned, such as where and how thermal mass are cut from the stack without impacting other critical factors, would be beneficial.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated 3.1 based on accomplishments.

- The project has met the time and energy target and is now concentrating on failure mechanisms.
- The project team made a low thermal mass Nuvera fuel cell and used a high-pressure purge that they believe is good for start-up from freezing. Is this the best method? We really don't know. It is not clear that we learned much about what one does generally to deal with freezing conditions. Perhaps a resistive heating cycle based on a brief short-circuit operation period would have worked better. It is also not clear that this method would have worked at all if more water were frozen in the cell.
- The team has demonstrated good energy management for the shut-down and start-up. It was not clear how aging affected this from the presentation. This project needs further work, understanding, and validation of the durability and energy behavior over time.
- The project demonstrated DOE's goal of 50% of rated power in <18 s, and identified the main failure mode.
- The start-up energy and time from -20°C to 50% rated power for the system are impressive and comfortably meet DOE targets. The improvements in start-up energy from last year to this year also suggest significant progress in the past year. Specific changes and their potential impact on durability or longevity of the stack and performance over time are not clear, and therefore it is not certain that the changes made don't also have negative consequences.

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated **3.1** for technology transfer and collaboration.

- The project team includes an integrator, membrane electrode assembly (MEA) manufacturer, gas diffusion layer (GDL) supplier, and a university.
- Though two university groups participated, there seemed to be little theoretical input.
- This was a good project team to address the effect of the materials and water management on the stack behavior. The projects involved a larger group of collaborators to address and understand the issues with the freeze/thaw and the materials durability and aging.
- This was an excellent team comprising an MEA manufacturer, a carbon supplier, and a university. The team also held a freeze workshop.
- The workshop is a good way to show collaboration/coordination with other institutions. The project has strong partners, but it is unclear how the partners have worked together to provide the improvements in performance presented. There is little in terms of publication from this group based on this project (for example, the PI this year, Conti, and last year, Cross, are not authors on the few publications listed). This further reflects the low level of information released from this largely publicly funded project that limits its value to the fuel cell community.

Question 5: Approach to and relevance of proposed future research

This project was rated 2.8 for proposed future work.

- The future plans are to incorporate durability consideration into the start-up protocol, and to evaluate the feasibility of an H₂ purge.
- The next step follows from the previous. It is not clear that any general conclusions will be derived, but it will not be worthless. The team has taken a very practical approach.

- Future work should continue to loot the validation of the energy management, as well as the stack design, to examine the effects of durability/aging on these parameters.
- There is insufficient detail to really evaluate this; however, it appears that now that test protocols have been identified, that integration of next generation fuel cell components will not be a problem.
- The future work proposed is vague and only inferred from two bullets on the summary slide or by interpolation from the overall approach slide. The plans may lead to improvements, but it is not certain whether future advances will be possible. Again, this is due to a general lack of detail throughout the presentation.

Strengths and weaknesses

Strengths

- This is a good team.
- The project has identified the key issues of thermal mass and its relationship to power density (current density at rated power).
- Though two university groups participated, there seemed to be little theoretical input.
- The team took a good overall approach to modifying the stack, MEA component, and operating profiles to address the two barriers of energy requirement.
- The team demonstrated realistic testing protocols, and collaborated with a materials and components supplier that can supply state-of-the-art and improved components.
- The project meets or exceeds a number of key DOE targets.
- The project produced a working model. It's nice when a project gets to a state where there is an actual product on the horizon.
- The project continues to focus on the effects of aging and durability on the materials, and the effects of these aging changes on the energy performance and operating profiles.

Weaknesses

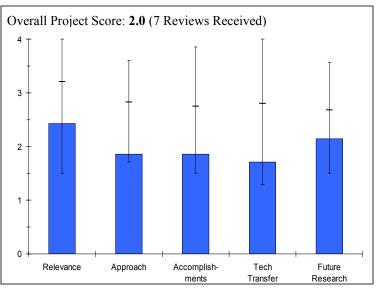
- The project has taken an engineering option and is not structured to developing a fundamental understanding of start-up/shut-down or material durability/compatibility.
- The project has not systematically looked at the effect of the shut-down protocol.
- The project needs more consideration of what is happening to the ionomer during freeze/thaw.
- The rationale, specific materials, and choices for this project are not presented in enough detail to understand whether or not there are critical shortcomings to the approach, or provide value for the general fuel cell community to apply similar approaches. This should be able to be done to a greater extent without meaningfully compromising proprietary information (or be done in the absence of public support).

- The project team should develop a method to characterize the MEA at the end of the purge cycle (beginning of the start-up cycle).
- The next step follows okay from the previous step.
- The team needs more polymer science.

Project # FC-39: Development of Thermal and Water Management System for PEM Fuel Cells *Zia Mirza; Honeywell*

Brief Summary of Project

The overall objectives of this project are to 1) improve proton exchange membrane fuel cell (PEMFC) performance and life by maintaining the humidity of the inlet air stream at a high level (>60%); 2) eliminate the need for an external water source by transferring water from the stack exit air stream to the inlet stream; and 3) design, build, and test high-performance full-size radiators to meet the 80 kW fuel cell stack cooling requirements. Specific objectives are to 1) validate the performance of fullscale humidification devices sized for an 80 kW PEMFC by testing the Emprise enthalpy wheel and the Perma Pure membrane module; 2) evaluate planer membrane humidification devices; 3)



perform performance testing at sub-ambient conditions; 4) increase the performance required to dissipate lowquality heat; and 5) optimize the weight, size, and cost.

Question 1: Relevance to overall DOE objectives

This project earned a score of **2.4** for its relevance to DOE objectives.

- Advanced humidification systems are important.
- Balance-of-plant is not a technically critical area for fuel cell research. It is an engineering area to the design and development of fuel cell systems, and it is a competitive area.
- System water and thermal management are important aspects of automotive fuel cell development, although they are of secondary importance to catalyst performance/cost, membrane development, and durability.
- This doesn't seem to address the major issues of fuel cell development: cost, durability, or infrastructure. These are some worthwhile paper studies, but it isn't clear how this is helpful to larger DOE goals or to improving the overall technical readiness of the fuel cell system.
- This project serves objective E.
- Core components for an automotive fuel cell system are developed.

Question 2: Approach to performing the research and development

This project was rated **1.9** on its approach.

- This project primarily is obtaining humidification components which are off-the-shelf items, and then evaluating them.
- Any fuel cell developer has already done this.
- No technical criticality is identified. The two humidifier technologies are off-the-shelf, and the approach is to perform design verification testing. No research is evident.
- The program has focused on materials that are well known in the community, and which in general are not expected to meet system overall targets.
- This project does not seem to have an approach that, even if it succeeds in its stated goals, will enhance the prospect for fuel cell commercialization.
- The testing of planer materials has some value if combined with novel material development.

• This is a very large budget for a component that only changes the overall system cost by \$30 (for the radiator, slide 15). It is not clear how this effort is unique from what individual automotive original equipment manufacturers (OEMs) and stack manufacturers are developing on their own to meet customer requirements.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated 1.9 based on accomplishments.

- There was a lot of discussion about radiator design; however, the automotive OEMs know how to make costeffective radiators. They make approximately 10-15 million per year.
- Humidification devices were purchased from other vendors.
- Little progress was observed.
- It is not clear from the results shown if microchannel radiators have some promise. Rather than focusing on a "value function," please show more test results and comparisons to baseline technology (commercial automotive radiator). Tests as-shown seem inconclusive.
- The project team appears to be making some progress, but nothing that fundamentally changes the cost model or system performance.
- Considering the budget for this project, more results and/or more substantiated results might be expected. The project team purchased and validated humidification devices and developed a cooler.

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated 1.7 for technology transfer and collaboration.

- The DOE and the fuel cell technical team do not count as partners; all projects are reviewed by these organizations.
- There does not seem to be any real collaboration with ANL, other than providing some data to ANL for modeling purposes.
- Any effective collaboration is not seen.
- This program would benefit from exploring more novel materials to test for water transport, not just the wellknown Perma-Pure tubular membrane humidifier and Emprise Enthalpy Wheel.
- Collaboration indicates minimal exchange with other research and manufacturing institutions. It appears that there is one-way delivery of information to Argonne's modeling effort, and participation in technical team reviews, but very little interaction with stack integrators.
- The FreedomCAR Technical Team is the only partner in the project. It is assumed that DOE, even though quoted as a partner, cannot be considered a development partner.

Question 5: Approach to and relevance of proposed future research

This project was rated 2.1 for proposed future work.

- Future work consists of modifying a test stand and testing components. There are no development activities to this project.
- Planer membrane testing may hold some value.
- The program should fully document test results. Do microchannel radiators provide a marked advantage?
- The project team should document: expected cost vs. conventional automotive radiators, delta-P vs. airflow, Q transfer vs. airflow (slide 11 just shows at one condition), and the expected impact of fouling.
- To be useful, membrane water transfer data should show operating conditions, molar flow rates, temperature, pressure, etc., not just relative humidity (RH).

Strengths and weaknesses

Strengths

- This is a solid hardware engineering study!
- The systems approach is good.

Weaknesses

- This project primarily evaluates existing technology and is not value added to developers.
- There are no development activities to this project.
- This is previously covered ground, with little potential to advance the state of the art.
- The project has minimal impact on DOE's overall goals.
- The value/cost ratio might be improved. For a smaller budget, the project had scored higher. In case the development is indeed that expensive, the presentation did not convey that message.

- SI units would be nice!
- This project's funding should be discontinued.
- In the remaining time, the project team should focus on testing planer membrane water transfer materials (if available) and document the radiator results in comparison to baseline conventional automotive radiators as noted previously.

Project # FC-40: Nitrided Metallic Bipolar Plates

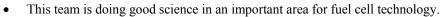
M.P. Brady, T.J. Toops, and P.F. Tortorelli; Oak Ridge National Laboratory

Brief Summary of Project

The overall objective of this project is to demonstrate the potential for metallic bipolar plates to meet the automotive durability goals at a cost of <\$5/kW. Oak Ridge found promising initial performance of stamped and nitrided Fe-20Cr-4V in cyclic single-cell fuel cell tests. Durability studies of stamped and nitrided foils benchmarked to untreated stainless steels and graphite are underway.

<u>Question 1: Relevance to overall DOE</u> <u>objectives</u>

This project earned a score of **3.7** for its relevance to DOE objectives.

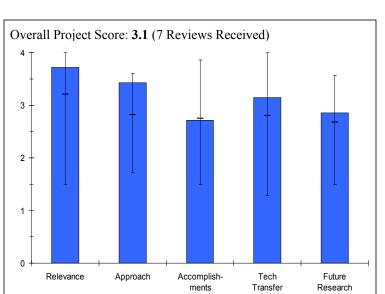


- This project addresses barriers A, B, and C under task 5, the development of bipolar plates.
- Bipolar plates play a critical role in meeting DOE stack and system targets.
- Metal plates for proton exchange membrane fuel cells (PEMFCs) have been thought necessary to achieve compact, automotive hardware.
- Several auto original equipment manufacturers (OEMs) are fielding metal plates, and that activity strongly supports DOE goals. Even so, the majority of PEM stacks today are using carbon-based plates, and these materials have also proven satisfactory for both performance and durability.
- The objectives of the project address the cost/durability of bipolar plates in a very good manner, and the breakout of the process steps and cost association of performance and cost with each step are commendable.

Question 2: Approach to performing the research and development

This project was rated **3.4** on its approach.

- It is appreciated that the team is going after a low-cost ferritic alloy such as Fe-20Cr-4V or Fe-23Cr-4V. Ni and Mo are highly price-volatile. The drive to shorter pre-oxidation/nitridization thermal cycles for low cost can also be appreciated.
- The project's approach is to develop a nitrided stainless steel that is cheap durable and can be stamped.
- The project team took an excellent approach to low-cost, rugged, and durable bipolar plates.
- The team should check the influence of worked or scratched surfaces on corrosion resistance.
- It would have been better if the presentation began with a review of the extensive previous work on the nitriding of stainless steel, and the use of such corrosion protection concepts in PEM stack engineering. Instead, the presentation tended to assert that new approaches were being pioneered, which is not the case. It would have been better if the presentation showed test results using earlier nitriding recipes, and then explained why the new concepts are an improvement.
- The "embossed" flow field shown is a long way from the precise geometries required to assure uniform flow and good stack performance. It was not apparent that the alloy selected, and the nitrided foils, are sufficiently ductal to allow such successful stamping.
- The approach to examining the alteration of metal alloys with respect to the resistivity and corrosion, relative to targets, is well-illustrated. The use of analytical techniques to determine the relationship between process, alloy surface change, and properties is very good. The correlation of surface properties and analyses of alloys which meet performance goals (but maybe not cost) and the alloys currently being investigated needs to be done to



gain better insight into what is causing the irregular surfaces; how much difference exists; and the limited nitridation of the Cr at the surface. Examination of the surfaces of the grooves to determine how much variation exists between the unstressed and stressed surfaces after the nitridation process needs to be determined. Examining smooth foil surfaces does not give a complete picture.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated 2.7 based on accomplishments.

- It was a good idea to increase Cr content from 20 to 23 weight percentage in an attempt to form more continuous CrxN and CrxOy layers for better protection. There is concern that the interfacial contact resistance (ICR) is still too high.
- A nitrided steel has been identified, but the milestone for demonstration of a 15 cm² single cell has been postponed.
- The team has made good progress evaluating new lower-cost stampable metal alloys, despite reduced FY09 funding.
- The materials science was okay, although the results were not novel; however, there is a long way to go from the current status to large size, uniform, and corrosion resistant plates.
- The investigation of process steps and analyses has provided insight into problems associated with irregularities at the alloy surfaces; however, the need to increase the membrane thickness to conduct successful single cell tests suggests that the surfaces of the plates are entirely too rough for the membrane integrity (additional cost of thicker membranes, with higher resistance, has not been included in the projected cost estimates). The go/no-go decision of Milestone 2 cannot be complete until a solution to the inadequate nitridation of the surface is understood, because the single cell tests do not suggest that either a cost-effective process or an acceptable alloy has been determined. Perhaps a treatment of an alloy that meets the performance goals should be examined to determine the degree of surface differences.

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated **3.1** for technology transfer and collaboration.

- I was glad to hear that there will be collaboration with an OEM soon; this is critical. Also, perhaps a bit closer collaboration with LANL on the actual fuel cell testing would be to overcome some of the technical difficulties there.
- A large team of diverse skill sets has been assembled. An OEM should be involved; however, whether or not Milestone 2 is passed, in theory the OEM could help attain the milestone.
- ORNL needs some stack design competence in this program. Precise flow channels are required to achieve uniform flow distribution among the many plates in a PEM stack. The degree of uniformity is a design issue which must be addressed early. This team needs a partner who is competent in computational fluid dynamics and knowledgeable in fluidic design engineering of PEM stacks.
- It appears that the list of participants and their roles are appropriate, but the costs associated with each and the degree of participation is not clear. Perhaps more analysis work needs to be done; for example, examine potential welding/joining problems of plates, variations in surface across a stamped plate, and alterations in the treating process.

Question 5: Approach to and relevance of proposed future research

This project was rated 2.9 for proposed future work.

- I would recommend adding the following to the go/no-go evaluation:
 - Analyze aged membrane electrode assemblies (MEAs) and product water from fuel cell durability tests to look for evidence of leached metals;
 - Analyze the metal foils for near-surface compositions following stamping, and compare with beforestamped to ensure no issues develop in that process that could interfere with the efficacy of the oxidation and nitridation treatments;

- Measure the surface energy of the nitrided surface;
- Work with OEMs to ensure the formability of these alloys enables stamping at length scales and tolerances relevant to automotive flow field designs.
- I'm not sure why they are now proposing to test commercial steels. Wasn't the point of the project to develop new steels? Also, the team should be evaluating larger surface area steels of at least 25 cm².
- It is logical to evaluate more readily available commercial alloys and the potentially lower-cost plasma arc lamp.
- Durability in the fuel cell environment (low ICR and high corrosion resistance) and stampability must remain the primary criteria (over alloy cost).
- Formability and joining with an industry partner for a demonstration on short stack is a must.
- Many have shown that Au-coated stainless steel delivers an okay performance. Although gold may be thought costly, Au-coated test articles might be useful for looking at planarity, resistance, and other stack design issues. Once a gold-plated plate design is shown to be useful, then the nitriding gun can be focused.
- The exposure of stainless steel plates to open circuit (high) voltage seems sacrificial. Steel corroded at high potentials; the low energy form of iron is Fe₃O₄, after all. There is no need to test to destruction, and adequate durability can be demonstrated by sensible testing. Operating a stack well past the "red line" seems risky, and proves nothing other than a sense for adventure.
- Extension of the second milestone go/no-go decision is correct, but a detailed plan for both examining options and definition of a resolution is necessary before the third milestone should be considered. After all, that is what a go/no-go decision is for. If the funds from the third phase can be readjusted to accommodate a resolution to the second phase problems, this would help reach an important goal as to what is needed to achieve an improved plate material.

Strengths and weaknesses

Strengths

- The team has demonstrated good science and collaboration with an alloy manufacturer.
- New steels with nitridation look promising.
- Nitrided metal plates, once successfully developed, have many advantages over other bipolar plates (thin, high mechanical strength, high electrical and thermal conductivity, light weight, and low-cost).
- Clearly, ORNL knows steel as well as anyone, and Allegheny Ludlum is a quality concern as well. ORNL has coating tools and experience.
- A well-defined approach to examining an alternate, potentially cost-effective method for producing metallic bipolar plates has been defined. The combination of alloy analyses, cost projections, and single-cell tests has been done in a coordinated fashion.

Weaknesses

- The team has issues with fuel cell testing, and there is a lack of involvement of an OEM.
- Single-cell testing should be on an industry standard of 25 or 50 cm², not 15 cm².
- There have been many, many attempts at nitriding stainless steel for PEM plates. It would have been more convincing if ORNL reviewed earlier work, and spoke to how new ideas (ORNL ideas) showed hope for greater success.
- Although the costs may be increased, a metallic alloy that has the necessary attributes, i.e., surface properties and nitridation success, should be included in analyses to illustrate specific differences between alloys under investigation and proven material. Industrial materials might be included as potential options.

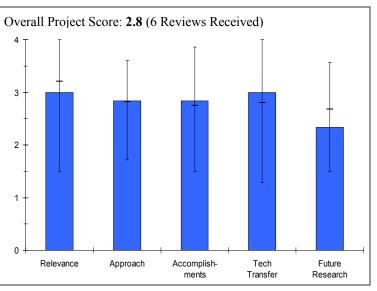
- More hard work on the new steels is needed.
- A table in the Annual Merit Review presentation showing the bipolar plate technical targets and project status would be helpful.

- It makes more sense for ORNL to work with an existing quality stack developer, and fabricate and coat stainless steel parts to replace the bipolar plates within those designs, which are already known to yield adequate stack performance. Indeed, it might be possible to assemble a hybrid stack made from mainly existing proven plates interlaced with some number of "experimental" nitrided plates.
- Delay Milestone 2 go/no-go decision until a reasonable plan of action to resolve surface inadequacies has been defined. Reallocate funds from the third milestone to illustrate potential improvements with tests on a single cell being adequate. Determine additional properties such as welding and uniformity of nitridation control to illustrate the merit of the proposed approach. Costs projections seem to be well-understood.

Project # FC-41: Next Generation Bipolar Plates for Automotive PEM Fuel Cells *Orest Adrianowycz; GrafTech International Ltd.*

Brief Summary of Project

The overall objective of this project is to develop the next generation of automotive bipolar plates based on an engineered composite of expanded graphite and resin capable of operation at 120°C. The goals for Year 1 are to 1) develop a graphite/polymer composite to meet the 120°C fuel cell operating temperature; and 2) demonstrate the manufacturing capability of new materials to a reduced bipolar plate thickness of 1.6 mm. The Year 2 goals are to 1) manufacture high-temperature flow field plates for full scale testing; 2) validate performance of new plates under automotive conditions using a short (10cell) stack; and 3) show viability of the published cost target through the use of low-



cost materials amenable to high-volume manufacturing.

Question 1: Relevance to overall DOE objectives

This project earned a score of **3.0** for its relevance to DOE objectives.

- Bipolar plate materials are one of the largest fractions of fuel cell cost. Bipolar plate materials benchmarking is important.
- Bipolar plates are an integral part of every fuel cell stack and contribute significantly to performance, durability, and cost.
- The availability of bipolar plates for 120°C operation is an important prerequisite to successful testing and implementation of 120°C membranes and membrane electrode assemblies (MEAs).
- Bipolar plates play a key role in stack cost, mass, and size (packaging), and is thus an important and proper area for DOE support.
- The bipolar plate is a considerable contribution to the overall weight and volume of the fuel cell, and DOE targets are clearly established to address cost and performance; this program addresses those concerns, but it's not immediately clear how this is directly leading to cost reductions, or improved manufacturability.
- While the plan to fabricate graphite plates, which can operate at 120°C and achieve a thickness of 1.6 mm is described, and is commendable, these do not correlate with the generally stated barriers that are being addressed as described on the first slide. Isn't the plan to develop a novel plate that can provide higher temperature operation without sacrificing any performance or cost attributes?

Question 2: Approach to performing the research and development

This project was rated **2.8** on its approach.

- The cost advantage for both materials and manufacturing processes, and a generic formability limit should be evaluated before full-scale stack fabrication and testing.
- One disadvantage of this bipolar plate material is volumetric power density.
- A 1.6 mm of plate thickness as a target is not a proper metric, because it is dependent on flow field design variations. Gas impermeability of embossed materials is more appropriate and generic.
- The project exhibits a logical task structure.
- The team has a clear grasp of requirement targets and has addressed them systematically.

- The team could benefit from prioritization of these targets. Key targets include, but are not limited to: ultimate (high production volume) cost and stack volume [bipolar plate (BPP) thickness] potential, durability and conductivity. These need to be addressed specifically in the program and final report.
- The team needs to address detailed manufacturability metrics- key attributes in the bipolar plate. The bipolar plate has a few key parameters related to performance: resistance and feature tolerances, which, in turn, affect plate-to-plate pressure drop variability. Permeability is more of a safety/efficiency performance metric that will have a small effect on overall cell electrical performance.
- The way that the bipolar plate affects the overall stack is in manufacturing cost, some electrical resistance, and in flow distribution. Once the minimum level of electrical resistance has been met, further improvements tend to be dwarfed by MEA resistance. Therefore, cost and manufacturing tolerances for flow distribution will be key. These issues need to be addressed more specifically.
- The fabrication approach, identification of the proper binding materials, testing physical properties and assembling/testing single cell test units all address the correct means for evaluating high-temperature graphite plates. The plan for testing the fuel cell at high temperatures without insuring a high-temperature MEA seems to be shortsighted. Since the tests could not be completed at high temperatures, it would seem that operating at a temperature as high as the MEA would accommodate for a longer period of time for analyses, at least under conditions that could be compared to other plates, would be reasonable. The cost analyses were not found/shown. Planning to do a ten cell stack at 120°C seems like an unreasonable expectation, since no MEA capable of 1,000 hrs was identified.

Ouestion 3: Technical accomplishments and progress toward project and DOE goals

This project was rated 2.8 based on accomplishments.

- Bipolar plate materials with Bensoxazines resin, corrosion resistivity, formability (emboss) and cost should be evaluated.
- For formability, the formability limit should be identified.
- Is gas impermeability (0.8 mm) verified with embossed materials? If not, it should be tested with processed materials, as 0.8 mm is too thick for automotive applications; it should be less than 0.3 mm.
- MEA test data is very poor, why?
- Cost estimates have not been reported yet.
- Progress has been made in materials (graphite and resins).
- I still have questions on cost and volume (achievable power density).
- What is the anticipated cost in large-scale (500K systems/yr) production?
- BPP thickness is given as 1.6mm, which still may be challenging for packaging. Is this best anticipated for this material set? If not, how much can this be reduced?
- The PI states that composite plates are superior to metal in conductivity, but metal plates are much thinner, offsetting this. What counts is the overall area-specific resistance (ohm-cm²). How do their plates compare to metal here?
- The team needs to state contact and overall resistance.
- They have characterized several carbons and resins, but haven't quantified how these changes will affect cost. As mentioned before, the bipolar plate will not have much of an effect on performance, except for ohmic losses (if the plate is very poor), and will have more of an effect on cost.
- While the mechanical tests that were described to be done were reported as successful, and mechanical test data were shown, no test data on the single cell at a temperature commensurate with the MEA and at high electrical potential were demonstrated, no gas permeability data were exhibited, no high-temperature coolant durability data were provided, and no cost comparisons were generated. This project is not complete until the supporting information is provided. No 10 cell stack should be tested until the goals for the tests are defined to be useful, i.e., at a temperature commensurate with the MEA stability.

<u>Ouestion 4: Technology transfer/collaborations with industry, universities and other laboratories</u></u>

This project was rated **3.0** for technology transfer and collaboration.

• A generic requirement of bipolar plate design would be helpful to evaluate the formability limit.

- Cell testing at 120°C appears to have been problematic.
- The team that has been assembled seems to be appropriate with the expertise available; however, the choice of high-temperature MEA before tests started, and the choice of single cell test conditions seems out of character for the fuel cell members of the team.

Question 5: Approach to and relevance of proposed future research

This project was rated **2.3** for proposed future work.

- For this project, materials benchmarking is good enough. Full scale testing seems to be superfluous.
- Stack testing for 1,000 hours may provide some indication of durability characteristics, but longer-term testing will be required to fully validate the plates.
- What is the heat capacity (mass C_p , kJ/K/cm²) of the bipolar plate?
- What is the anticipated cost in high-volume production?
- What is the PI's estimate of minimum possible thickness while meeting the other DOE targets?
- Please supply area-specific electrical and thermal conductivities (ohm-cm², W/cm²/K).
- The project seems to be moving in the direction of corroborating a good judgment, but doesn't address the overall needs of the technical community, or help in predicting cost reductions. We need to see cost reductions at a moderate volume, and changes in either raw material cost or processability that can be quantified.
- The project is 90% complete, and the remaining planned work will wrap-up the project.
- While the project is nearly, if not entirely, completed, there certainly needs to be more information provided to support any claims that the choice of materials for graphite plates can meet the gas impermeability, coolant durability, scale-up possibility, and cost targets for the described <0.8 mm thick graphite plates. The results provided look promising, but supporting information is necessary. The final stack tests should demonstrate at least a long duration test at higher potentials and a temperature commensurate with a stable MEA (at least 80°C), and post-test analyses should be compared to current graphite plates at those conditions. Supporting cost analyses must be provided.

Strengths and weaknesses

Strengths

- The team has identified alternative materials for the bipolar plate. The use of natural graphite is a cost and performance (electrical conductivity) advantage vs. graphite composite materials.
- The team's expertise in graphitic materials and plate development is good.
- The project team is moving quickly towards a finished product.
- They have a good plan to develop/fabricate high-temperature graphite plates.

Weaknesses

- This material has a generic disadvantage for stack power density. The cost advantage vs. metallic bipolar plates is questionable.
- Estimating plate cost appears to have been postponed till the end of the project. There will probably not be enough time to make changes before the end of the project if cost estimates do not meet DOE targets.
- There are fundamental limitations of graphite composite based materials vs. metal plates (thickness, cost?).
- Performance results are very scattered (slide 21), and don't instill confidence that the process or cell assembly is under control.
- The previous year's comments suggested "Poor channel formability might create problems for certain stack designs and/or create high contact resistance or poor fit if tolerances of the plates aren't well controlled."
- The project team gave qualitative assurances that these issues would be treated, but we see no quantitative data on tolerances, or throughput.
- The team made a poor selection of MEA for fuel cell tests and/or fuel cell test conditions.
- There was a lack of supporting data to verify claims for cost, gas impermeability, high-temperature coolant durability, and reproducibility of plate fabrication within tolerances.

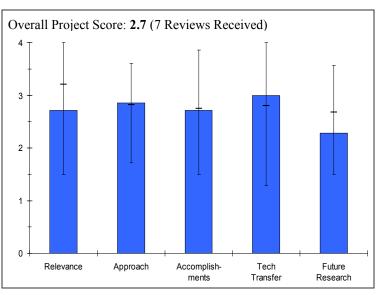
- It would be good to focus on materials testing with more detailed materials requirements. The FreedomCAR Fuel Cell Technical Team may be able to provide detailed attributes and metrics. Full scale testing is not recommended.
- Testing cells at 120°C should be carried out at higher current density, at least 400 mA/cm².
- We need a cost analysis. What is the ultimate potential cost per plate?
- The team needs to determine the ultimate minimum thickness due to the importance of volumetric power density (automotive packaging).
- The above two, plus durability, will determine if graphitic/composite bipolar plates can compete with metal plates for automotive fuel cell commercial viability.
- The project team needs to add manufacturability/reproducibility studies so that yield, process time, etc. can be quantified by outside reviewers.
- The project team needs to complete the final report with data that supports or clarifies the claims listed above.

Project # FC-42: Low Cost, Durable Seals for PEM Fuel Cells

Jason Parsons; UTC Power

Brief Summary of Project

The objective of this project is to develop low-cost, non-silicone, durable seal materials and sealing techniques amenable to high-volume manufacture of proton exchange membrane (PEM) stacks. The project goals are to 1) improve mechanical and chemical stability of seals to achieve 40,000 hours of useful operating life; and 2) obtain a material cost equivalent to or less than the cost of high-performance silicones in common use. Material properties meet most ultimate program goals – FCS2 is expected to meet all program goals.



Question 1: Relevance to overall DOE objectives

This project earned a score of 2.7 for its relevance to DOE objectives.

- Low-cost, durable seals are needed for PEMFCs.
- While the need for durable, cost-effective seals is clear for fuel cell applications, the general low level of disclosure of the actual elastomers and specificity of the seal development to UTC's fuel cell design make this project's outcome of somewhat questionable value to the overall fuel cell program.
- The project is focused on two key barriers in fuel cell's durability and cost.
- The project is relevant to the DOE fuel cell program objectives. Cost effective, durable seals are necessary for successful commercialization of the technology.
- Although fuel cell efficiency and durability are worthy topics, gaskets for PEM stacks necessarily are of less importance. This is especially so for a company that has claimed an important position in the global PEM stack industry, and necessarily has extensive PEM seal technology under its belt.
- The need for durable, stable seals for fuel cells is necessary, and objectives regarding temperatures and time of tests generally align with the DOE goals. The description of materials/polymers that are under consideration for testing and evaluation should be identified in order to establish a well-defined database for future use in evaluating other options.

Question 2: Approach to performing the research and development

This project was rated **2.9** on its approach.

- The project team took a clear approach of material selection and evaluation.
- *Ex situ* accelerated stress tests should be correlated to fuel cell data for proven rapid material evaluation.
- The general approach for rapidly screening candidates and various levels of testing that have been established are very good and make for an effective development program. There is concern that leachability tests have not been performed early in material evaluation. Also, the focus on the Integrated Molded Seal MEA element of this program may be too ambitious and specific to UTC.
- The general materials development, compatibility, and testing approach seem sound for the seal development. Their approach has limited testing in fuel cells to confirm the compatibility and applicability of these materials, in particular, under fuel cell cycling conditions.
- The approach is sound and very thorough. *Ex situ* tests are being employed to screen candidate materials. The testing includes both physical and chemical characterization under conditions expected in operating fuel cells. An extensive database of material characteristics has been compiled for the few candidates under consideration.

UTC is planning to develop a unitized MEA seal package that requires the seal material to be compatible with the MEA materials. Other MEA materials may not be compatible. The project was selected on the premise that the seal material would be available to other developers. If the material is not compatible with other MEA material sets, this benefit would be lost.

- The real goal is to edge-seal an MEA. Although it was not mentioned, this would mean bonding to the membrane, which is not necessarily dimensionally stable, tends to flow under compressive stress, and is difficult to bond. There was no consideration of the most difficult engineering task, forming the seal.
- Even with supported membranes, one still needs to seal on an acidic, chemically, and dimensionally unstable polymer.
- Henkel contains technical excellence that should have been tapped early. It is most likely that they already know the problem, or know folks who do. Every successful stack manufacturer has figured out the sealing problem.
- Cost may still be an issue; if so, costs should have been addressed.
- The tests that are outlined for evaluating the polymer candidates are in-line with the fuel cell conditions. However, no description is provided on the process that the initial polymeric materials undergo that would be useful in determining what parameters could be important in the future advancement of sealing materials. The integration of efforts is a logical approach. Only static tests are described, but cyclic tests should be included in the screening process, since all automotive fuel cells will see significant cyclic operation.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated 2.7 based on accomplishments.

- The project team conducted a good material evaluation, and materials were developed that meet most goals. However, as the material formulations are not provided, this limits the value of this project to other developers.
- For this project to have general value, much more detail should be disclosed regarding the formulations that have been evaluated. It will likely be helpful to know how the various elastomer chemistries that were evaluated by Henkel performed against the various project requirements. It would also be nice to see hydrogen permeability measured for these materials.
- They have made good progress in developing hydrocarbon elastomers with the target properties to provide for liquid injection moldable (LIM)-type seals. They appear to have conducted limited testing in real fuel cells.
- Progress is evident, but it is difficult to assess the effectiveness of the project. Only three materials advanced to the testing stage. It is not known how many others have been screened. Even a notional idea of the composition of the materials is not known. It is not clear if the materials are hydrocarbons, fluoropolymers, or blends. Testing at Virginia Tech appears thorough and capable of stressing the materials in an appropriate manner.
- This simple task began in April 2007, and still is not completed. There is no way that the described existing work should have cost the funds spent to date.
- The Fenton reagent is a very aggressive agent, based on oxidation with the ferric ion. Many perfectly good sealants will be attacked by the aggressive ferric ion, because most everything in the Merck Index is.
- A Fenton reagent test seems foolish—simply evaluate under anticipated worst conditions.
- The team's progress is commendable. A cyclic test comparison is missing. Marginal limits in hardness, 100% modulus, and tear strength suggest that supporting information should be provided as to why these limits were found to be acceptable, e.g., couldn't do better in timeframe, material wasn't found to be better, process was limiting. Do the accelerated tests adequately illustrate failure under nominal fuel cell conditions where surface area exposure is limited and penetration of reactant (peroxide, for example) is an important issue?

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated **3.0** for technology transfer and collaboration.

- There is a good set of partners with clear interactions, especially with Virginia Tech.
- Good balance exists among the elastomer developer, the OEM, and materials characterization experts.
- This is a good team to address the development and testing of new seal materials. The project team seems to have a well-coordinated and close collaboration.

- Three organizations, in addition to UTC, are involved. Input from other developers regarding their seal requirements is not evident.
- Virginia Tech seems to be assigned simple materials characterization testing, a rather commercial task that could be done by any number of companies, and certainly by UTC.
- The choice of experimenters and participants seems to be appropriate for the defined tasks. Coordination of the information developed and team interaction has not been shown, and communication of results and analyses is to be determined in tests to be conducted. It would be appropriate to show the coordination of tests chosen to other materials besides silicon polymers that could be potential candidates for baseline comparisons, since some of the properties of the chosen materials are marginal (see slide 9).

Question 5: Approach to and relevance of proposed future research

This project was rated **2.3** for proposed future work.

- It seems that the overall outcome of the project would be strengthened by more focus on full-scale durability testing in fuel cells with more traditional over-molded design.
- The development of the elastomer materials addresses the chemical and physical characteristics of the seal targets. However, the testing of the seal materials is planned in single cells and not stacks, which may not provide all the information on the durability of the seals. Further, it is not clear if the program plans to test the seals under real world cycling conditions in the fuel cell testing.
- There is much to do in very little time.
- The latest and presumably best material appears that it will not be released in time for the final short stack build.
- The details of activities of bonding the fuel cell membrane to the gasket in ways that permit the membrane to shrink and swell without stress cracking was not addressed and needs to be.
- It would be beneficial to show the correlation of accelerated tests, and some combinations of tests, with actual operations. Cyclic tests should be included in testing protocol. A wide range of fuel cell operating parameters still needs to be evaluated. Material compositions should be identified to some extent, even if proprietary information cannot be shared. The correlation between the analyses of final test articles, tests conducted, and materials examined should be targeted in order to provide a solid conclusive analysis of materials potential for use in fuel cells. Are gas permeability tests considered?

Strengths and weaknesses

Strengths

- The out-of-cell testing/accelerated testing is good, and correlation to actual fuel cell performance should be emphasized.
- It appears to be a solid team with strong complimenting expertise to tackle these technical issues, and they have worked effectively together.
- The team has made good materials developments and testing of the elastomeric materials with the target properties of an LIM-based hydrocarbon seal material.
- The team has a good understanding of the requirements for seals, at least in the case of UTC's needs. It is a good, capable team.
- Industrial and academia partners were chosen with good skills for this project.
- A wide range of evaluation tests were covered.
- Tests are to include actual fuel cell assembly for correlation to static tests.

Weaknesses

- Material formulations eventually need to be publicized; otherwise, this project has limited value to any other fuel cell developers.
- There was not enough disclosure of the materials being examined. The project is perhaps too specific to UTC's applications.
- There was limited testing of fuel cells and stacks to ensure the material met the fuel cell durability.
- It is hard to justify the resources for the limited information generated.
- The classification of gasket compositions (FCS1, etc.) served no purpose. Commercial gaskets are beginning proposed. There was no description of why the existing UTC PEM stack gaskets are unsatisfactory and need

FY 2009 Merit Review and Peer Evaluation Report

replacement, nor was there any description of what others are using for gaskets. It is easy enough to buy a commercial stack and shine a Fourier transform infrared (FTIR) on the gasket.

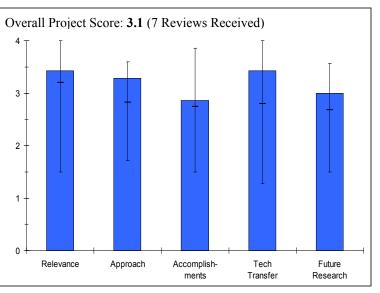
- Interim single-cell fuel cell tests of material should be included to verify the validity of accelerated tests.
- No cyclic condition tests were included in accelerated tests.

- It seems essential that more details of the elastomers evaluated be shared. It also is important that hydrogen permeability be measured for at least the final candidates and reported.
- The team should explore a means to get the FCS3 material into the test stack.
- The project should conclude in September 2009.
- Cyclic tests of materials should be included to examine effects compared to static tests.
- Some single-cell fuel cell tests might be conducted in the interim to ensure that acceleration tests are as applicable as possible.
- Discussion of why marginal limits were found to be acceptable for continuation of tests should be provided.

Project # FC-43: Diesel Fueled SOFC System for Class 7/Class 8 On-Highway Truck Auxiliary Power Dan Norrick; Cummins Power Generation

Brief Summary of Project

The objectives of this project are to 1) demonstrate on-vehicle and evaluate a solid oxide fuel cell (SOFC) auxiliary power unit (APU) with integrated on-board reformation of diesel fuel; 2) develop a transparent method of water management for diesel fuel reformation; 3) develop controls to seamlessly start, operate, and shut-down the SOFC APU; 4) evaluate hardening the SOFC APU to enable it to operate reliably in the on-highway environment; and 5) develop the overall system for performance, size, cost, and reliability targets.



<u>Question 1: Relevance to overall DOE</u> <u>objectives</u>

This project earned a score of **3.4** for its relevance to DOE objectives.

- This project is very relevant to the Fuel Cells subprogram's emphasis on SOFC fuel cell power systems for mobile auxiliary power applications. The primary fuel is diesel as appropriate for highway truck applications.
- This project uses a challenging approach to truly test the feasibility of SOFCs as power conversion devices. The objectives of building and mounting a complete fuel cell system on a truck, reforming diesel fuel, solving water management, and simulating vibration conditions are all part of a true test of feasibility. This is an excellent demonstration of the SOFC part of the Hydrogen Program.
- This project focuses on the development of diesel-fueled SOFC-based APUs for truck applications and fully supports DOE RD&D objectives.
- This project appropriately supports DOE objectives for APU applications.
- This truck APU is an excellent introductory application for SOFC technology.
- The truck APU application would provide an environmental mitigation technology not strictly a principle goal, but one that might gain in importance. Fuel savings was well demonstrated, but it is not clear that multiplied by the number of trucks it makes a significant contribution to reducing imports.
- This project supports the DOE targets and plans for truck APUs in existing and re-directed program described by Sunita Satyapal on May 18, 2009.
- The project should demonstrate a viable SOFC solution to anti-idling.

Question 2: Approach to performing the research and development

This project was rated **3.3** on its approach.

- The project has adopted a logical approach to total system design and hardware performance optimization that incorporates a total system perspective.
- This project identifies and focuses on the most significant barriers of SOFC development. Many SOFC demonstrations are conducted by stack developers who are experts in the development of cells and stacks, but not necessarily the complete system. In this case, Cummins has significant experience in building portable power systems. Here, they have developed a fuel cell power system that responds to the current weaknesses of their SOFC component, while taking advantage of its strengths. Cummins recognizes that a SOFC system must include battery storage to become practical. Their second design emphasizes this further with larger batteries. This is an honest approach to the demonstration of SOFC systems.

- The "system" approach to performing the work is logical and reasonable. Progress has been made on addressing thermal management of the system and diesel reforming. No information was given regarding the identified barriers of transient operation, power density, and vibration and shock tolerance.
- Technical barriers have been well defined and are appropriate for truck APU applications. These include thermal management, degradation, zero-water diesel reforming, mechanical robustness (shock and vibration), and cost.
- This project comprehensively addresses the application requirements.
- The project team has set an initial 5-year (10 khr) lifetime target, but a final10-year target.
- Cummins has been working in this area for a number of years, so they are well aware of the challenges and opportunities associated with SOFCs for mobile applications. Overall, the work plan is appropriate. It would have been good to see some information regarding how they plan to deal with S impurities in the fuel.
- The project appears to contain all the critical technology pieces to achieve a successful system along with the key technical requirements identified. It is not clear from the presentation whether the specific technology chosen can meet the goals.
- The project team uses an excellent overall technical approach based on Cummins extensive experience in APUs.
- Sulfur tolerance was not discussed.
- 1.5 years is the payback time.

Ouestion 3: Technical accomplishments and progress toward project and DOE goals

This project was rated 2.9 based on accomplishments.

- Good progress has been made since this project was restarted. Scale-up of output power per module is significant.
- Much progress has been made in overall SOFC systems development. However, the stack technology chosen for this project has slowed the overall progress of the project. It is not clear which is the main cause, however; in general the SOFC has not made enough advances on fuel and sulfur tolerant anodes. Also, although the tubular SOFC stack design is known for its ease of gas sealing and is tolerant to thermal cycling, cell interconnection becomes more complicated and expensive.
- DOE needs to support development of new ideas on electrode, cell, and stack designs to solve these issues. The past several years have focused on the demonstration of fixed design technologies.
- The key technical accomplishments to date include completion of overall system design and hot box design. The degree to which progress has been made toward the other defined objectives (such as transparent method of water management for diesel reformation and controls) is unclear from the presentation.
- Analysis and design is 95% complete, subsystem test and development are 90% complete.
- The project team is slightly behind on milestones, but not to a degree unexpected in an R&D program. In addition to technical difficulties, funding appears to have lagged.
- The project team is not meeting DOE program targets (100 W/kg, 100 W/L aggressive) on power density, balance-of-plant (BOP) parasitic losses, efficiency, and fuel; however, the team has indicated progress.
- Subscale stack testing reflects good thermal-cycling performance. Long-term testing is being done with one cycle per day.
- The project team demonstrated waterless CPOX with ULSD, which is significant to the application.
- Overall the project shows good progress. It's not clear whether the tubular technology from Protonex will be able to offer satisfactory performance in terms of mechanical robustness and low degradation rates.
- Good tight packaging. Technology development has resulted in components that fit well into the tight package. However, this is based on conceptual-level pictures. The actual component performance was not adequately discussed or shown. The individual cell performance is unclear and therefore an estimate of the cost is impossible. No cell dimensions were given. O/C of 1.3 is good but the length of test was not specified. It is well known that a fuel processor can adsorb carbon deposition for several hundred hours before failure.
- The project team is making good progress.
- The project team has developed a transparent method of water management for diesel fuel (ULSD) reformation and of controls to seamlessly start, operate, and shut down SOFC APUs. These are significant accomplishments.

- <1% degradation in 10 thermal cycles was attained by the SOFC.
- The simplest possible fuel processor is being used. It is extremely compact with an inexpensive design. It has demonstrated stable operation of a SOFC stack on ULSD with no added or recovered water. This is excellent. The project team has demonstrated tight thermal integration.
- The SOFC APU is only a little bigger and heavier than diesel APU.

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated **3.4** for technology transfer and collaboration.

- Meaningful collaborations are in place and active with partners who complement the skills and expertise of Cummins. It should be noted however that one of the original partners is currently inactive.
- Cummins has organized a capable team to achieve the project's objectives. It is clear that Protonex has a significant role in the SOFC component development. It is unfortunate that the OEM could not stay active in project.
- Collaborations have been excellent.
- Excellent integration with Protonex LLC and International Truck and Engine Corp. (no longer present). Welldefined roles and responsibilities. International helped define technical requirements earlier in the project - vital given the ultimate commercialization goal.
- The collaboration between Cummins and Protonex appears to be well coordinated.
- Good collaboration between a packager (Cummins) and technology provider (Protonex) and an OEM, although the OEM is currently inactive.
- Collaborators in this project include Cummins Power Generation, Protonex LLC, and International Truck and Engine Corp.
- Cummins knows APUs and the market and its customers. They are the best.
- This is good team containing excellent industrial partners. However, the truck company is now inactive.

<u>Ouestion 5: Approach to and relevance of proposed future research</u>

This project was rated **3.0** for proposed future work.

- The proposed future work builds on this year's progress and will continue to move the project toward its established goals and objectives. Prototype fabrication and testing is critical to successful completion of this project.
- Cummins is moving forward with its partners in the new design by addressing the shortcomings of the SOFC with a flexible BOP. The overall weight and volume of the system will be improved by reducing the size of the power conditioning and the number of fuel cell modules. This creates the need to rely more on battery storage, which seems to be a fair trade-off.
- Proposed future work is reasonable; however, a detailed plan with defined objectives and schedules may be needed.
- Not much detail was presented on risk mitigation and design alternatives.
- Overall, the proposed future work is appropriate; it would have been helpful to hear more about how the issues with the SOFC cells/stacks are going to be tackled.
- Looking at a battery/fuel cell system is good. This is an old and relatively obvious system, but it is good that it is the future direction. Not much else was discussed.
- The project team's future plans include:
 - System BOP design;
 - Protonex delivery of SOFC sub-assemblies;
 - System checkout ready for vehicle install; and
 - o Vehicle tests.
- The project barriers are well defined and excellent approaches have been used to resolve them.

Strengths and weaknesses

Strengths

- This is a good system design that is flexible to the abilities of the SOFC module.
- The hybridization between the SOFC and battery storage is inevitable, and other SOFC developers should admit this need. DOE should consider supporting development of advanced SOFC advanced battery systems to take advantage of their synergistic benefits. By themselves, neither can answer all power systems needs.
- The project has a strong system development approach.
- The project focuses on key technical areas: SOFC; diesel reforming; and thermal management.
- The application has strong market potential. Cummins is a leader in the market.
- Development of the transparent method of water management for diesel fuel (ULSD) reformation and of controls to seamlessly start, operate, and shut-down SOFC APU are significant accomplishments.

Weaknesses

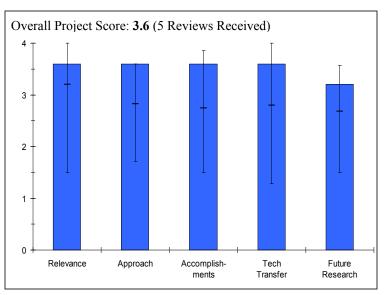
- There is risk in connecting all of the cells in series.
- In general, it is expensive to interconnect tubular cells together and have good power output.
- Emphasis has not been placed on addressing certain issues such as SOFC degradation and start-up/shut-down of the fuel cell.
- Cost targets should be explicit, with regular analysis and reporting to DOE. Cost targets should be tied closely to the intended application alternatives (e.g., diesel APUs). Cost is an integral and critical element of a technology development program using DOE support for public benefit.
- To be fair, the SOFC stack is the critical element. Insufficient detail was provided to permit a substantial assessment. A non-disclosure agreement would be required.
- Efficiency may not meet target 35%. System is only 18% at 1500 W. SOFC needs improved power density. Fuel utilization is only 63%.

- The Cummins team is on the right track for real-world SOFC demonstration. However, to reach the deployment stage, DOE needs to allow for more fundamental work for the SOFC stack developer to develop high-sulfur and other impurity tolerant anodes, as well as economical cell interconnection. In addition, research needs to be done to develop high-volume manufacturing processes and procedures to reduce cost.
- The project team should use metrics to measure progress for each technical task.
- The project team should evaluate degradation (if any) and start-up/shut-down of the hot box, especially the SOFC.
- The project team should consider anode recycle to enable ATR reforming. This is more complex and expensive, but has greater operating margins and efficiency. Has this been considered? R&D Dynamics has high-temperature recycle blower prototypes. Perhaps the current SOFC stack hot box/module design precludes this option? Insufficient detail was provided in the presentation.

Project # FC-44: Solid Oxide Fuel Cell Development for Auxiliary Power in Heavy Duty Vehicle Applications *Gary D. Blake; Delphi*

Brief Summary of Project

The objectives of this project are to 1) develop auxiliary power unit (APU) system requirements and concepts with major truck original equipment manufacturers; 2) design, develop and test the needed subsystems for the approved concept; and 3) build and demonstrate a diesel-fueled truck APU system for the Department of Energy. Delphi is currently focused on 1) completing the solid oxide fuel cell APU hardware build and procurement; 2) initiating the subsystem hardware testing and design iterations; and 3) performing subsystem testing and controls development, initial solid oxide fuel cell APU system brass board integration and design iteration. Delphi is on target for



meeting timing and budget and is committed to introducing solid oxide fuel cell diesel technology in full-scale production for heavy duty truck applications.

Question 1: Relevance to overall DOE objectives

This project earned a score of **3.6** for its relevance to DOE objectives.

- The successful design, building and testing of a mobile APU will demonstrate the solid oxide fuel cell (SOFC) as a viable energy conversion device. The 5 kW scale, use of diesel fuel, and vehicle application all provide a rigorous tests of the technology. This project completely supports the SOFC part of the Hydrogen Program.
- This project aims at developing SOFC-based APUs for heavy duty trucks and fully supports DOE RD&D objectives.
- This project appropriately supports DOE Hydrogen Program goals for the APU application. The project team is keeping spin-off applications/alternative uses of the technology in mind.
- The APU has good applicability from an environmental perspective, which may reach a federal level of attention in the future.
- Reviewing the presentation of Sunita Satyapal on May 18, 2009, this project supports the new fuel cell systems program direction APUs.
- Truck idling emits 11-million tons of CO₂; 200,000 tons of NO_X; and 5,000 tons of particulate matter and consumes >1 billion gallons of diesel fuel.
- The Delphi unit will exceed the 35% efficiency goal for 2010.

Question 2: Approach to performing the research and development

This project was rated **3.6** on its approach.

- Delphi has an aggressive approach toward meeting and exceeding the DOE targets.
- Delphi is addressing two critical issues of sulfur and carbon, which are significant barriers to SOFC deployment.
- The planar SOFC is more sensitive to mechanical shock, vibration, and thermal cycling in a mobile application; however, it has a better power density than other designs. What kind of shock damage will the stack survive?
- This project focuses on the approaches to address the technical barriers relating to diesel reforming and system integration. Work on SOFC degradation and start-up/shut-down is needed.

- DPS 3000 enhancements address key technical barriers: fuel compatibility, power, and efficiency. Autothermal reforming (ATR) is key to meeting the DOE efficiency target and is enabled by anode recycle.
- System integration appears to reflect a near-commercial product.
- Scale-up of cells to >100 cm² in active area is very technically feasible and will result in system simplification and lower cost very appropriate.
- Some of the key issues specific to an APU are being addressed. A focus on carbon and sulfur issues is a good focus. Excellent focus on original equipment manufacturer (OEM) demos with complete system packaging.
- The work is well designed, feasible, and integrated well with other efforts, especially with SECA. All barriers defined and removed.
- Truck cab heating will be totally separate initially. Further full integration is being considered.

Ouestion 3: Technical accomplishments and progress toward project and DOE goals

This project was rated **3.6** based on accomplishments.

- Delphi has been working on similar systems for some time. It seems that the diesel reforming barrier has been significant and that the endothermic (H₂O, CO₂ recycling) reformer unit will help solve this issue.
- The short-term on-truck data looks promising.
- Is there longer lifetime and thermal cycling data?
- Significant progress has been made in hardware demonstration, especially in OEM demos (PACCAR/Peterbilt and Daimler/Freightliner).
- The data is well characterized for application operational requirements and the 2.5 4 kW power requirement.
- Delphi's internal targets closely match DOE targets with the exception of start-up time. However, the project will not achieve stated DOE goals of 100W/kg and 100W/L. Those targets are perhaps overly aggressive.
- The project team is on track with respect to key milestones.
- Vibration testing has shown promising results with respect to SOFC stack robustness.
- The project has demonstrated prototypes in on-truck operation (short term). Excellent performance.
- Maximum stack test duration to date is 5,000 hours, 1%/1000 h degradation. The ultimate target is 20,000 h.
- The project presentation did not address cost status a key metric in the technology's viability.
- Power densities look excellent. Cell area was specified. Using a recycle to perform a reformation rather than partial oxidation is difficult but was apparently achieved. There was significant positive impact relative to efficiency. A full system test with two OEMs was successfully accomplished. Given the importance, more discussion was needed on diesel reforming, accomplishments, and difficulties.
- Two major highly visible successful OEM demos were completed in 2008. Completed 3 or 4 milestones 50 % on fourth critical milestone.
- Degradation is less than 1% in stack 5,000 h testing in stack accomplished.

<u>Ouestion 4: Technology transfer/collaborations with industry, universities and other laboratories</u>

This project was rated **3.6** for technology transfer and collaboration.

- The collaborator's specific contributions to the project are not clear other than the role of consultant.
- The project team works with PACCAR and Volvo Truck. Further OEM input is expected. Multiple demonstrations have taken place with truck OEMs (Peterbilt and Daimler).
- Excellent development of system requirements through multiple OEM input and demonstration.
- PACCAR, Volvo Truck, and Electricore Inc. are key automotive partners included in the project. Project is professionally coordinated.
- Team involvement of OEM allows load profiles -potential power requirements of 2.5 kW and 4.0 kW to be meaningfully determined.

Question 5: Approach to and relevance of proposed future research

This project was rated **3.2** for proposed future work.

- The future work is focused on finishing subsystem testing and completing design and development of the whole system.
- Specific barriers have not been outlined and addressed in future plans.
- Proposed future work is consistent with technical progress. The focus of "subsystem testing and development iterations" is unclear.
- Future plans include full APU system testing in 2009 and commercial package in 2010. These plans are appropriately aggressive; it appears that Delphi has the progress-to-date, focus and capabilities to achieve these targets.
- Activities are focused and are critical to commercialization.
- The project is over 70% complete. Future work for FY09 and FY10 is well defined and executable:
 - Finish subsystem testing and development iterations;
 - Conduct 24-month critical decision milestone review;
 - Complete system module testing and development;
 - Begin full SOFC APU system testing;
 - Build commercial packaged SOFC APU; and
 - Demo test, 24-hour truck user profile using battery interface and vehicle simulation (20,000 hour planned, 5,000 hour completed).

Strengths and weaknesses

Strengths

- Delphi has long and broad experience in developing SOFC systems.
- Delphi has used its experience with natural gas (NG) systems to successfully redesign for a diesel system.
- Delphi has a strong system development approach.
- Delphi has a strong focus on subsystem and system demonstration.
- State-of-the-art SOFC technology has very high performance.
- Excellent professional team.
- High APU efficiency supporting program goals.

Weaknesses

- Fundamental issues of SOFC anode durability are a weakness and have not been discussed in the presentation. Are these issues being addressed?
- Cost targets and estimates have not been addressed.
- It appears that several critical issues such as performance degradation and control including start-up/shut-down may not be adequately addressed in this project.

- Delphi is on track for real-world SOFC demonstration. However, for developers to reach the deployment stage DOE needs to allow for more fundamental work on SOFC anodes to develop high-sulfur and other impurity tolerance and direct reforming of CH₄ and C₂s in the stack. Research needs to be done to develop high-volume manufacturing processes and procedures to reduce cost.
- Some work needs to be initiated in this project to assess degradation, control, and start-up/shut-down issues.

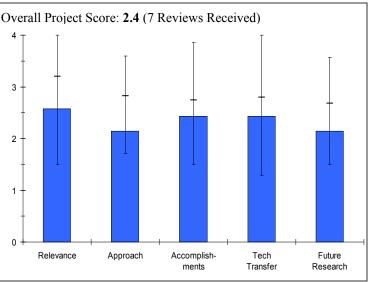
Project # FC-45: Solid Acid Fuel Cell Stack for APU Applications

Hau H. Duong; Superprotonic, Inc.

Brief Summary of Project

The main focus of the project is to develop a solid acid fuel cell (SAFC) stack that operates on diesel reformate with performance characteristics approaching or exceeding most of the U.S. Department of Energy's 2010 technical targets for an auxiliary power unit. This project has demonstrated SAFC functionality and stability on methanol, propane, and diesel fuels. Future work will include the scale up of SAFC membrane electrode assembly size and quantity, building a 300-W SAFC stack, and designing a 3-kW SAFC system.

Question 1: Relevance to overall DOE



objectives

This project earned a score of **2.6** for its relevance to DOE objectives.

- This project introduces a novel electrolyte similar to the phosphoric acid fuel cell (PAFC). The PAFC had problems of low power density, handling of electrolyte before start-up, and platinum electrodes. These made the technology expensive.
- The ability to function in high CO makes the project worthwhile. However, the heavy loading of platinum electrodes makes it difficult to reach DOE cost objectives.
- Why this concept is better than phosphoric acid fuel cells isn't clear. What are its benefits compared to PAFC?
- The project focuses on the development of solid acid fuel cell stacks and fully supports DOE RD&D objectives.
- The project's stated goals appear to support the DOE Hydrogen Program's goals for APUs; however, there is no connection between the project details and a particular application of national interest. Furthermore, the state of development is quite immature to the point that meeting the 2010 goals is impossible.
- The APU represents an excellent potential application for SOFC technology.
- APU applications have good environmental characteristics and may reach a federal level of attention in the future.
- This project is not projected to meet the APU 2010 target of 35% efficiency.
- Conductivity is not equivalent to PEMFC.
- It is unclear what cathode and anode were used with CsH₂PO₄ proton-conducting electrolyte.
- Even higher temperature, 200°C operation does not offset the lower temperature PEFC system inefficiencies.

Question 2: Approach to performing the research and development

This project was rated **2.1** on its approach.

- The approach of this project was to fabricate and demonstrate cell and stack operation. Over the duration of the project, cells have been scaled from 3 to 15 to 125 cm². Twenty cell stacks have been built and tested in a variety of carbonaceous fuels. Long-term and thermal cycling tests are proposed.
- The main issue of heavy platinum loading on electrodes still needs to be addressed.
- There is no indication of how this concept addresses the cost barrier. This concept doesn't appear to offer any cost advantages compared to PAFC.
- No clear approaches have been shown to address the issues of durability and performance improvement under practical conditions (e.g., high fuel utilization).

- The presentation did not address, in a substantial manner, the technical barriers (cost, durability, and stability), paths for resolution, and status.
- The project is fairly limited in scope, focusing just on the fuel cell stack. Given some of the significant limitations of the solid acid electrolyte, it's not clear that it's a good candidate material for the APU application. The material is brittle and weak at room temperature. Even if it is more plastic at operating temperatures, the authors did not present any evidence that cells/stacks based on this material will survive thermal cycling. Cost issues were not satisfactorily addressed.
- Technical targets appear adequate for an APU application. Much of the discussion of technical characteristics of solid acids appeared to be idealistic rather than based on extensive data. Conductivity was given on a 1/T plot, which is not a good way to present data in a time-restricted review. It is difficult to draw out technical characteristics. The presenter did not seem to understand key technical aspects of the technology. The presenter discussed tolerance in relation to the electrolyte but did not discuss electrode tolerance, which is generally the more critical issue. The presenter gave the impression that this is an electrolyte development project not even close to an APU project. Some modeling results were presented. Electrodes and other stack components are not addressed. The use of diesel at 250°C could be fairly problematic given there is higher hydrocarbon slip. It is very difficult to control carbon deposition at this temperature.
- The overall approach is good. The project team has made the right level of advancement and scale-up.
- Stability in water vapor and carbon dioxide in anode and cathode gases may need to be addressed. CO and H₂S tolerance was tested.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated **2.4** based on accomplishments.

- The project team has made impressive progress in the past year in cell power density. It has increased to 0.65 W/cm² at 250°C. The 20-cell stack has been tested on synthetic reformate, propane, methanol, and diesel reformate fuels.
- The project has demonstrated tolerance to reformates. However, the degradation rate of ~0.06%/hr on reformate is a significant weakness and will have to be greatly improved to meet the durability target of 2,000 hours.
- V/I polarization curves show a current density max of about 350 mA/cm² on hydrogen, and about 300 mA/cm² on reformate. This isn't consistent with claims of power densities of ~320-600 mW/cm² on slide 6.
- Progress has been made in demonstration of operation on a variety of reformate gases and stack design/fabrication.
- In light of the Hydrogen Program's 2010 targets, this is a very immature technology.
- The production target of 500 mW/cm². Claims to have achieved >600mW/cm² this year; however, details are not provided. All data presented is substantially lower.
- Power density appears low (most data ~100 mW/cm²), with substantial degradation 0.06%/hr on reformate. Newer performance is ~1-2%/100 hr. is very high.
- There appears to be durability issue. Can this technology be viable for commercial application?
- Numerous milestones have been missed.
- Cost entitlement and potential are not addressed.
- Much of the work is focused on development of fabrication procedures for the SAFC MEA. Thus far, the areal power densities obtained are quite low (requiring many cells to obtain the desired stack power level), and while a very limited amount of results over time were reported, it's clear that the degradation rates are very high.
- Other than a few plots related to the electrolyte, very little actual technical discussion is present. A project can't successfully evolve when primarily focused on electrolyte characterization to a 300 W stack. There are major material issues that have to be addressed before this could even be considered. There is no mention of any work other than characterizing the electrolyte. The level of technical discussion does not support the later milestone discussion. It is highly questionable how the milestones were met.
- Progress has been made. Stack performance on all reformates except diesel are acceptable.
- The project team tested one or more (unclear) 20-cell, 20-cm² cell stacks for 16 days on reformates. Reformate was not done *in situ*. It can only be assumed that the fuels were externally reformed and predicted compositions were used. Non-commercial platinum anodes and cathodes were used.

<u>Ouestion 4: Technology transfer/collaborations with industry, universities and other laboratories</u>

This project was rated 2.4 for technology transfer and collaboration.

- California Institute of Technology (Caltech) was the inventor of the technology.
- Richard Mistler, Inc. (Mistler) helped in coating formulations.
- Superprotonic should consider teaming with a fuel cell system integrator.
- Collaboration with other academic institutions (outside Caltech) and fuel cell developers is encouraged.
- Collaboration included Caltech and Mistler.
- It was hard to tell how much coordination/cooperation exists between the partners.
- The project team collaborated with an academic institution. There was no indication of industry input or interest.
- Coordination with Caltech is appropriate.

Question 5: Approach to and relevance of proposed future research

This project was rated **2.1** for proposed future work.

- Investigators plan to scale up stacks to 300 W and 3 kW. Long-term and thermal cycling short stack tests should demonstrate cell durability.
- Platinum loading needs to be reduced.
- The plan for future work is logical, but it's doubtful that the project team has the time or resources to complete the work as planned.
- The proposed future work appears to be too general and needs to include metrics and work on durability improvement.
- The proposed work focuses on scale-up; however, the small-scale data presented suggests that the technical barriers for the 3-kW APU application are much more fundamental than would allow scale up. There is also the issue of stability/degradation and the ability to operate for 10-20,000 h. These are issues that will likely take considerable resources and time to address.
- It seems inappropriate to devote resources to the design of a 3-kW stack/system unless the authors can show significantly improved power density and stability for their current cells/stacks (and also provide some evidence that the materials and fabrication processes involved in preparing the stacks could be cost-effective; it was noted that noble metals are utilized as electrode materials).
- The future work appears unrealistic with a large focus on full stacks verses technology characterization. There are substantial degradation questions that were not adequately addressed. Until these questions are fully addressed, there is little reason to proceed further.
- Future stack plans for FY2009 are appropriate:
 - Build and characterize a 300-W SAFC stack operating on hydrogen fuel;
 - Employ micro-porous layer deposition using tape casting;
 - Employ anode and cathode catalyst layer deposition using sprayer;
 - Employ CDP (25-50 micron) electrolyte densification using compaction; and
 - Fabricate 125-cm² SAFC MEA using above processes.
- Additional work will require more funding.

Strengths and weaknesses

Strengths

- CO poisoning is reduced by increased temperature.
- Aluminum bipolar plates can be used.
- Solid electrolyte has plastic mechanical behavior at operating temperature.
- The use of a solid proton-conducting electrolyte instead of liquid phosphoric acid is a benefit.
- The cell and stack fabrication is a strength.
- Operation has been demonstrated on a variety of reformate gases.

Weaknesses

- The electrolyte is water sensitive.
- There is high platinum loading in electrodes.
- There was no mention of the projected cost impact of the electrolyte.
- A number of technical barriers relating to durability, performance in reformates, and stack design/operation have not been addressed.
- The state of development is quite immature to the point that meeting the 2010 Hydrogen Program goals is impossible.
- Low efficiency is a weakness.

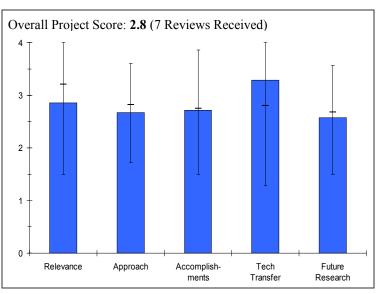
- This project needs to include a cost evaluation.
- Significant effort should be focused on reducing the use of platinum.
- The project team should work to identify causes for observed performance degradation and develop approaches to mitigate this issue is strongly recommended.
- Assessment was difficult because the details were not presented. However, a detailed cost entitlement analysis supplemented with a cost estimate based upon actual experimental data would be useful in assessing the state of development. Explicit degradation targets based upon a techno-economic analysis are needed.
- Longer term R&D project requiring more time and funding.

Project # FC-46: Low-Cost Co-Production of Hydrogen and Electricity

Fred Mitlitsky; Bloom Energy

Brief Summary of Project

The objectives of this project are to 1) demonstrate cost-effective, efficient, reliable and durable solid oxide fuel cells (SOFCs) for stationary applications; and 2) determine the economics of hydrogen and electricity co-production for comparison to stand alone hydrogen production facilities. The Alaska site build was completed. The planar SOFC system is installed and operational with key metrics achieved. The full-scale hydrogen pump has been integrated with the planar SOFC. Partial pressure swing adsorption design and prototype testing are being performed in parallel. The cost of hydrogen was analyzed using the DOE H2A model.



Question 1: Relevance to overall DOE objectives

This project earned a score of 2.9 for its relevance to DOE objectives.

- This project, the demonstration of stationary SOFC power generation under realistic operating conditions, is very relevant to the Fuel Cells subprogram goals and objectives.
- Using carbon-based fuels, steam, and a fuel cell to make hydrogen is an interesting idea. However, there can be some question on its economy. A comparison between this and other hydrogen/electricity generating technologies would be useful as an initial determination of the viability of the approach. This project has the potential to support hydrogen production goals.
- The focus of this project is on SOFC system tests. Is the overlap with SOFC programs supported by DOE's Fossil Energy (FE)?
- This project explores SOFCs for co-production of H₂ and electricity. It is not clear how this effort addresses the stated DOE Hydrogen Program's fuel cell goals. Is it categorized as an auxiliary power unit (APU) project?
- Overall, the relevance to DOE objectives (improvement of hydrogen generation and fuel cell technology) is good.
- Co-production of hydrogen and power seems of less significance than producing either hydrogen or power. It is not clear that supplementing gasoline with natural gas (NG) accomplishes much from a strategic fuel standpoint.
- This project should:
 - Demonstrate cost-effective, efficient, reliable, and durable planar solid oxide fuel cell (PSOFC) systems for stationary applications;
 - Demonstrate the feasibility of a delivered cost of hydrogen below \$2.50 per gge DOE target; and
 - Give information concerning the economics of hydrogen and electricity co-production to compare with stand-alone hydrogen production facilities.

Question 2: Approach to performing the research and development

This project was rated 2.7 on its approach.

• The approach taken for this project is straightforward and directed toward field-testing of a fairly standard SOFC power system. The approach supports the project goals and objectives.

- The technical barriers relating to fuel processing, stack operation, and hydrogen purification are not clearly spelled out.
- It seems that the capital equipment cost of two independent systems can be expensive. Why is this technology preferable to other hydrogen/electricity generation technologies?
- The project appears to focus on demonstration. A number of technical barriers have not been addressed (e.g., fuel cell performance and durability). The benefits of hydrogen production by electrochemical pumps or swing absorption for this system are unclear.
- Demonstration and scale are appropriate.
- The project integrates independent third party validation and economic analysis.
- The presentation was very "high level," making it difficult to assess the specific approaches being used to overcome challenges.
- The project team discussed application of H2A model but didn't discuss methodology or detailed assumptions. The team did discuss some global results and attributed them to the H2A model, which does not provide confidence in results. A system diagram was presented. It requires two fuel cells and a reformer to produce hydrogen and power when in principle the reformer is producing hydrogen. It would seem better to either use the reformer followed by purification or electrically driven electrolysis. The system doesn't indicate purification system or external heat source for the hydrogen concentration.
- This project uses an elegant, simple design for difficult environmental conditions.
- Excellent approach for operation:
 - 25 kW power;
 - Operation on natural gas;
 - Operating at 480 V;
 - Grid parallel operation;
 - \circ Remote monitoring; and
 - \circ One-year demonstration.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated 2.7 based on accomplishments.

- Significant progress was achieved during the past year focusing on the field-testing, including extensive operational data collection.
- There is no description of what point the developmental work started or discussion of specific technical barriers, so it is difficult to evaluate what progress has been made.
- Each SOFC stack was rated at 25 kW and 480 V (slide 9). What fraction is the power conditioning section of the system? Is it included in the cost estimate?
- Although the stack technology is presented as a black box, the system setup and testing was quick (9-13 hours from delivery). However, there are no details of what lessons were learned during the setup of the system.
- Progress has been made toward demonstration of fuel cell operation and co-production of electricity and hydrogen. No work was indicated in the presentation to demonstrate or improve durability.
- Intermediate goals and objectives are reasonable and appropriate, reflecting appropriate progress.
- The project team claims the 50 kW PSOFC system has been operational since December and met key metrics. Testing of a full-scale H₂ pump integrated with 25kW SOFC stack should start soon.
- The project team's accomplishments include:
 - 45% LHV NG efficiency (electric only), peak of 51.1%;
 - Approximately 70% availability target, actual in the >90%;
 - Grid-parallel operation;
 - Greater than 2,000 hours of operation to date;
 - o 95% fuel utilization in anode recycle mode;
 - \circ 19kg/day H₂ production;
 - PPSA will enable 80% fuel recovery, 95% CO₂ removal; and
 - \$4.53 H₂/gge, at 33% electrical efficiency (proposal was \$4.82 target), if get 0.12\$/kWh credit, get \$0.97 H₂/gge.
- The fact that the authors were able to get two separate 25 kW systems up and running is encouraging. Unfortunately it's hard to tell how successful/viable those demonstration units really are. We were provided

with power output over time, but not given information regarding changes in operating voltage and/or current during that time that were made to sustain the desired power level, so it's not possible to tell what sort of degradation may have been occurring. Also, the average AC efficiencies reported in the tables appear to be inconsistent with the efficiencies shown in the graphs in the supplemental slides.

- The project team discussed pressure swing adsorption (PSA) as a significant technical accomplishment without explanation. PSAs are standard equipment. Very little presentation of, (if any) technical or economic results. 45% electrical efficiency on natural gas is not particularly good for a 25 kW system. Electrical efficiency should be in the 50% + range. There was a substantial reduction in power a few months into the test, but no explanation given. This could be major problem. Impossible to judge future viability of technology from data given.
- SOFC run data looks good running for over 4,000 hours and operating at 38.2 kW.
- Project achieved 97% availability.
- Project team demonstrated remote monitoring.
- Good progress has been made to-date.
- 45% lower heating value (LHV) net electric efficiency in electric-only mode is possible. DOE should examine method used to calculate electrical efficiency.
- There was little discussion about H₂ and PPSA.
- It is unclear whether the degradation level was measured.

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated **3.3** for technology transfer and collaboration.

- There are good collaborations in this project. The partners played an important supporting role and provided independent validation.
- Bloom Energy seems to have assembled an effective team to build and demonstrate its technology; however, it is not clear what each team member's contributions are.
- The project may benefit from interactions with organizations working under FE programs.
- This project includes diverse partners and good coordination:
 - The demo was done at Udelhoven Oilfield System Services;
 - \circ H₂ Pump LLC has been providing hardware;
 - Giner Electrochemical Systems, LLC has been providing equipment; and
 - University of Alaska has provided independent validation.
 - The collaboration between partners appears to be well coordinated.
- The project team was able to install the system at an airport, which required coordination with several local organizations.
- Excellent team for manufacture, equipment, and testing:
 - o Bloom Energy: Planar SOFC system, hydrogen testing, and project management;
 - Udelhoven Oilfield System Services, Anchorage, AK: General Construction;
 - H2 Pump LLC, Latham, NY: Equipment;
 - Giner Electrochemical Systems, LLC, Newton, MA: Equipment; and
 - o University of Alaska, Fairbanks, AK: Independent Validation.

Question 5: Approach to and relevance of proposed future research

This project was rated 2.6 for proposed future work.

- Plans for future work focus primarily on completion of the field demonstration and appear to be adequate to achieve this objective. In addition, the economic analysis will be updated and completed, and the hydrogen production component will be demonstrated.
- Since specific barriers are not mentioned, it is difficult to determine if planning for future work is focused on overcoming barriers.
- The plan for future work does not provide details or proposed approaches/directions to address certain barriers such as degradation and performance or system operation improvements.

- The key element in going forward is a detailed assessment of the capital cost of the system, including the SOFC stack and balance-of-plant (BOP). This analysis should take into account the degradation and overall life of the SOFC stack as the technology stands today.
- The proposed future work appears to be in line with the overall project goals.
- There was no real discussion of future work.
- This is a nice project that has identified and managed risks.
- Plans to overcome barriers and have a successful demonstration are excellent:
 - Complete PSOFC system demonstration (1 year);
 - Complete hydrogen production demonstration;
 - Complete PPSA build, test, and investigation; and
 - Complete cost and economics analysis.

Strengths and weaknesses

Strengths

- The system seems to be well designed and developed by the performance data, but not enough of the right data is given to be sure.
- The system power output appears stable, based on the data given.
- The project team's hardware and prototype demonstration is a strength.
- This is an excellent team and a simple design.

Weaknesses

- The SOFC and H₂ separation units do not appear to be heat integrated. It is not clear how efficient and cost effective the system is.
- Approaches to resolve certain barriers are lacking.
- DOE should examine the method used to calculate electrical efficiency.

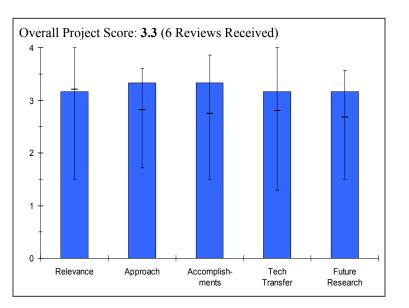
- The project team should be more forthcoming on the technology and cost barriers.
- In addition to the demos, part of the effort should be focused on addressing certain key barriers in the development of such a system. Metrics and detailed plans need to be developed.
- DOE should examine the method used to calculate electrical efficiency.

Project # FC-47: Development of a Novel Efficient Solid-Oxide Hybrid for Co-Generation of Hydrogen and Electricity Using Nearby Resources for Local Application

Greg Tai, Mike Homel, Bruce Butler, and Anil Virkar; Materials and Systems Research, Inc.

Brief Summary of Project

The overall objective of this project is to develop a low-cost and highly efficient 5 kW solid oxide fuel cell (SOFC)-solid oxide fuel-fed electrolysis cell (SOFEC) hybrid system co-generating both electricity and hydrogen to achieve the cost target of <\$3.00/gge when modeled with a 1,500 gge/day hydrogen production rate. The project focuses on materials research and development, stack design and fabrication, and system design and verification. The 2008-2009 objectives for this project were 1) 5 kW SOFC-SOFEC hybrid system development and 2) 5 kW SOFC-SOFEC hybrid system evaluation.



Question 1: Relevance to overall DOE objectives

This project earned a score of **3.2** for its relevance to DOE objectives.

- This is a clever idea for using carbon-based fuels and steam to make hydrogen. However, there may be some questions on its economy. A comparison between this and other hydrogen/electricity generating technologies would be useful to determine the viability of the approach. This project has potential for meeting the Hydrogen Program's goals.
- This project aims at developing a system capable of co-producing electricity and hydrogen and fully supports DOE RD&D objectives.
- It's not clear how this project supports the stated DOE Hydrogen Program's fuel cell goals. Is it considered an auxiliary power unit (APU)?
- The subjects of the work (improvement of SOFC and hydrogen production technology) are relevant to DOE objectives.
- Hydrogen production via water electrolysis in an SOFC is an interesting approach.
- The project will lead to the development of a low-cost and efficient 5 kW SOFEC-SOFC hybrid system cogenerating both electricity and hydrogen and achieving the cost target of <\$3.00/gge when modeled with a 1500 gge/day hydrogen production rate.

Question 2: Approach to performing the research and development

This project was rated **3.3** on its approach.

- The hybridized 13-cell SOFC/20-cell SOFEC stack design seems like a good design for heat integration. Is the gas manifolding too complicated to continue in this direction?
- How well is the 5 kW design thermally integrated?
- Does use of LSCM as a reversible cathode work well enough? This material has not been fully proved as an active, conductive electrode.
- The project approaches are logical and focus on resolving certain barriers in the SOFC followed by stack and other component designs, then integration and testing.
- This project looks at H₂ generation by electrolysis and a low-cost, efficient 5 kW SOFEC-SOFC system for cogeneration <\$3/H₂ gge.

556 FY 2009 Merit Review and Peer Evaluation Report

- Approach is fairly comprehensive, culminating in proof-of-concept fabrication and operation.
- The approach, involving hybrid SOFEC/SOFC stacks, is interesting and worthy of investigation.
- There is a good balance between component and system development. It would seem more efficient to produce power or hydrogen, versus combining the two functions. In most cases, the power-producing SOFC will not produce sufficient heat to substantially contribute heat to the electrolysis function (i.e., combining the functions doesn't necessarily produce a synergistic system). Having the power and electrolysis co-located could be very problematic in maintaining a balanced thermal profile within the respective stacks.
- The project team has a well-documented and conceived approach and a well-integrated SOEC/SOFC concept to optimize thermal integration.
- An excellent engineering analysis of performance and cost can be expected.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated 3.3 based on accomplishments.

- The team has designed and fabricated the cells for a 5 kW SOFEC-SOFC hybrid system and has tested cells, 2cell stacks, a 13-cell SOFC/20-cell SOFEC stack, and a 40-cell 1 kW SOFC stack. The team will need to assemble the 5 kW unit and test it before July. More analysis and development of the cathode will probably be needed. What about the anode material? The Ni-cermet has poisoning and coking issues when using carbonaceous fuels.
- The key achievements include development of cathode materials stable under redox conditions, 1 kW stacks built and tested, 5 kW components fabricated, and long-term stability tests.
- The project appears to be progressing well towards 5kW construction and operation, given the apparent underfunding.
- Results to date are encouraging, although degradation rates appear to be quite high. It will be interesting to see if the approach can be extended to the larger 5 kW scale. More information regarding the expected cost of materials and fabrication would have been useful.
- The project team has presented a reasonably good level of technical detail. It is clear that the LSCM cathode is only moderately active –the price that is paid for claimed stability in reducing and oxidizing conditions. The electrodes can be problematic in this application. It may require extensive work to demonstrate that they are truly stable for extended life beyond a thousand hours or so. Extensive microanalysis work needs to be done. In particular, substantial transmission electron microscopy (TEM) work needs to be done.
- SOA SOFC performance with the LSCM electrolyte has been excellent.
- The project team has conducted long-term stability tests of hydrogen production to reduce cost. The team has finalized the design of hybrid modules with improved thermal and flow management.
- The project team has designed, fabricated, and tested main balance-of-plant components.
- The project team has fabricated cell/stack components for the 5 kW system.
- The project team has assembled and evaluated the 1 kW SOFC stack with the new design.

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated **3.2** for technology transfer and collaboration.

- The partners in the project are known for their experience in the field and can contribute to the project. It is not clear however why anode fracture and residual stresses are an issue as to require focused attention.
- Excellent coordination has taken place among resources with appropriate skill sets and capabilities:
 - University of Alaska at Fairbanks (UAF) anode failure and residual stresses;
 - Missouri University of Science and Technology (MST) cathode and seal materials development; and
 - University of Utah (UU) interconnect development.
- Project collaborations are difficult to evaluate; collaborations weren't discussed much in the presentation.
- There has been good collaboration for technology development. MST and UU add substantial component expertise.
- Excellent team:
 - UAF: anode fracture mechanisms and modeling of residual stresses (S. Bandopadhyay);
 - o MST: cathode & seal materials development (H. Anderson; R. Brow); and
 - UU: interconnect development (A. Virkar).

<u>Question 5: Approach to and relevance of proposed future research</u>

This project was rated **3.2** for proposed future work.

- The 5-kW unit still needs to be demonstrated and a cost analysis needs to be completed for this project. In addition, experiments and analyses demonstrating biomass or coal operation would help the idea obtain broader support.
- The plan is straightforward for the proposed future work. Development of test protocols, including startup/shut-down and controls and metrics, may be needed to support the 5 kW system demonstration.
- The future work is appropriate and includes system assembly and operation and cost analysis.
- The planned scale-up of the technology seems appropriate, but cost-effective resolution of performance degradation issues should take higher priority.
- Future work is focused on producing a full system with a cost estimate. It is questionable whether detailed component R&D is done, particularly in regard to stability of electrodes in a wide range of conditions and thermal integration and profiles in the stacks.
- Future work is well-planned and will result in testing and analysis:
 - SOFEC-SOFC hybrid module assembly, integration and burn-in;
 - o 5-kW hybrid system assembly;
 - System testing and evaluation;
 - o Implementation and optimization of system controls; and
 - Hydrogen production cost analysis using H2A model.

Strengths and weaknesses

Strengths

- Materials and Systems Research Inc. (MSRI) has extensive experience in fabricating solid oxide cells and stacks, and has excellent research-level stack production facilities.
- MSRI also has a good understanding of SOFC materials development and testing.
- Key technical barriers have been identified and addressed.
- The project team has used logical approaches.
- Excellent SOFC co-generation system performance and design.

Weaknesses

- Not much has been said about fuel processing and impurity removal. Impurities affect the operation of the fuel cell anode.
- More explanation of the design of the balance of plant is needed.
- System integration can be improved.
- The project team needs to eliminate some piping in the hybrid design.

- The viability of this approach should be addressed by a comparison of this and existing hydrogen generation technologies.
- The project team should consider expansion of the tests on the type of fuels used, especially biomass and coal.
- The project team should develop metrics/success criteria and test protocols.
- The level of detail and rigor in the cost analysis is critical to assess the true status of the technology, and should include such factors as system degradation and stack life.

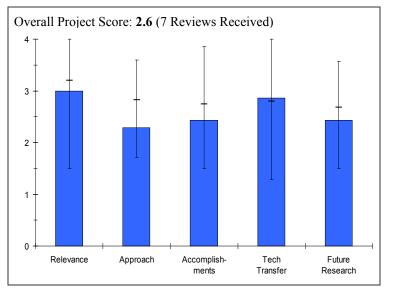
Project # FC-48: Silicon Based Solid Oxide Fuel Cell for Portable Consumer Electronics

Alan Ludwiszewski; Lilliputian Systems, Inc.

Brief Summary of Project

The objective of this project is to improve the cost, durability, and performance of the MEMS-based solid oxide fuel cell (SOFC) technology for consumer electronics applications. Project objectives are to 1) increase the MEMS SOFC array power density toward a level sufficient to support a commercial product launch; and 2) improve vacuum sealing materials and processes to extend lifetime at higher operating temperatures.

<u>Question 1: Relevance to overall DOE</u> <u>objectives</u>



This project earned a score of **3.0** for its relevance to DOE objectives.

- There is a great need for increased energy density in power sources for portable consumer electronics. Fuel cell technology will allow longer operation times than a battery system, so there is an opportunity here to support the main objectives of the Hydrogen Program. Nevertheless, Lilliputian technology competes with direct methanol fuel cells (DMFC), which have made great progress and operate at room temperature. The PIs need to demonstrate and openly document high energy density, low cost and long life over and above DMFCs.
- The project focuses on the development of silicon-based SOFCs for portable consumer products and fully supports DOE RD&D objectives.
- This project supports the DOE Hydrogen Program's 2010 consumer electronics goals; however, it is difficult to see how this work supports national energy goals and interests security, availability, cost, and environmental.
- The subject of the project (portable SOFC power systems) is relevant to DOE objectives.
- It is not at all clear what role portable electronics plays in the hydrogen or R&D objectives.
- DOE Hydrogen Program stated objectives include development and demonstration of cost-effective, reliable, durable fuel cells for portable power applications.
- Initial product targets are below DOE 2010 targets for sub-50 W systems.

Question 2: Approach to performing the research and development

This project was rated **2.3** on its approach.

- There must be a practical limit to the cell size where current path length and heat integration give way to the small cell area. Generally, the larger the cell area, the cheaper the materials cost is until high current cannot be transferred out of the stack. It is not clear how well MEMS technology can achieve cost targets with so many small, interconnected units.
- Will the large MEMS fuel cell array depicted on slide 5 have a significant heat disposal requirement? What has been done to model and design for this?
- The fuel-type and cathodic activity determine the SOFC operation temperature. How do fuel impurities affect operation? How is the air and fuel flow controlled for each module? There is a significant materials issue preventing the silicon substrate from oxidizing. What is the role of the silicon substrate, is it really needed?
- It was unclear how cell performance and sealing would be improved; no details were given on approaches to address these issues.
- 1-25 W range for consumer electronics is not the optimal application for a high-temperature fuel cell. An assessment of the cost entitlements should show that.

- The work plan to achieve the specific objectives (higher power density and improved vacuum sealing) was well organized and consistent with other aspects of the technology.
- Seal work is detailed but not pursuing any new concepts. Clearly looking crystallized glasses; which has proven to largely be a dead end. The project is at a very low level of maturity. Much work needs to be done.
- Lilliputian Systems' MEMS-based SOFC technology could be a scalable, cost-effective, environmentally robust approach to addressing the consumer electronics application.
- The project team has an excellent understanding of markets.
- There are 192 cells in the array.
- The team used an electrical heater to start up the device. A 4-minute start-up time may be too long.
- No thermal cycling and degradation data discussed. 300 thermal cycles were attained of the necessary 3000 thermal cycles.
- SOFC component materials were not discussed.

Ouestion 3: Technical accomplishments and progress toward project and DOE goals

This project was rated **2.4** based on accomplishments.

- It seems that this technology has not progressed very far since 2002. Specific cell and stack performance information would allay this suspicion. What is the power density or power output? What do polarization curves look like? What is the fuel utilization and what happens to the heat from excess fuel?
- The issue of vacuum sealing is a difficult problem with an operating 800°C device in close proximity to the vacuum seal.
- Progress has been made on improving cell power but significant challenges remain on sealing.
- 300 thermal cycles have been completed to date. Seal degradation 250-hour life, need at least 2 khr. Apparently a modified glass composition was developed; however, it could not be tested in the timeframe of the project.
- It appears that increased power density was obtained, although it's not clear if the achieved power density is sufficient for the proposed application. Also, power degradation rates should have been addressed in the presentation. Sealing obviously remains problematic, and it doesn't appear that the authors have identified a viable sealing material at the present time. Finally, it's hard to tell if the proposed technology can be cost-effective.
- Considering it would normally take several hundred million dollars to develop a relatively new fuel cell design, this project is at the expected level of low maturity. Nothing was said about thermal issues, which would be a major question in this size. Self-sustainability is very tenuous and potentially reduces efficiency substantially. However, good detailed work on a few aspects such as producing the silica backbone and seals although ultimately the glass approach has been more or less shown to be a dead end.
- Significant progress in very difficult undertaking was made in:
 - Increasing array power density (2.5x) toward that of button cell benchmarks (this is major accomplishment now at low end of commercial product);
 - Exceeding the target of 50% power improvement with improvement of 85% attained;
 - Implementation of automated dispense equipment with custom control enhancements, increased throughput, and improved repeatability;
 - o Improvement of vacuum seal temperature/lifetime performance;
 - o Improved understanding of die/sealing glass interactions; and
 - Manufacturing fuel cell chips with the improved processes and a 2.5x improvement in power.
- The total current tested lifetime was not discussed. Items like cooling and fuel utilization were not discussed. Butane fuel processing was not discussed.

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated **2.9** for technology transfer and collaboration.

- Alfred and MS&T are helping with the vacuum sealing and electrode issues. No original equipment manufacturers (OEM) have been identified who will provide production capacity and cost reductions.
- Alfred University and Missouri S&T bring excellent credentials with respect to glass science and sealing.

- The collaboration with partners appears to be well coordinated and productive.
- Alfred University and Missouri S&T provide excellent SOFC component support. There has been no industry interaction.
- The project team has partnered only with universities: Alfred University, Missouri S&T, and no industrial partner.

<u>Ouestion 5: Approach to and relevance of proposed future research</u>

This project was rated 2.4 for proposed future work.

- It is not clear how much the performance needs to be improved to achieve a viable product. The PI is retaining important performance data in order to be able to determine where the main issues lie.
- Scale-up to volume production may be too early? It is unclear whether all the issues relating to manufacturing have been resolved.
- This project is complete. Future work should focus first and foremost on cost if everything worked well, is this application of SOFC technology economically viable? Does it offer significant advantages over other existing and under-development technologies for the application?
- Not much detail was provided regarding future work, but it makes sense for the focus to remain on power density (and stability) and sealing quality.
- Several hundred million dollars in development is likely pending. The project team is nowhere near having a product as implied.
- Project complete.
- The target first product is a USB charger capable of delivering 2.5 W with the following single cartridge performance: power density: >25 W/l; energy density: >500 Wh/l; and run time per cartridge: >30 h.

Strengths and weaknesses

Strengths

- For applications with extremely small power requirements (mW levels), this technology may become viable.
- SOFC power densities should be larger than other technologies if the operation temperature of 700°-800°C can be successfully contained in such a small space.
- The tiny cell size could makes it easier to increase voltage output without losing power by minimizing current path lengths.
- Cell design and manufacture.
- Understanding of customer requirements.

Weaknesses

- It is not clear from this presentation that the technology can be scaled large enough to provide 3 4 W of net power.
- It is not clear how the heat is disposed for large 22 x 8 cell arrays.
- It is not clear which fuel has been demonstrated with the technology. Has butane been demonstrated?
- Approaches to address technical barriers are unclear.
- Seal stability and isolation from silicon structure (interaction between silicon structure and the SOFC) is a key issue.
- Low power density.
- No industrial partner.

- The PI needs to be more forthcoming with performance data.
- The PI needs to state clearly how this particular technology can meet performance requirements because of their design, materials and methods.
- Emphasis on establishing all of the key cell operating characteristics is recommended.

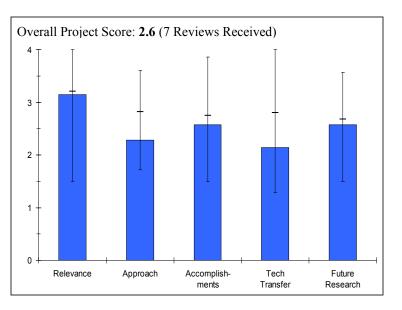
- Future work should focus first and foremost on cost if everything worked well, is this application of SOFC technology economically viable? Does it offer significant advantages over other existing and under-development technologies for the application?
- Focus on durability and stability, if the economics justifies the application.

Project # FC-49: Biogas Fueled Solid Oxide Fuel Cell Stack

Praveen Cheekatamarla; NanoDynamics Energy, Inc.

Brief Summary of Project

The main objective of this project is to develop and demonstrate a 400 W stack module using advanced solid oxide fuel cell (SOFC) technology. Specific objectives include 1) electric power generation from different biogas compositions; 2) costeffective SOFC manufacturing; 3) increased energy efficiency; and 4) the capability to integrate in to commercial systems such as micro combined heat and power and portable power. A new SOFC fabrication route was successfully implemented. Future work will focus on thermal shock resistance and long-term endurance of the SOFC operated on biogas.



<u>**Ouestion 1: Relevance to overall DOE**</u> <u>objectives</u>

This project earned a score of 3.1 for its relevance to DOE objectives.

- This project using a renewable fuel source coupled to SOFC electrical generation is relevant to the goals and objectives of the Fuel Cell Program.
- The use of biogas as fuels for SOFCs is a critical move to demonstrate that SOFCs can be an efficient green technology. This project helps expand the scope of the Hydrogen Program.
- The project fully supports DOE RD&D objectives.
- It is not clear which of DOE Hydrogen Program's fuel cell goals this project is pursuing the "low weight" and thermal cycling suggest a truck APU. But if that is the case, why biogas?
- This project is relevant to DOE objectives (i.e., fuel cell technology for portable power, renewable energy).
- Presumably, the DOE Biomass Program has a use for such a fuel cell. Certainly, the U.S. Department of Agriculture (USDA) does in rural areas. Relevance to the Hydrogen Program appears tenuous.
- The project supports DOE EERE through:
 - Research and development of advanced fuel cell technology for portable power applications;
 - Renewable energy-biogas is a domestic, renewable resource, which offsets the use of non-renewable resources with corresponding emission reduction and energy security benefits; and
 - Viable, cost effective process for efficient power generation.

Question 2: Approach to performing the research and development

This project was rated **2.3** on its approach.

- The technical approach adopted in this project focuses on the development of advanced SOFC technologies coupled with a biogas fuel input. The approach includes design, fabrication, and testing of a complete power system.
- Most of the project effort is spent on developing a tubular SOFC "stack" or module. Tubular SOFC designs are interesting because of the ruggedness of individual tubes and the elimination of seals. The major problem with tubular cells is economically interconnecting tubes together to increase voltage output.
- The major point of the project is the use of biogas to fuel SOFCs. Is there a need to develop an integrated fuel processor to generate biogas from bio-solids? Are there potential partners who could help address this important issue?

- Approaches to performing the work are reasonable. Ways to improve fabrication yields need to be developed.
- The project identifies cell yield as a barrier; however, based on the presentation, it is in no way evident what is novel about this SOFC technology that causes there to be cell fabrication yield issues.
- The approach is to fabricate "lightweight" cells, but no comparison or reference is provided.
- Critically, the approach does not address cost in any meaningful way.
- Emphasis on optimization of fabrication yields seems premature. It's more important to focus on fundamental challenges (performance degradation over time, increasing fuel utilization, thermal cycle stability, demonstration of 400 W stacks).
- Statements of approach were highly generalized and unsubstantiated; therefore the reviewer was not able to render a judgment.
- The project team identified most barriers. The team is somewhat inexperienced.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated 2.6 based on accomplishments.

- Good progress since the beginning of the project at the start of FY09. Advances in performance, using H₂ fuel, are impressive. Operation on synthetic biogas will require additional optimization.
- The technical accomplishments that have been made so far are designing, fabricating and testing single cells in hydrogen and simulated biogas. Single cell performance is good, >0.525 W/cm², assuming the cell voltage is not less than 0.7 V. Stack design and building is in the early stages. The real test will come in interconnecting cells into bundles or modules. A 400 W stack will need a minimum of 42 cells. The PIs should give more information on standard operation metrics (e.g. fuel utilization, polarization curves, or current at 0.7V) to demonstrate that cell performance meets DOE objectives.
- Technical achievements include electrode material and microstructure optimization, biogas testing, and stack operation. Current cell fabrication yields (at about 50%) are too low and need to be improved.
- Presentation of power and volumetric density does not address the balance-of-plant (BOP), which is substantial in terms of volume and weight. No comparison to other SOFC technologies is presented. How does this compare to the state of the art? The power density of >500 mW/cm² on a button cell is not impressive in this regard, even on biogas. Power and efficiency numbers appear to be presented on a stack basis. They have little bearing on ultimate system performance, given that state-of-the-art SOFCs can operate at very high fuel utilizations and voltages with economically viable power densities. In this case, a meaningful discussion of cost is not presented.
- Thermal cycling performance appears good although this may be only a button cell, in which case it means little in regards to full system cycling capability.
- Progress has been made, but performance over time and the ability to scale up to stack level have not yet been adequately addressed.
- Technical accomplishments were highly generalized and contained no specific information to review. Some volumetric power density data was presented but it was based on single cell volumetric power density, which is fairly irrelevant given that most of the volume will be BOP. Areal power density would be relevant but not reported. Information presented is very vague.
- New SOFC fabrication route was successfully implemented. This process offers numerous benefits over conventional methods: cost effective, automated, lightweight fuel cells with high energy efficiency.
- SOFCs with high volumetric (3.4 kW/liter), gravimetric (2.56 kW/kg), and specific power densities (0.63 W/cm²) were fabricated and tested on hydrogen and biogas. Is this SOFC only single cell? Tubular design is not correctly accounted for.
- SOFC cells demonstrated up to 50% and 40% electrical efficiencies on hydrogen and biogas respectively.
- There is only 32% stack/system efficiency on H₂.
- However there were achievements:
 - \circ Achieved >525 mW_e/cm2 producing >9.5 We on biogas;
 - Thermal shock tests: 120 cycles conducted; and
 - Endurance tests: 250 hours achieved.
- Unfortunately, there is a 12-16% drop in power with biogas as the fuel. There is only 26% efficiency.
- Stack/cell design, sizes, and fuel utilizations were not adequately identified.

<u>Ouestion 4: Technology transfer/collaborations with industry, universities and other laboratories</u>

This project was rated **2.1** for technology transfer and collaboration.

- Collaboration consists primarily of a university partner who provided analytical support for the project. Other collaborations, including a user community representative, would be useful.
- The State University of New York (SUNY) at Buffalo partner is not a subcontractor. This project could use system development partners, especially in the reforming of biomass to biogas.
- The only collaboration is with SUNY on an as-needed basis.
- The project uses some university support on an as-needed basis; otherwise, all work is done in house.
- Informal collaboration only with SUNY.
- Virtually no collaboration. However, it is commendable that the project procures microanalysis as needed.
- Collaborations were limited to SUNY.

<u>Ouestion 5: Approach to and relevance of proposed future research</u>

This project was rated **2.6** for proposed future work.

- Plans for future work appear to be adequate, although the design and testing of the 400 W stack will be challenging and new technical issues will likely be encountered.
- The stated next steps of this project are to demonstrate long-term cell performance and to collect tubular cells into modules with high power output. More importantly, a critical step should be to show that real biogas, including all its impurities, can be internally reformed in this SOFC system while maintaining high power output. The project team should have better addressed how it plans to accomplish these important tasks.
- The purpose of certain proposed tasks is unclear:
 - Fabricate 150 cells with integrated catalytic layer (what is the justification for the number?); and
 - CFD analysis of 1.2 kW (is the focus is on 400-500 W stacks?).
- Future work should focus primarily on durability (long steady-state run times), degradation (which was not discussed), and particularly cost.
- The proposed future work is okay overall, except for emphasis on fabrication yield.
- Determining what barriers exist is very difficult, but list of future actions is reasonable.
- Plans are probably aggressive:
 - \circ 400 W stack build 11/2009;
 - CFD analysis of 1.2 kW stack –10/2009; and
 - Stack feasibility demonstration on biogas.

Strengths and weaknesses

Strengths

- Good cell performance in simulated biogas.
- Good thermal cycling performance of single cells.
- Cell manufacture.
- Electrode materials and microstructures.
- Stacks operating on biogas.
- Achieved $>525 \text{ mW}_{e}/\text{cm}^{2}$ producing >9.5 We on biogas. Utilization and cell/stack size is unclear.

Weaknesses

- No provision is made for demonstrating cell/module performance in real biogas.
- No clear design is mentioned on how cells will be bundled to increase voltage output without loosing power or thermal cyclability.
- Cell reproducibility and long-term stability not well defined.
- Overall, too little information was presented about the cell construction and materials to permit a full assessment of performance and cost potential.
- There is little endurance testing.

• The lack of experience presents a possible challenge in building large stacks.

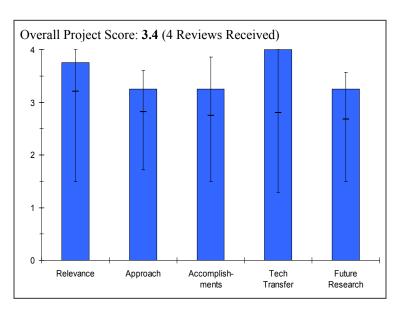
- The project team should incorporate plans to study operation on actual biogas; e.g., biogas from water treatment operations.
- The project should be expanded to include biogas production method and demonstration of technology using real biogas
- The project team should focus on long-term operation (at least 1000 hrs) with demonstration of no coking on biogas.
- Future work should focus primarily on durability (long steady-state run times), degradation (not discussed), and particularly cost.

Project # FCP-02: Component Benchmarking Subtask Reported: USFCC Durability Protocols and Technically-Assisted Industrial and University Partners

Tommy Rockward, Rod Borup, and Fernando Garzon; Los Alamos National Laboratory

Brief Summary of Project

This task supports LANL technical assistance to fuel cell component and system developers as directed by DOE. This task is expected to include testing of materials and participation in the further development and validation of single cell test protocols. This task also covers technical assistance to the U.S. Council for Automotive Research (USCAR) and the USCAR/DOE Freedom Cooperative Automotive Research (FreedomCAR) Fuel Cell Technology Team. This assistance includes making technical experts available to the Technical Team as questions arise, focused single cell testing to support the development of targets and test protocols, and regular participation in working and review meetings.



Question 1: Relevance to overall DOE objectives

This project earned a score of **3.8** for its relevance to DOE objectives.

- This program supports the DOE R&D objectives.
- It is important to provide consistent measurement methodology/protocol to pursue fuel cell R&D.
- Support for developers from national labs is important to maintaining a highly scientific approach while keeping characterization and analysis costs within a reasonable budget for those developers that cannot afford in-house equipment and dedicated personnel.
- The project fills a void in the Hydrogen Program by making advanced testing and analytical procedures available. The LANL fuel cell team has the expertise to assist other research organizations.

Question 2: Approach to performing the research and development

This project was rated **3.3** on its approach.

- This project provides a wide variety of support to companies and universities engaged in fuel cell R&D.
- Basically, the team is consulting as required.
- Activity to standardize testing methodology/protocols would be good.
- The approach appears to be to wait for DOE or others to contact LANL for assistance. LANL could be more proactive and identify those researchers having limited capabilities and offer assistance to them.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated 3.3 based on accomplishments.

- This project has supported many important efforts.
- The presentation/poster identified a number of interactions that produced positive and beneficial results to other research organizations. The examples for analytical capability are impressive.

<u>Ouestion 4: Technology transfer/collaborations with industry, universities and other laboratories</u>

This project was rated **4.0** for technology transfer and collaboration.

- Excellent collaboration.
- Excellent collaboration with a wide range of partners and institutions.
- There are a large number of collaborators.

Question 5: Approach to and relevance of proposed future research

This project was rated **3.3** for proposed future work.

- The project team has a good plan. The approach builds on current successful interactions.
- New.
- Future work is not identified on the charts. Holding a class in 2009 appeared to be the only planned future work.

Strengths and weaknesses

Strengths

- Excellent collaboration.
- This project provides a wide variety of support to companies and universities engaged in fuel cell R&D.
- Testing and consulting capability.
- Experienced researchers and facilities at LANL.

Weaknesses

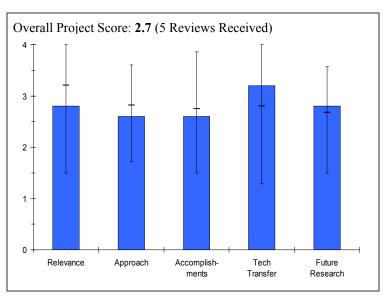
• The project team needs to focus on future work.

- The project team should develop standardization of measurement methodology and protocols for fuel cell materials evaluation.
- The project team should continue this activity and become proactive in support of other Hydrogen Program projects.

Project # FCP-03: Research & Development for Off Road Fuel Cell Applications *Richard J. Lawrence; IdaTech*

Brief Summary of Project

The objectives of this project are to 1) have Toro measure loads and report vehicle modifications and specifications, 2) report on shock and vibration profiles and lifetime, 3) complete shock and vibration of the fuel cell system, 4) have Donaldson measure contaminants and develop an air filter, and 5) install a proton exchange membrane liquid-fueled system in a golf course maintenance vehicle. The critical assumptions for this project are that the fuel cell system can 1) physically fit into the vehicle, 2) can provide the required energy during field-testing, and 3) function under applications' shock and vibration loads. Potential solutions include 1) modifying the vehicle, 2) improve controls and response;



and, 3) incorporate shock and vibration test results.

Question 1: Relevance to overall DOE objectives

This project earned a score of 2.8 for its relevance to DOE objectives.

- This project provides off-road demonstration of a methanol fuel cell maintenance vehicle.
- Fuel cell demonstrations in a real-world, near-term application are important to outreach and support commercialization of fuel cells.
- This project is relevant to the DOE Fuel Cell Program in that it provides a demonstration of the technology in a near-term application and can potentially provide feedback to the materials development efforts within the DOE program. Reforming technology will likely become more important in the DOE program for stationary applications. The project addresses issues related to air filtration and shock and vibration.
- The project pursues the goal of an early market introduction and penetration. Additional scientific goals are not pursued.
- Objectives A through E are not addressed.
- The project could align with most aspects of the Hydrogen Program and DOE RD&D objectives, but as presented the information would not be very supportive of the Hydrogen Program.

Question 2: Approach to performing the research and development

This project was rated **2.6** on its approach.

- The vehicle uses an IdaTech 3-kW methanol fuel cell. (R&D on this existing technology started in 2004 and was stopped in 2005.) A maintenance crew uses the vehicle at a golf course. The fuel cell was already developed using DOD funding, so the project made good use of the existing system. Shock and vibration testing provided useful data.
- Golf course maintenance vehicles are a good near-term market that can help increase fuel cell sales volume and therefore reduce cost.
- The approach is practical, which keeps the project simple. The project uses existing technology developed at IdaTech and modified it for this application. The poster did not present air filtration and shock and vibration targets and how well IdaTech met them. The engineering of the system in the vehicle appeared to be well done.

- The project focused on making a system work, and the system was successfully proven to work. Though the system works as a hybrid advanced design, methods for determining the battery size versus the fuel cell size were not applied. An average systems efficiency of 40% was stated, but not substantiated.
- From a market introduction point of view, the project focuses on a very reasonable application.
- The approach was not clearly stated in the presentation. The approach appears to be to install a fuel cell in a golf maintenance vehicle and drive it around the golf course.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated 2.6 based on accomplishments.

- The project team has obtained about 60 hours operation on a golf course (start/stop, not continuous). A lot of spurious shut down problems have hindered data collection. Many wiring problems have been encountered. Voltage and power curves were obtained, but they are not very understandable.
- The testing was performed under realistic conditions.
- The vehicle is up and running on a golf course. Operating data is being acquired that will assist in further development of the power plant. The intended customer Toro is actively involved in system definition. Data showing the effectiveness of the air filtration would be helpful.
- The system was proven to work.
- Fuel cell performance was measured, but were strain gauges attached to the fuel cell system? What was the level of vibration? What methods were used to dampen the vibration or shock to the system? The technical accomplishment presented was "see it works." This is not at the level of understanding of why it works. There is no data on fuel or fuel efficiency.

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated **3.2** for technology transfer and collaboration.

- There have been interactions with Toro, although Toro is not really an active participant. University of California at Davis (UC Davis) is a partner. Rivers Edge golf course provides a demonstration site.
- Collaboration appears to be good. Toro is actively involved in developing the definition and specification for the final commercial product. However, what is not clear yet is whether or not the fuel cell maintenance vehicle will be commercially viable. UC Davis performed shock and vibration testing on a vibration table.
- A good industry consortium exists, yet the approach left the impression of being too practical not sufficiently making use of existing cutting edge design insights and tools. An academic partner might help improve this weakness. The potential role of that institute is suggested to be control and hybridization of fuel cells.
- There has been outstanding collaboration within the scope of the effort.

Question 5: Approach to and relevance of proposed future research

This project was rated 2.8 for proposed future work.

- The project team will do public outreach at the upcoming Bend High Desert Conference. On-board data acquisition will be installed this year and should provide better quality data, 24 hours per day. The project team wants to get into parks and recreation.
- The additional testing planned appears to be appropriate. A second-generation system will be built that will incorporate learnings from the vehicle currently undergoing testing. Design for manufacturability will be developed with input from Toro.
- The project is basically finished. Insofar, this point is not really relevant any more.
- What barriers are being addressed by the future work? How will this effort be calibrated? What will full time data acquisition acquire; vibration data, shock data, or fuel cell performance data?

Strengths and weaknesses

Strengths

- The project team uses fuel cells developed under government funding. Some good public outreach. Lots of electrical problems have been encountered and this provides insight into the use of "already developed" equipment.
- The is a near-term application.
- So far, the project has developed and tested hardware in a maintenance vehicle on a golf course. A second-generation vehicle is planned.
- There has been strong industrial cooperation, which even survived a period in which DOE did not fund the technology.
- IdaTech makes a good fuel cell system.

Weaknesses

- More systems are needed to provide a "real" test.
- Only one ultimate user is represented on the team.
- The team has used a very industrial trial and error approach.
- What fuel was used? The project team claims liquid fuel was used, but the type of fuel used was not provided in the presentation. The presentation did not answer the questions required by DOE (e.g., future work did not identify barriers). What were the performance indicators for the technical accomplishments?

- The project team should get information on cost objectives commercialization plan none was presented. For continued funding, this should be made clear.
- The project team should evaluate whether controls and battery selection (type, size) can be improved to reduce cycling of the fuel cell stack, and therefore improve its life.
- The project would benefit from more input by the ultimate user community (e.g., golf course superintendents and other building owners). If the community is enthusiastic about the vehicle, it would strengthen the business case for Toro.
- The project team should add an institute to the project with practical experience in control and hybridization of fuel cells.
- This program needs a major overhaul. Vibration and shock data should be quantified. Fuel efficiency needs to be identified. Design characteristics for dampening shock and vibration should be discussed.

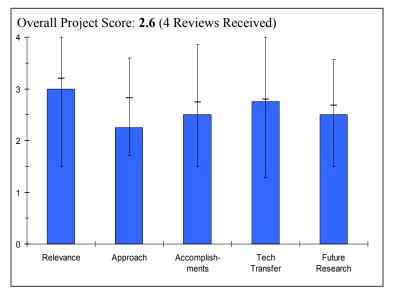
Project # FCP-04: Renewable and Logistics Fuels for Fuel Cells at the Colorado School of Mines

Neal P. Sullivan, Robert Braun, Anthony M. Dean, Robert J. Kee, Ryan O'Hayre, and Tyrone Vincent; Colorado School of Mines

Brief Summary of Project

Objectives for this project are to 1) develop solid oxide fuel cell materials for robust operation on diesel fuel; 2) identify optimal hydrocarbon fuel reforming strategies; 3) create thermally stable fuel-reforming catalysts and supports; 4) employ system modeling to optimize auxiliary power unit configurations; and 5) utilize modelpredictive control to integrate system hardware.

<u>Question 1: Relevance to overall DOE</u> <u>objectives</u>



This project earned a score of **3.0** for its relevance to DOE objectives.

- Multitask (5 different groups) solid oxide fuel cell (SOFC) auxiliary power unit (APU) systems for heavy vehicles. Improve performance, increase efficiency, and develop understanding of thermal management and transient operation.
- SOFC APUs are relevant to the Hydrogen Program.
- The project includes different tasks that address various aspects of operating solid oxide fuel cells on diesel or biofuels, including sulfur tolerance, tar-free fuel reforming, and durable reforming catalysts and supports.
- General objective of broadening fuels suitable for SOFCs is certainly relevant. DOE's refocus on stationary, portable, and auxiliary power in the near term increases the project relevance.

Question 2: Approach to performing the research and development

This project was rated 2.3 on its approach.

- Develop new SOFC materials for greater durability and robust operation using low sulfur diesel fuels. Evaluate various fuel reforming and integration strategies. Do cell and stack modeling to understand operational characteristics, thermal management. Translate physics-based models into system models. Optimize APU configuration and performance. Projects attempts to do wide-ranging fuel cell APU effort, and ultimately bring results from different groups together to improve fuel cell APUs using diesel fuel.
- The approach seems similar to work performed under SECA- investigation of non-nickel catalysts, modeling efforts, etc.
- The heat exchangers efficiency was surprisingly low improving this should be a top priority.
- There are two significant barriers to SOFC: durability and cost. The project is examining only durability. It would be more applicable if the project team could quantify how its improvements in durability and efficiency will help in cost reduction.
- The project team does not seem very focused. The team is modeling two similar but different reforming approaches: CPOx and ATR. The team is also trying to develop catalysts for two very different fuels: diesel and biomass tar.
- The project is exploring nickel-free anodes for sulfur tolerance, and barrier layers for durability.
- It is not clear how proton-conducting ceramics fit the overall project objectives; such proton conductors operating at 400°-700°C would require a very significant effort to develop effective non-precious-metal cathode electrocatalysts. Also, a proton-conducting fuel cell would require a very different system configuration from

that of an oxide-ion-conducting fuel cell, since the product water would be produced on the cathode side rather than the anode side.

- Reaction modeling is being used to understand, and then inhibit, the formation of tar (high molecular weight compounds) during fuel reforming. Thermally stable supports and catalysts are being studied for activity and durability.
- System modeling is being used to identify opportunities for system performance improvements.
- Activities within subtasks seem appropriate. However, the project scope is likely too broad to significantly advance the state of the art. The project proposes to explore everything from fuel reforming and fuel cell catalysts (and reforming catalyst supports), to operating strategies, to system modeling, to model-predictive control of operating systems.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated **2.5** based on accomplishments.

- The project team developed improved microstructures for LSCM anode materials and evaluated protonconducting electrolytes. The team modeled an ethylene kinetic model for APU conditions and showed underpredicted CH₄ and over-predicted C₄H₆. Better understanding was gained on how to prevent deposit formation through better upstream mixing. The team synthesized catalyst supports and new catalysts that resist deactivation at high temperature. The team developed a better understanding of inefficiencies in system using CPOX reforming, recuperator, SOFC APU. The team also developed a better understanding of thermal management – this is the best part of this project. The team performed single tubes response modeling using simplified predictive control model.
- The data indicates that the catalysts selected do not perform very well.
- Progress from last year is difficult to determine, since no baseline data was presented.
- This project is only about halfway through its scheduled term. Therefore, complete results are not in yet. Some of the desired materials structures have been obtained but the materials have not been tested for activity.
- Modeling of the reforming processes is yielding useful insights into the factors and parameters that promote (and inhibit) tar formation, such as unsaturated and aromatic precursors and imperfect mixing of reactants.
- Fuel cell and system modeling is also providing helpful insights into potential for system-level improvements and process control.
- The short time since the project started and the overly broad scope (lack of focus) have led to limited results to date.

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated 2.8 for technology transfer and collaboration.

- The project team interacted with three companies: Protonex (provides data), Reaction Systems (provides catalysts), and CoorsTek (low-cost materials processing). However, there wasn't any strong collaborative research and it is not clear how results are transferred to industry that would do commercialization.
- There appears to be good collaboration between the team participants.
- In addition to several co-investigators at the Colorado School of Mines, the collaborators include an industrial SOFC developer, a catalyst developer, and a major ceramics supplier (for the proton-conducting materials development task?).
- Collaboration and coordination appears good at the project level, but it may be limited within subtasks.

<u>Question 5: Approach to and relevance of proposed future research</u>

This project was rated 2.5 for proposed future work.

• The project team plans to continue to evaluate next generation SOFC materials, including new anodes and new proton conducting electrolytes; expand reforming strategies and experimental evaluation of feed gases, such as toluene; and conduct catalyst aging and stability tests. The team will perform CFD modeling of systems and

propose optimal configurations of liquid fueled SOFCs. The team also plans to further evaluate and refine system control models.

- It is good that they intend to begin examining long-term durability.
- It is unclear whether the project team has a catalyst that is active enough to warrant long-term testing. The team may benefit from screening a few more candidates while performing long-term testing on the best so far.
- The project team needs to improve the heat exchangers.
- The project team has not demonstrated a suitable catalyst for diesel reforming, yet it intends to begin investigating catalysts for a more difficult fuel (biomass tars). The team needs to focus its effort. If this is for a diesel truck APU, then the effort should focus on diesel.
- The materials prepared in Task 1 will be characterized in terms of some of the performance characteristics. There is little or no indication, however, of how the performance will be improved.
- In Task 2, a combination of reaction modeling and experimental validation will be pursued to define the conditions necessary for fuel reforming without tar (or coke) formation.
- The catalysts' reforming activity will be characterized in Task 3, along with aging tests, but there was no discussion of how catalyst improvements will be achieved.
- In Tasks 4 and 5, efforts will continue to improve the performance and control models. The effectiveness of some of the approaches, such as high-fidelity CFD modeling or modeling for "robust operation," is not clear within the context of the overall tasks.
- The subtask plans are good, but at the overall project level, this effort is likely too unfocused to succeed.

Strengths and weaknesses

Strengths

- Good academic groups are present in most areas of this project.
- The project is well funded. The modeling work is interesting.
- The project is following a multi-prong approach to address different aspects of diesel and biofuels-based fuel cell systems.
- The project team is working with industrial companies that are developing ceramics, catalysts, fuel cells, and systems. Thus, any materials or process improvements achieved in the laboratory can be tested out in an operating platform.
- This is a multi-disciplinary team with appropriate test equipment and use.

Weaknesses

- This project is very spread out and difficult to coordinate. The project team has used a scatter approach that attempts to cover most aspects of fuel cell APU. Newer proton conducting materials will take a long time to bring to commercialization. There is no commercialization plan. There is no real plan for long-term testing.
- The project team lacks focus. The team should select one fuel and select one reformer technology [autothermal reforming (ATR) or catalytic partial oxidation (CPOX)].
- Amount of progress on catalyst work is unclear. The Protonex APU (600 W) seems low power for a truck APU where 1 5 kW would be more reasonable.
- One weakness appears to be the activity investigating proton-conducting electrolyte materials. As mentioned above, if such materials are developed successfully, very substantial additional developments will be needed in electrocatalysts, fuel processing, and system configurations. It would not be a simple transition from an oxide-ion conducting fuel cell system to a proton-conducting fuel cell system.
- Project scope is too broad to advance the state of the art.

- The project team should focus the project into one or two areas probably thermal modeling. More collaboration with industry and transfer of results are needed.
- If this is for a diesel truck APU, then the team should focus on diesel and not get distracted by examining a fuel that will never be used in the vehicle application. Biomass tars are cleaned up in the biomass gasification process so they do not foul the rest of the system. The team should focus its modeling efforts on a single reforming technology (ATR or CPOX). The team needs to consider larger systems for a truck APU since 600 W is too small.

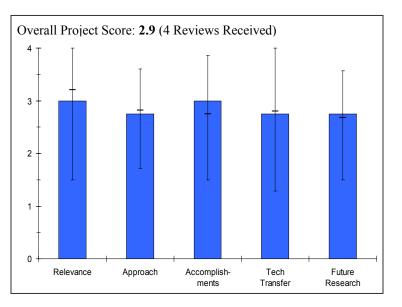
- Finally, the Solid State Energy Conversion Alliance (SECA) program did a lot of work in this area. The project team should engage some of the prominent SECA participants to benefit from past work.
- The overall program appears to be structured well, with the exception, perhaps, of the subtask on developing proton-conducting ceramics for use as the electrolyte in ceramic-based fuel cells.
- The project team should focus down to one or two closely related tasks.

Project # FCP-06: Fuel Cell Research at the University of South Carolina

John W. Van Zee; University of South Carolina

Brief Summary of Project

The objectives of this project are to 1) develop novel materials (e.g. Nb-doped) for improved corrosion resistance and improved fuel cell components; 2) develop a fundamental understanding of performance loss introduced by fuel contaminants and durability loss fuel induced by contaminants; 3) develop a fundamental understanding of the degradation mechanisms of existing gaskets and the performance of improved materials; 4) develop a fundamental understanding of acid loss and acid transport mechanisms; and 5) predict performance and lifetime as a function of load cycle.



<u>**Ouestion 1: Relevance to overall DOE**</u> <u>objectives</u>

This project earned a score of 3.0 for its relevance to DOE objectives.

- This project is concerned with the durability of stack components, cost of catalysts, electrodes and seals, and hydrogen quality.
- Corrosion resistive catalyst support is important area to improve membrane electrode assembly (MEA)/catalyst durability.
- Non-platinum group metal (PGM) catalyst can be a transformational technology for fuel cell commercialization.
- The project is addressing issues of stable non-carbon supports for electrocatalysts, fuel impurity effects on fuel cells, seal durability, and water vapor adsorption/desorption in PBI-based high-temperature polymer electrolyte fuel cells.
- All of these tasks are important for fuel cell development, except that the task on hydrogen impurity effects applies primarily to transportation fuel cell systems, and the task on water sorption in polybenzimidazole (PBI)-based MEAs applies only to non-automotive systems.

Question 2: Approach to performing the research and development

This project was rated 2.8 on its approach.

- It appears that DOE selected four subprojects on durability of seals, development of non-carbon catalyst supports, H₂ impurity effects, and characterization of PBI-H₃PO₄ membranes.
- The project team needs to identify rationale for titania-based materials selection for catalyst support.
- The project team needs to more specifically identify what kind of modeling development could be pursued for H₂ quality.
- Generic characterization of seal materials is good.
- This project is investigating doped-titania as electrocatalyst supports as potential replacements for carbon.
- The impurity effects task has focused primarily on carbon monoxide (and more recently on CO plus ammonia), which has already been investigated at length by others.
- In the task on gasket/seal durability, the project is essentially characterizing the aging performance of commercial sealant materials, with the objective of predicting seal life, rather than developing improved sealant materials.
- For the PBI water and acid loss measurements, the project team has devised an experimental apparatus specifically suited for these measurements.

Ouestion 3: Technical accomplishments and progress toward project and DOE goals

This project was rated **3.0** based on accomplishments.

- The project is wrapping up. The tasks on gaskets and seals and non-carbon supports have been completed. The project has collected and published data on the effects of CO and NH₃ in fuel hydrogen. The project has also developed techniques for the measurement of isotherms and rate constants for interaction of water vapor with PBI-H₃PO₄.
- More analysis is necessary for alternative catalyst support data and investigation of performance enhancement.
- In the task on carbon-free electrocatalyst supports, a 25atom% Nb content in titania is more than a typical "doping" amount. Also, 4% hydrogen peroxide production is greater than what fuel cell developers would like to see. The project team has observed good performance and, apparently, good stability (preliminary).
- In the task on fuel impurity effects on fuel cells, they have observed slow rates of poisoning by CO, leading to hysteresis in short-time measurements.
- In the task on water sorption in PBI membranes, the team has determined water vapor sorption and desorption rates as functions of temperature. The team has not, however, reported any electrochemical performance or membrane conductivity data.

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated **2.8** for technology transfer and collaboration.

- Each of the four subtasks had significant collaborations and partners.
- The project has extensive collaborations with industry and national laboratories.

Question 5: Approach to and relevance of proposed future research

This project was rated 2.8 for proposed future work.

- The project is in the final stages. The plan is to continue to disseminate results through presentations and journal publications.
- For seal, focus on generic materials characterization for fuel cell seal, not seal concept, such as gasket.
- This project is scheduled to end by October 2009. As such, no additional work is planned in the task on dopedtitania-based electrocatalyst supports and in the task on seal durability.
- The project team will complete the work on CO and combined CO and ammonia poisoning.
- The project team will conduct additional work on water balance measurements in PBI membranes during transient operation of single cells.

Strengths and weaknesses

Strengths

- Qualified PI and team members.
- Extensive experience.
- Good lab facilities.
- Good collaborations.
- Controlled experimental capability for catalyst activities.
- The project has an extensive array of analytical and characterization tools available for the different tasks.

Weaknesses

- The project is a collection of four unrelated subtasks.
- The four major tasks are quite disparate and there appears to be little interaction between them (or among the different groups of researchers addressing the four tasks).
- There was no indication of how the results of this work are being, or will be, used by other researchers or fuel cell developers, except for the task on fuel impurity effects on fuel cell performance.

Specific recommendations and additions or deletions to the work scope

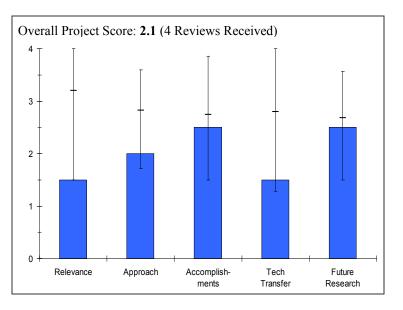
• The various tasks in this project are 90% to 100% complete. Therefore, it is difficult to make any meaningful recommendations for the remaining work yet to be completed.

Project # FCP-07: Development of Kilowatt-Scale Fuel Cell Technology

Steven S.C. Chuang; The University of Akron

Brief Summary of Project

The overall objective of this project is to develop a kilowatt-scale coal fuel cell technology. The results of this research and development efforts will provide the technological basis for developing megawatt-scale coal fuel cell technology. The objective for 2008 was to investigate the factors governing the anode catalyst activity for the electrochemical oxidation of carbon in coal. The objectives for 2009 were to 1) evaluate the long-term anode and cathode catalyst activity as well as interconnect durability; and 2) refine the coal injection and fly ash removal systems.



Question 1: Relevance to overall DOE objectives

This project earned a score of 1.5 for its relevance to DOE objectives.

- This doesn't appear to fit in with the rest of the Hydrogen Program. It appears to fit in with the Office of Fossil Energy (FE) since it uses coal.
- Properties focused on direct electrochemical oxidation of coal, with no hydrogen production or utilization involved. It represents an interesting and potential alternative to coal burning for electricity generation, but it is at its infancy. It does not fit into stationary or early market applications or transportation.
- It is hard to see the relevance of this project to the DOE EERE Fuel Cell Program. If such a coal-fueled system could be successfully developed, it would be more germane to the DOE FE effort. It would appear to apply to larger sized generators. Emissions of CO₂ will be less than from a coal-fired power plant due to increased efficiency, but will still be substantial.
- This project employs solid carbon as a fuel in a solid oxide fuel cell (SOFC) fuel cell, and as such, has little direct relevance to the bulk of the hydrogen fuel/proton exchange membrane (PEM) fuel cell centric DOE program. However, this should not be viewed as a negative, but rather as a positive aspect. This is a novel approach that has potential to be a useful technology and is worth further investigation. If the Hydrogen Program is to be re-focused to consider other fuels and approaches with the potential for greater impact in the near term, then this effort may very well be much more in line with next year's program objectives.

Question 2: Approach to performing the research and development

This project was rated **2.0** on its approach.

- This project uses a high-temperature fuel cell, with direct coal with a saturate H₂O anode feed, Anode catalyst is a large 3-5 micron particle size.
- This is an interesting approach, essentially examining the direct conversion of coal in a high-temperature fuel cell, however the likelihood of success is rather small, and there appears to be no actual data showing that the direct conversion of coal is achievable.
- The concept demonstration is in its infancy. Proof-of-concept still needs to be demonstrated. Many issues remain to be revealed let alone addressed, such as oxygen crossover and anode poisoning.

- The project is overly ambitious for the funding provided. The investigator is focusing efforts on finding stable anode materials in the coal dust environment. However, ash-free coal is planned for a large part of the testing. It is not clear how the fly ash removal system will be able to cope with the fly ash that is released in the reaction.
- At the current stage of development, the project approach is good. The PI is addressing appropriate issues (catalysis, materials development, cell fabrication).

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated 2.5 based on accomplishments.

- 500 hours of durability have been demonstrated with hydrogen.
- The project team is currently using Ni anode and will add Cu + Ce in the future.
- A coal injection system has been designed.
- Durability data to date is questionable as it is not with coal and is not with the catalyst intended for eventual use.
- A large fraction of the funding has been spent already this does not seem to match the timeline or results produced. The major accomplishments appear to be to have identified two significant problem areas of anode poisoning and oxygen crossover, as expected for this crude fuel oxidation.
- For the limited funding and time since the beginning of the project, progress is reasonable. Anode stability over 500 hours has been demonstrated using hydrogen as fuel. A long-term test is planned with low-ash carbon as fuel. Fabrication of the coal injection system and fly ash removal systems is underway.
- The PI is making good progress towards understanding the implications of the unique aspects of this effort. For example, dealing with a solid fuel this eliminates the benefit of a porous, three dimensional electrode structure as is common with gaseous reactants. As a result, a thin, non-porous anode structure is preferred, and is being pursued. This in turn should allow for a lower operating temperature, which will enhance production of CO₂ relative to CO, and simplify the interconnect and sealing issues. The progress along these lines is promising. However, there is still considerable thought needed to address the fuel utilization/fly ash mitigation problems associated with this concept. The solution to these problems will likely not be as simple as having a vertically oriented anode as the PI believes.

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated 1.5 for technology transfer and collaboration.

- The project team is working with the Ohio Coal Development Office and First Energy; however, it is not clear how the interactions with the other partners are contributing to the development of the system.
- There are no apparent partners with SOFC experience.
- Three collaborators are mentioned but their roles are not clear. The Ohio Coal Development Office is probably a funding agency and is not likely to bring technical expertise to the project.
- More contact with other groups that are perhaps more experienced in SOFC technology would be helpful. The overall progress of the effort would probably be faster. However, given the unique nature of the problem (oxidizing a solid fuel in an SOFC), it may not make a huge difference. Again, the bigger issue will be in regards to fuel handling for eventual stack designs, particularly how is the stack to be configured to allow for high fuel utilization, how is fuel to be fed into a stack, etc. There are significant engineering issues here that need to be addressed to move this concept out of the laboratory. At this point, its not clear to me if Chemstress (who as a partner on this project, should have some responsibility for these issues) is really a partner and will be intimately involved in the design of a stack, or if they are merely in place to build a stack eventually.

Question 5: Approach to and relevance of proposed future research

This project was rated 2.5 for proposed future work.

- Anode catalyst formulation will be modified to minimize carbon formation on the nickel catalysts.
- Coal injection system has been designed; and will be implemented.
- It is not clear how the anode catalyst will be developed. The project team should pick one major problem and address it with the limited resources remaining, e.g., how to remove fly ash residue from the anode surface or

interface with the carbon fuel. This project seems doomed to failure if solid impurities like trace metals in the coal build up on the catalyst surface, preventing coal oxidation.

- The project team should try using ultra-pure carbon and if the time decay of the polarization curves on slide 9 are still seen, then there is an even more significant fundamental issue than contamination poisoning.
- The future work is laid out and addresses the most significant issues challenging the concept. The path to developing interconnects that cost 50% less than present interconnects is not well laid out. The proposed future work is ambitious for the amount of funding provided.
- The PI's plans for addressing near-term issues relating to catalysis, interconnects, and cell fabrication are logical. Longer-term issues relating to stack design and operating have not been adequately addressed as mentioned above. This is definitely an area where considering many alternate possibilities would be helpful and should be encouraged.

Strengths and weaknesses

Strengths

- Good funding partners.
- This is a novel approach using a readily available fuel: coal.

Weaknesses

- Direct conversion of coal has not yet been demonstrated.
- Progress to date is with hydrogen, which is already proven. There doesn't seem to be evidence that the direct coal conversion will work.
- There is a lack of partners with high-temperature fuel cell expertise. The PI should ask the SOFC community for help.
- Power density is low and there is not much discussion on how it will be increased.
- How to handle/deliver a solid fuel within a fuel cell stack?
- How to handle/exhaust solid waste (fly ash) produced within the stack?
- Solid fuel coupled with 2-D anode architecture suggests that the limiting current density achievable may be relatively low. Will very large area electrodes be required? If so, what is the ultimate power/energy density achievable with this approach?
- At what scale is this approach really feasible? Is it appropriate for kW size systems such as APUs? Or, is it really only suitable for stationary applications? My hunch would be that more conventional SOFC systems using natural gas or liquid fuels would be more widely applicable, but good engineering could prove otherwise.

Specific recommendations and additions or deletions to the work scope

• The project team should review the work on materials development in the DOE-FE SECA to determine relevance to this project.

Project # FCP-08: Center for Fundamental and Applied Research in Nanostructured and Lightweight Materials

Julie King; Michigan Technological University

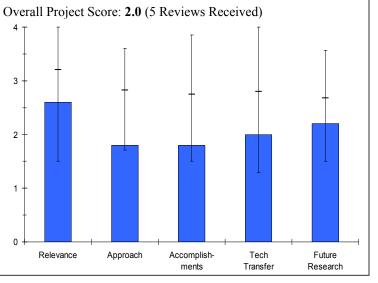
Brief Summary of Project

This project involves fundamental and applied research in the development and testing of lightweight and nanostructured materials to be used in fuel cell applications and for energy storage. The research covers three areas, including: 1) heat and water management; 2) development of new electrode materials; and 3) enabling technologies for membrane synthesis.

Question 1: Relevance to overall DOE objectives

This project earned a score of **2.6** for its relevance to DOE objectives.

• The project has 3 different approaches



(and in some cases with multiple tasks under each approach). The approaches based on thermal and water transport, catalysis, and advanced membranes all have some relevance to fuel cell needs. Each of the approaches presented is limited in that they have not shown that they address the critical needs for any of these areas (e.g., conductivity (thermal or electrical) or cost data for injection molded bipolar plates; mass activity and durability for catalysis; and high-temperature/low relative humidity performance and durability for advanced membranes).

- Each of the project areas is relevant to DOE objectives.
- The program serves objectives A through E.
- It is a materials' program in which different materials are being developed. Not every material addresses all of the DOE targets yet, the whole program does.
- Each of the individual projects has relevance to DOE program goals; however, much of the actual effort seems to be materials of interest to the PIs, and not of direct relevance the DOE Hydrogen Program. The carbon foam/nickel hydroxide work is an example. Advances in carbon foam materials could certainly contribute to DOE Hydrogen Program goals, but there does not appear to be any reason for diluting this effort with a foray into battery materials. Similarly, the electrospinning work seems to be completely focused on spinning a polymer (PLLA) that is not of interest to the fuel cell community.
- Only part of this project appears to be relevant to DOE objectives. The part on "new electrodes" would be more appropriate for a battery or ultracapacitor project than a fuel cell effort.

Question 2: Approach to performing the research and development

This project was rated 1.8 on its approach.

- The study is disjointed and has little cohesion and no synergy amongst the various PIs. Even within a specific topic area there are widely different tasks such as injection molded flow fields and fundamental aspects of water transport under water and thermal transport. The study of electro-catalysts based on heterogeneous catalysis of ethylene hydrogenation on non-conducting supports is not an appropriate platform for investigation. Using polymers with poor durability like poly lactic acid will not allow useful materials to be developed.
- The approach for areas 1 and 3 is reasonably good. The area 2 approach is not as good. More attention should be focused on the electrochemical reactions that are of interest H₂ oxidation and O₂ reduction instead of examining ethylene hydrogenation. Also, depositing metals on non-conductive oxide supports is not relevant for fuel cell electrocatalysis.

- Research targets are on bipolar plates, thermal cyclability, and gas diffusion layer (GDL) improvement. Means to achieve this are: development of testing protocols, tailoring of a carbon foam as a support for fuel cell electrodes, development of nanostructured polymer membranes, and enabling of rapid production techniques.
- Three main areas are targeted: Heat and water management, new electrode materials, and technologies for membrane synthesis.
- The approach is well structured and fully addresses the barriers in an appropriate way. The membrane development seems to be very basic and should be observed yet, not questioned at this stage.
- The focus is not completely on fuel cells but also on batteries. Although synergies are appreciated, the program might be more focused.
- Bipolar plate work is adequate, although more attention could be paid to mechanical properties now that thermal and electrical property goals are in sight. Very little relevant progress on other topics, so it's difficult to assess the approach.
- This project is a collection of three independent research efforts that are unrelated to one another. Approaches within these individual "sub-projects" are not particularly new and do not assure progress towards the technical barriers. Only the development of improved bipolar plates and selected aspects of hybrid-membrane deposition offer certain promise.
- Significant fraction of electrode materials seems to be tailored for batteries and ultracapacitors instead of fuel cell electrodes. This approach does not promise good progress in a fuel cell project.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated 1.8 based on accomplishments.

- To date, data generated by the project shows no progress towards addressing any objectives or barriers.
- Technical accomplishments are few, and some of the presented accomplishments do not demonstrate significant progress toward goals. Doping of fluorescent materials into electrospun polymer fibers has not been shown to constitute progress toward DOE objectives.
- Bipolar plates: the in-plane conductivity meets set targets, yet through-plane the conductivity is in the order of 1/3 to 1/5 of the target. Testing of thermal conductivity shall be finalized by December 2009. Respective optimization is not mentioned. As for the GDL, an environmental testing chamber was fabricated as the first contact angle measurements were carried out. A GDL compression device was fabricated and taken into operation; no major results were attained yet.
- Carbon material development for electrodes targets batteries, supercaps, and fuel cells. A production method was developed. It is irritating that properties mentioned in this review are not relevant to fuel cells. The specific advantages of the carbon over existing solutions were not clearly presented. The addition of nickel to the anode is not self-explanatory, nor has it been explained. This section might need some clarification.
- Catalysts with core-shell structures here called pseudomorphic overlayers are a development with high potential and first success has been made. Yet, again it seems necessary to keep it on a fuel cell track in a fuel cell program.
- The production technology for membranes focuses on fibers. It should be clarified how these fibers will eventually contribute to the formation of a gas tight membrane.
- Assessing the program, it needs to be taken into account that the program just recently started and very little funding was spent in FY08. For the time and money given, the results are very good and thus rated outstanding. For FY09, support should be given to keep the program on a fuel cell track.
- Only the composite bipolar plate effort can make any claim of real progress towards addressing a DOE goal/barrier. The rest are making small steps with materials that are not relevant.
- The absence of fuel cell performance data, electrochemical test results (e.g., for electrode materials), as well as of membrane conductivity and performance data, make evaluation of the technical progress in this project very difficult.
- Charge and discharge data, appropriate for batteries, are irrelevant for fuel cell electrode development. Also irrelevant are results pertaining to ethylene hydrogenation.
- The purpose of building catalytic layers on electronically non-conductive supports is difficult to justify. The reasons for measuring hydrogen adsorption or, for that matter, development of anode catalysts in general, and using precious metals in particular are also unclear.

<u>Ouestion 4: Technology transfer/collaborations with industry, universities and other laboratories</u>

This project was rated **2.0** for technology transfer and collaboration.

- It is a single institution collaboration. Even within the project, no cohesion or synergies exist.
- Specific contributors to the program are developing the different materials. There might not be a strong interaction between the different partners yet, but this is not necessarily to be expected at this point in time. Dana Corp. provides technical input. RIT and GM were mentioned as well. There is a common DOE project with GM.
- In conclusion, the program is well tied to industrial experience and requirements.
- This is a collection of individual efforts that are not linked in any meaningful way. The individual PIs do not seem to have a good familiarity with prior work in several of the areas they are investigating.
- There appears to be no collaboration between various, distinctively different parts of this effort. The effort clearly lacks coordination.

Question 5: Approach to and relevance of proposed future research

This project was rated 2.2 for proposed future work.

- Proposed future work is a continuation of work to date, which has shown no progress in overcoming barriers and has little relevance toward advancing the program.
- Future work is reasonable.
- Only the bipolar plate work is relevant and some thought has been given to future plans (collaboration with Dana Corp.).
- Similar to the development effort to date, proposed research is not particularly novel. Also, continued fragmentation of this project does not promise significant progress.

Strengths and weaknesses

Strengths

- For the most part, the project is relevant to DOE objectives.
- New ideas for materials' fabrication.

Weaknesses

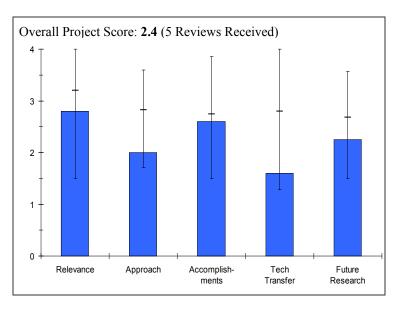
- Approaches and results to date provide no value in advancing the field or addressing key issues in fuel cell technology. There is no synergy in the project.
- Some of the work being done seems unlikely to yield anything useful in terms of DOE objectives. Catalysts supported on non-conductive oxides are irrelevant to fuel cells.
- A strength and weakness is the classical approach of materials' scientists to develop materials for a range of applications. The project needs to keep its focus on fuel cells.
- There is no over-arching theme to bring individual elements together.
- This project has a very poor focus on DOE needs/goals.
- It is very hard to get a good read on a program when one PI is presenting the work of 6 PIs, but has essentially no familiarity with the details of the work of the other PIs.
- At best, these efforts duplicate work being performed elsewhere or previously.

- This project should be cut. Nothing of merit exists to build upon from the work presented.
- If project cannot be cancelled, insist that the effort be focused on materials relevant to fuel cells not batteries, not bio, and not catalysts supported on alumina.
- There seems to be little justification for maintaining funding for this project.

Project # FCP-09: Engineered Nanostructured MEA Technology for Low Temperature Fuel Cells *Yimin Zhu; Nanosys, Inc.*

Brief Summary of Project

The objective of this project is to develop a novel catalyst support technology based on unique engineered nanostructures for low temperature fuel cells that 1) achieves high catalyst activity and performance; 2) improves catalyst durability over current technologies; and 3) reduces catalyst cost. Nanosys, Inc. has developed novel inorganic, nano-technology support structures using functionalized silicon nanowires that 1) are highly durable, have high conductivity and large surface area; 2) have controlled porosity which improves catalyst utilization; 3) have improved Pt alloy catalyst particle dispersion on the support; and 4) maintain well controlled catalyst loading characteristics.



Question 1: Relevance to overall DOE objectives

This project earned a score of **2.8** for its relevance to DOE objectives.

- The project proposes to address the three most critical barriers for MEA components, but only focuses on one component of the membrane electrode assembly (MEA) the catalyst and support, and for direct methanol fuel cell (DMFC) small portable applications.
- This project is relevant to the DOE goal of reducing carbon corrosion and increasing catalyst stability. Replacing carbon black with another material or composite may achieve a more thermally and oxidatively stable catalyst support.
- This is nice work that addresses new support materials for fuel cell electrodes that avoids the use of carbon. This is very relevant for MEA durability. Some of the tests shown are not so relevant and need to be modified for open circuit voltage (OCV) and humidity cycling with hydrogen feed. Work is focused on DMFC, which is not relevant to DOE goals. Behavior with low relative humidity (RH) hydrogen would be more relevant.
- This project addresses the critical barrier of catalyst and catalyst/support durability. Testing has been for DMFC applications, while DOE Hydrogen Program has been focused on H₂ fuel and systems that have potential crossover between H₂ and DMFC.
- This project is relevant to the development of DMFCs for portable power applications. However, its focus is only marginally relevant to improving the performance of these devices.

Question 2: Approach to performing the research and development

This project was rated **2.0** on its approach.

- The project is based on the vapor liquid solid approach for generating nanostructured catalyst support fibers. This is an inherently slow and costly approach. The high-temperature SiC coating process may also add additional cost limitations.
- The project lacked detail on why it was expected that the particular Si/C/nitride support would be expected to be more stable than state-of-the-art materials.
- "New" support materials still contain carbon. Discussion on why oxidation/corrosion is expected to be less would be helpful.

- No standard C corrosion data was available. No electrochemical area (ECA) measurements were available. No end-of-life (EOL) microscopy was available.
- The project team has done good work making electrode supports, dispersing catalysts, etc. Tests are focused on DMFCs, which is not so relevant. Behavior with low RH hydrogen feed would be better. Also, the project assumes dimensions of the nanowires are optimized. Some transport modeling is needed to develop a model that could place the choice of dimensions on a sound footing.
- The approach leads to more controlled porosity and appears to provide better catalyst dispersion. Potential cycling tests cycle over a limited potential range at relatively low potential where corrosion is not expected to be an issue. Potential hold test is at a low voltage, again where limited corrosion is expected. DOE suggested protocols involve cycling between 0.6 and 1.0 V for catalyst durability studies, and a potential hold test at 1.2 V for catalyst support durability.
- This project seeks to improve the stability and utilization of the anode catalyst in direct methanol fuel cells by replacing the amorphous carbon support or unsupported PtRu catalyst with PtRu deposited on carbon-coated SiC nanowires. The main issue with the stability of DMFC anodes is not support-related but is the stability of the catalyst composition itself. This project does not address this issue.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated 2.6 based on accomplishments.

- The project is complete and some milestones were achieved. However, the project team did not overcome the DOE barriers targeted.
- Si/C nitride nanowires production technology was previously known.
- Formation of nanoparticles technology was previously known.
- The project successfully married the technologies and produced Si/C nitride wires with catalyst.
- The testing plan was very lacking and could have used some more fundamental testing.
- The accomplishments are impressive for the work performed, but some important durability studies are absent including OCV and humidity cycling with hydrogen feed. There is too much DMFC work here for the program goals.
- Results suggest some advantages in catalyst dispersion, increased surface area, porosity, and durability. Durability testing has been performed under relatively mild conditions; so testing under DOE protocols to see if the durability advantage remains is of interest.
- The project has accomplished quite a bit in a short amount of time. However, it is not clear how this project addresses the overall barriers because it focuses on replacing the anode support for DMFCs where the support stability is not the biggest issue with the anode. Utilization may be improved with this approach, but the overpotential for this reaction is extremely high leading to low cell power densities. This is the main issue with the cathode catalyst and not its utilization. This approach would have been more interesting and have made a bigger impact if it were pursued for the cathode catalyst.

<u>Ouestion 4: Technology transfer/collaborations with industry, universities and other laboratories</u>

This project was rated **1.6** for technology transfer and collaboration.

- This project appears to have been done very quickly with earmarked funding from the company's congressional members. There has been little interaction with other partners for the technology advancement.
- No collaborations were noted.
- Collaborations with others have been non-existent. The project team needs to collaborate with some electrochemical modelers to determine what the best dimensions of the support structure should be and then vary the dimensions accordingly.
- Collaborators were not listed. No collaborations were apparent.
- No apparent collaborations, with the exception of acquiring materials from component suppliers.

<u>Question 5: Approach to and relevance of proposed future research</u>

This project was rated **2.3** for proposed future work.

- Not applicable because the work is completed.
- The project team discussed testing in H₂ fuel cells. This should have been part of original project plan.
- The project is at an end. Plans for the future were not given.
- The project is complete. No future work has been planned.
- Water management with this catalyst layer would be of interest. Does the large pore size help or hurt water management?

Strengths and weaknesses

Strengths

- This project is one of very few that directly targets the replacement of "classical" carbon supports with a different material. The use of Si/C nitride materials may well prove much more thermally and oxidatively stable.
- Nanowire structure capability is shown and the ability to disperse conventional catalysts is demonstrated.
- The project team used a novel approach for catalyst support development. The project team has shown the ability to synthesize very small and monodispersed PtRu nanoparticles.

Weaknesses

- The project plan for testing is suspect. DOE goals are primarily for hydrogen proton exchange membranes (PEM). H₂ fuel cell testing should have been carried out. Classical carbon corrosion and ECA experiments should have been done. In-depth microscopy at beginning-of-life (BOL) and EOL, thermal stability, and oxidation testing should have been done.
- The project team assumed nanostructures are the best dimensions. There is a lack of electrochemical modeling and expertise to determine whether the right dimensions are achieved. Demonstrating ability to change dimensions at will for various applications would be good.
- Durability was measured under mild conditions.
- The project team is not addressing the main issue for DMFC anodes.

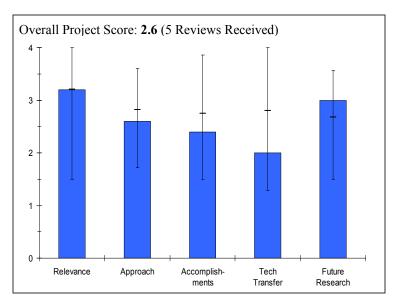
- The project team should add a electrochemical modeler and expertise. The project team should collaborate.
- The project team should perform durability tests under DOE suggested protocols.

Project # FCP-10: Alternative Fuel Cell Membranes for Energy Independence

K.A. Mauritz and R.F Storey; University of Southern Mississippi

Brief Summary of Project

The objectives for this project are to 1) synthesize stable aromatic hydrocarbon polymers containing acid ion-exchange groups tethered to the backbone via fluorinated side chains; 2) synthesize benchmark aromatic hydrocarbon membranes for properties comparisons and refinement of synthetic methods; 3) establish Nafion® benchmark data to which novel hydrocarbon membrane data can be compared on an all-other-things being equal basis; and 4) establish hydrocarbon membrane structure-property, proton conductivity characterizations and fuel cell performance data as relating to the Hydrogen Program proton conductivity technical achievement milestones.



Question 1: Relevance to overall DOE objectives

This project earned a score of **3.2** for its relevance to DOE objectives.

- The project targets the synthesis of new membrane materials for operation at low relative humidity (RH) and high temperature for H₂ proton exchange membranes (PEM), which are main goals for the DOE PEMFC development plan. The project team has a good plan for membrane design, synthesis, and in-depth testing.
- This program supports the DOE R&D objectives.
- This project is relevant as it looks at preparing new materials and looking at behavior under degradative stress. These techniques are valuable and relevant. The syntheses are also interesting. However, there is no rationale given for how these membranes will achieve the conductivity goals under low RH, and it is not at all clear how these materials that depend on the presence of water will be any better than Nafion®.
- The project team should address barriers identified in DOE Multi-Year RD&D Plan (found at http://www1.eere.energy.gov/hydrogenandfuelcells/mypp/): durability, cost, performance, water transport in the stack, thermal and water management, air management, or start-up/shut-down time, and energy.
- Determining baseline properties of Nafion® for comparison to other membranes does not really address these barriers. Others have pursued preparation of sulfonated poly(arylene ether sulfone) (sPAES) systems. Phosphonic acid derivatives and are of interest, but it is not clear what equivalent weight materials are being prepared. The project team needs to work at low equivalent weight/high ion exchange capacity.
- Development of hydrocarbon membranes with improved functionality is relevant to DOE program goals.

Question 2: Approach to performing the research and development

This project was rated **2.6** on its approach.

• The approach includes the synthesis of modified diphenol-type monomers to be used as comonomers in sulfone-ether type copolymers. The target modified monomers include tethered acid groups that may provide more mobility and free-volume in the material and enhance proton conduction. The initial target of using phosphonic acid (or a,a'-difluorophosphonates) may not be the best approach given that the pKa of these groups is much greater than that of sulfonic acid groups. Researchers discussed the use of sulfonate or a,a'-difluorosulfonate acid groups, which may be a better alternative.

- Collaboration with a world-class membrane testing group will prove most useful once viable membranes are produced. The testing group is currently running baseline experiments with commercially available materials.
- The project team has a good approach using materials that should have good stability.
- The degradation work and application of the dielectric relaxation methods are very useful. The development of the methods is tested on Nafion® and the syntheses methods are sound. The work promises to produce valuable results of use to others in the program.
- The strategy for addressing the technical barriers is not clear. Determining baseline properties of Nafion® and determining how it degrades may be useful, but unless you have strategies to address its failures, the work does not lead to advances. The strategy for addressing mechanical failure of Nafion® and low conductivity at high temperature/low RH is not apparent.
- DOE membrane targets are not identified, nor seemingly used to guide development. This seems to be more of a university learning activity at this point, rather than a high-functioning R&D effort with experienced investigators. Plans are okay, but the reviewer needs to see progress to make a judgment.

<u>Ouestion 3: Technical accomplishments and progress toward project and DOE goals</u></u>

This project was rated 2.4 based on accomplishments.

- The project is currently in early stages and consists mainly of monomer and polymer synthesis. Synthesis of new materials can be quite time consuming, so it is understandable that viable membranes are not yet in hand.
- The a,a'-difluorophosphonate diols may be interesting, however, it is recommended that the group move toward sulfonate and a,a'-difluorosulfonates.
- Successfully carrying out sulfone-ether condensation copolymerizations can be very tricky, particularly in ensuring that monomer ratios are correct and that polymerizations are completely dehydrated. It is suggested that the project team consult with J. McGrath at Virginia Tech.
- It is too early in the program to evaluate accomplishments.
- Progress is good although not clear regarding the polymer synthesis. Testing of methods is satisfactory and adequate.
- Membrane development work has not made membranes to test yet. Characterization work has observed features in dielectric loss spectroscopy with ageing, but it is not clear exactly what the features are due to.
- Progress to date is limited to some backbone synthesis and to characterizing a Nafion® membrane electrode assembly (MEA) as a benchmark (with nothing new apparent). Backbone has not been functionalized. Necessary equipment has been procured but is not yet operable.

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated **2.0** for technology transfer and collaboration.

- Good teaming of synthesis and characterization expertise. Partners are within the same university. Outside collaboration is suggested to strengthen project.
- An industrial partner would help in the evaluation of these new materials.
- Not much collaboration is evident. There should be more interaction with others in the program.
- Some collaborations are in place.
- The only apparent collaboration is unfunded activity (scope not defined) with the Illinois Institute of Technology. There is no mention of DOE membrane working group collaboration or coordination.

Question 5: Approach to and relevance of proposed future research

This project was rated **3.0** for proposed future work.

- The future work plan is well defined. Synthesis of new monomers will lead to work on copolymerization and membrane production. Membrane testing by dielectric spectroscopy and various microscopy techniques are planned.
- A good plan was presented.
- Future plans do not directly address DOE milestones.

- Proposed future work will move membrane development along. The project team needs to concentrate on low equivalent weight materials.
- The project team's plans seem adequate, but progress needs to be demonstrated.

Strengths and weaknesses

Strengths

- The teaming of synthesis and characterization expertise is strong. The materials approach accounts for the dual goal of low RH conductivity and temperature stability. Multiple synthetic targets have been suggested to reduce risk.
- Synthesis of new and interesting materials although incremental from those at Virginia Tech.
- Dielectric relaxation and mechanical measurements of degradation behavior are valuable.
- The characterization technique is novel.
- Polymer science and property characterization.

Weaknesses

- Moving from new monomer synthesis through membrane production can be very time consuming. Strict project planning must continue to ensure materials are produced with sufficient time to carry out the characterization.
- The project team has used of phosphonate functionality as proton conductors (less-acidic, higher pKa than sulfonate).
- This project does not address DOE milestones. No attempt has been made to understand proton transport mechanisms.
- The strategy for addressing barriers (durability and performance) is not clear.
- The lack of progress would indicate that the project did not have the capability to perform the work at the time of project award.

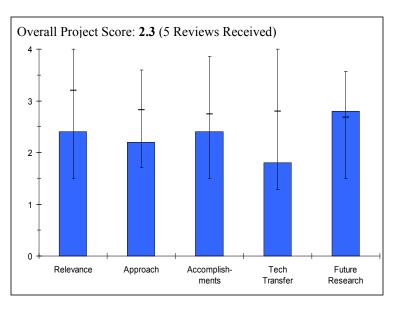
- The project team should focus on sulfonic acids.
- The project team should suggest ways to increase sulfonic acid content (lower EW).
- The project team should suggest ways to mechanically stabilize membranes (cross-linking, support material).
- An industrial partner would help in the evaluation of these new materials.
- The project team should address low RH conductivity.
- This project should be evaluated next year to see if meaningful progress is made.

Project # FCP-11: Extended Durability Testing of an External Fuel Processor for SOFC

Mark A. Perna; Rolls Royce Fuel Systems (US) Inc.

Brief Summary of Project

The overall objectives for this project are to 1) conduct long-term tests in a relevant environment for the external fuel processor for a 1 MWe solid oxide fuel cell generator; 2) determine long-term performance of critical components including catalysts, sorbents, heat exchangers, and control valves; 3) evaluate the impact of ambient temperatures (hot and cold environments) on performance and component reliability; 4) determine system response and performance of process controls for transient operation; and 5) identify any long-term failure mechanisms.



Question 1: Relevance to overall DOE objectives

This project earned a score of 2.4 for its relevance to DOE objectives.

- Durability studies are always of value; however, this study is looks at components two of which are only to be used during start-up operations. This system is not designed for frequent start-ups.
- This project examines durability and performance of a solid oxide fuel cell (SOFC) fuel reforming system for combined heat and power (CHP).
- This project provides demonstration of SOFCs (1 MW) using natural gas as fuel for stationary power. It provides demonstration of fuel processing subsystem durability and performance information. It also plans to provide demonstration of all season operation.
- 1 MW is the scale that Fossil Energy is looking at, so the principle (long-term testing) is applicable to the Fuel Cells Program. The scale is a bit large.
- The objective of this project is to test an external natural gas fuel processor for a 1 MWe solid oxide fuel cell power generator. This appears to be of low relevance to the overall hydrogen and fuel cell program for the following reasons:
 - o No megawatt-scale SOFC systems have been developed and demonstrated yet.
 - It is not clear what the application of interest would be.
 - It is not clear why water-free fuel processing is needed for stationary distributed power plants of this scale.
 - o It is not clear how this scale SOFC system fits in with the other activities in the Hydrogen Program.

Question 2: Approach to performing the research and development

This project was rated **2.2** on its approach.

- The study uses the full-scale components.
- It is not clear how degradation that is not visually detectable will be identified, or what (if any) post-test characterizations are planned.
- Durability and performance including start-up/shut-down are measured.
- The system intends to use pipeline natural gas.
- This system uses a very complex method to start-up the CHP unit, including O₂/N₂ separation, a syn-gas subsystem, and a start-gas subsystem. It also includes electric heaters for preheating and standby.
- The project team demonstrated multiple start-ups (10) and 1200 hours for the syn-gas subsystem.

FY 2009 Merit Review and Peer Evaluation Report

- The project team demonstrated 24 start-ups and 200 hrs for the start-gas subsystem.
- The project uses an already developed Rolls Royce SOFC, 1 MW unit built up from four 250 kW blocks. A catalytic partial oxidation (CPOX) is used to start up and system uses internal reforming to run using pipeline natural gas.
- This is a full-scale demonstration.
- If this unit was intended for a distributed residential area, then transient, load following behavior would also be of interest.
- The described approach was to test two different fuel processors for reforming natural gas, an internal one to generate the fuel gas for the SOFC (without an actual SOFC in the system to be tested), and an external one used essentially for start-up of the internal one. It was not explained why the external (start gas) fuel processor needed to be located outdoors.
- There was no discussion of a test plan, of the data to be obtained, or how those data would be used. The only metric given was the number of hours of operation and the number of start-ups and shut-downs.

<u>Ouestion 3: Technical accomplishments and progress toward project and DOE goals</u></u>

This project was rated 2.4 based on accomplishments.

- The project has just started.
- Durability testing has not yet been started and appears to be behind schedule.
- The project just started so there are few results.
- The project began only a few months ago, and hardware has been fabricated and installed.
- This project started very recently (in January 2009). The early months have been spent in building the indoor test rig and enclosure and in preparing specifications for the external test facility.

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated **1.8** for technology transfer and collaboration.

- Collaboration with an educational institution will help train students. The project team should use a metric to quantify student involvement.
- There has been minimal collaboration up to this point.
- Eventual collaboration is intended with the Ohio Department of Development and Stark State College of Technology.
- There have been no obvious collaborations.
- The partners seem to be coordinated and doing well. It is too early in the project to determine how close the collaboration is.
- No technical collaboration was identified with any organization other than Rolls-Royce Fuel Cell Systems.

Question 5: Approach to and relevance of proposed future research

This project was rated 2.8 for proposed future work.

- The main activity is testing the system for time on-stream and cycling.
- Plans for post-test studies are not well defined.
- The proposed future work appears as a serial methodology: testing the syn gas system, testing the start-up gas system, and then testing durability.
- At end of the project, the team will have 8000 hours of durability testing of the system, including desulfurizer. The project team will have winter/summer operation data. The team wants to do parallel operation with multiple fuel cell blocks. This will require a distributed air and fuel system and this could provide useful systems data.
- Subject to the weaknesses in the approach mentioned above, the proposed future work is to complete the project as planned.

Strengths and weaknesses

Strengths

- The project addresses durability of components.
- The project team has incorporated an academic institution, which will help train faculty and students.
- The project team uses an already developed system to test and get durability data. This project provides a good demonstration of SOFC running on pipeline natural gas.
- This is a large-scale demonstration project that will provide important data for industry on this technology. By operating outside, weather impacts will be evaluated. By operating year-round, temperature extremes and changes in natural gas composition will be evaluated.
- The personnel involved have an extensive background in fuel processing and they understand the issues and challenges involved.

<u>Weaknesses</u>

- Post-test studies are not clearly communicated.
- The team is relying on electric heaters for standby and preheating.
- This project employs a very complex system, with a standard reforming unit, a syn-gas subsystem, a start-gas subsystem and O₂/N₂ separation membrane.
- Durability testing has not yet been started.
- The project team has no commercialization plan.
- The project team is focusing on natural gas. It would be interesting to examine biogas in addition.
- The lack of technical objectives in the test plan is a significant weakness.
- The project needs to identify what maximum rate and extent of performance degradation would still qualify as a successful durability test.

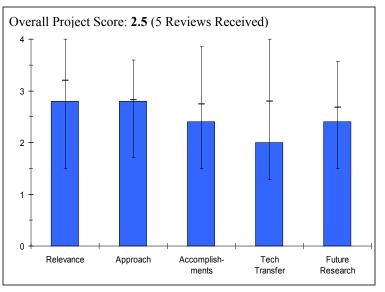
- The project team should define a metric to gauge faculty/student participation.
- The project team should include an analysis on what it would need to do in order to work on biogas.
- The project is very similar to Fossil Energy's SECA and FutureGen projects and would benefit from increased interaction with those programs perhaps by adding a partner from the SECA program.
- Since the project is so similar to SECA, it may want to be transferred to Fossil Energy.
- The project team should develop a technical test plan with quantitative performance targets over time.
- The project team should identify the classes of applications for which these megawatt-scale SOFC systems are targeted.

Project # FCP-12: Hydrogen Fuel Cell Development in Columbia (SC)

Kenneth Reifsnider; University of South Carolina

Brief Summary of Project

The general objective of this project is to contribute to the goals and objectives of the Fuel Cell element of the Hydrogen, Fuel Cells and Infrastructure Technologies Program of the Department of Energy by enhancing and supplementing the fuel cell research and development efforts at the University of South Carolina. The project research activities focus on the following technical objectives: 1) the development of metal-free oxygen reduction catalysts to reduce cost, facilitate manufacturing, and enhance durability of fuel cells; and 2) the development of redox stable mixed ionic and electronic conductors for bi-electrode supported cell symmetrical solid oxide fuel cell designs, to reduce cost by simplifying



manufacturing, enhance durability, and greatly reduce sensitivity to thermal cycling.

Question 1: Relevance to overall DOE objectives

This project earned a score of 2.8 for its relevance to DOE objectives.

- The project focuses on fuel cells.
- There is a very diverse portfolio of projects presented in this one poster. All of the projects are relevant to DOE's objectives in different applications of fuel cells. The impurity project would become more relevant if it were to focus on materials not already studied by other laboratories.
- Each of the project areas is relevant to DOE objectives.
- This project is an unfocused, broad and seemingly unconnected effort to "support" other funded work at the University of South Carolina. The shotgun approach is unlikely to yield relevant results to the DOE program.

Question 2: Approach to performing the research and development

This project was rated 2.8 on its approach.

- The scope is very broad and should be focused. The goals should be more specific. Milestones and project outcomes need to be more specific.
- The solid oxide fuel cell (SOFC) work should collaborate with the Solid State Energy Conversion Alliance (SECA) and leverage what has been done in this area.
- In general, the approaches pursued in these diverse projects do contribute to overcoming the barriers to commercialization of polymer electrolyte fuel cells (PEFC) and SOFCs to varying degrees. The SOFC projects appear to be at an early stage, but are following relevant approaches. The impurity project should focus on other impurities not already covered in DOE's portfolio of impurity projects.
- The approach is good overall, although insufficient information was presented for each of the project areas to fully demonstrate a good approach for attacking the various technical barriers.
- The approach to individual identified tasks is okay; but the unfocused, broad and seemingly unconnected effort is unlikely to result in significant advances toward DOE goals and technology targets.

Ouestion 3: Technical accomplishments and progress toward project and DOE goals

This project was rated 2.4 based on accomplishments.

- The project has just begun, so it is hard to judge.
- The non-platinum electrocatalyst project is generally effective, but makes claims regarding optimization of pyrolysis temperature that are not substantiated by the data. Is catalyst activity optimized at pyrolysis temperature of 1000°C? Or would even higher temperatures yield higher activities?
- Ammonia and sulfur dioxide contaminants have been studied extensively by LANL. With so many potential contaminants and given the urgency of determining the effect of these contaminants, it would be best for the University of South Carolina (USC) to examine contaminants that have not been or are not being studied by other organizations.
- Various results have been presented but it is difficult to gauge to what extent they represent significant progress during the project period. For instance, presenting the demonstration of a role of N content in C-based catalysts in determining activity doesn't seem like significant technical progress. Others have previously shown this, and anyway, the relationship is very complex.
- I was unable to assess what portion of the progress presented was accomplished under the funding from the program. The poster and presenter comments would indicate much of this work was authorized and funded elsewhere.

<u>Ouestion 4: Technology transfer/collaborations with industry, universities and other laboratories</u>

This project was rated **2.0** for technology transfer and collaboration.

- The partners seem limited to those located in South Carolina.
- A list of collaborators was given, but it was not clear what these collaborators contributed to in the presented work.
- I was unable to assess what portion of the collaborations presented was resulted from funding from the program. The poster and presenter comments indicate much of this work was authorized and funded elsewhere.

Question 5: Approach to and relevance of proposed future research

This project was rated 2.4 for proposed future work.

- The seals work does not seem very ambitious.
- The project team needs to identify the anticipated outcomes and benefits of its work. The modeling looks useful, but benefits from other areas of the work are not as clear.
- The presentation was lacking in proposed future work. Only a few broad statements were presented.
- Few plans for future work presented. Future work is in general relevant and reasonable, but decision points and alternate development pathways were not mentioned.
- To the extent the future plans presented are to be accomplished under existing funding for this program the proposed work is good. The scope is too broad, however, for meaningful advances under this funding in this time period. It is unclear what portion of the plans presented is to be accomplished with funding from the program.

Strengths and weaknesses

Strengths

- The project team is leveraging from many past projects.
- The project areas are generally quite relevant to DOE objectives and the approach seems good.
- Scientific breadth and approach to individual tasks.

Weaknesses

- The scope is too broad.
- The project is poorly designed and unlikely to significantly advance the technology toward DOE goals and targets by itself.

- Focusing of scope would help this project make meaningful progress.
- The project team should include more partners or at least interactions with institutions located outside of South Carolina.
- The SOFC work should engage the SECA program to leverage the SECA knowledge.
- The project team should consider drastic scope reduction and improve focus and deliverables. Otherwise, this project should be terminated.

Project # FCP-13: Martin County Hydrogen Fuel Cell Development

Jeffrey Bonner-Stewart; Microcell Corporation

Brief Summary of Project

The objective of this project is to transfer a microfiber fuel cell technology's manufacturing process from a research and development level to a manufacturing environment and evaluate various parameters including speed and product quality. Unicell throughput was increased due to enhanced systems and programming without affecting Unicell performance.

<u>Ouestion 1: Relevance to overall DOE</u> <u>objectives</u>

This project earned a score of **1.8** for its relevance to DOE objectives.

- The manufacturing technology under development seems applicable only to relatively low total power "stacks."
- Cost was not mentioned.
- Objectives are not tied to any fuel cell performance metrics. The person presenting the poster couldn't provide details.
- The project involves scaling up an R&D level technology to a mass-produced product. In principle, this is relevant to DOE objectives.
- The subject of this project may have some relevance to DOE objectives; however, the lack of technical content in the presented material makes assessment of the effort practically impossible.

Question 2: Approach to performing the research and development

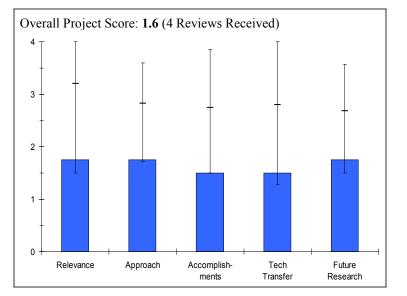
This project was rated **1.8** on its approach.

- Scaling up of the manufacturing process is important, but there is not enough information on how scaleup/optimization was achieved.
- Insufficient information is given about the intended applications and system packaging issues for those applications.
- The presenter did not have sufficient knowledge of the technical aspects of the project and of the cell construction.
- My only take away from the poster presentation and discussion with the presenter was that this project uses an alternative approach for fabricating fuel cells and stacks. No information was available on any performance requirements or important performance metrics.
- The approach is good in terms of addressing technical barriers to scale up.
- While extrusion of a complete MEA in a single nanofiber appears attractive, this presentation gives no information on whether the approach has been successful to date and does not allow one to judge prospects for overcoming various barriers that this project is targeting.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated 1.5 based on accomplishments.

- The goals of the project were met although the general applicability is not evident.
- Throughput was maintained with no adverse effect on quality.



- I'm not sure how to assess or evaluate the impact of the accomplishment, because it is not compared against any metrics.
- The lack of technical performance data (other than power per "unicell" of unspecified size) renders technical evaluation of this project's progress impossible.

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated **1.5** for technology transfer and collaboration.

- There appear to be no technical partners. Input from catalyst and membrane developer/manufacturer would have been beneficial.
- The technical collaboration that took place with North Carolina State University (NCSU) is unclear.
- The roles of two partner organizations in this project, Martin County Economic Development and NCSU, are not explained. All work appears to be have been carried out by Microcell.

Question 5: Approach to and relevance of proposed future research

This project was rated 1.8 for proposed future work.

- This program ended in March 2009. There is no DOE-funded future work planned.
- Proposed future work needs to include measurable performance metrics.
- The future plans appear reasonable on the surface, but the limited information on the poster and the limited technical knowledge of the presenter leave some questions unanswered.
- Relevance of proposed future work cannot be evaluated in the absence of technical content in this year's presentation.

Strengths and weaknesses

Strengths

- The project is making reasonable progress towards the goal of scaling up an R&D level technology to a manufacturing environment.
- Neither project strengths nor weaknesses can be determined in the absence of any substantial technical information.

Weaknesses

- It was nearly impossible to assess the status of the technology readiness level or the objective of this project from the context of a fuel cell power generator.
- Further work on refining the technology on the R&D level should be done before any efforts at mass-production are made.

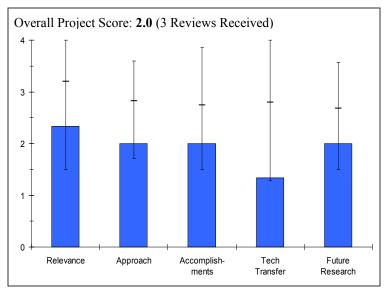
- This whole project needs to be thought through and its justification needs to be reevaluated.
- The funding of this project should not be continued.

Project # FCP-14: Fuel Cell Balance of Plant Reliability Testbed

Vern Sproat; Stark State College of Technology

Brief Summary of Project

The objectives of this project are to 1) develop test beds to address the challenge to the fuel cell industry of the durability and reliability of components that comprise the complete system (balance of plant); 2) develop the test plan to address the candidate balance of plant components and basic test bed design for long term operation; 3) use collaborations with component manufacturers to develop and enhance final product performance; 4) develop statistical models for extremely small sample sizes while incorporating manufacturer validation data for future evaluation of candidate components; and 5) use the test beds to enhance the education of the technical workforce trained in proton exchange membrane fuel cell system technology.



Question 1: Relevance to overall DOE objectives

This project earned a score of 2.3 for its relevance to DOE objectives.

- This project seeks to generate a reliability database for proton exchange membrane fuel cell (PEMFC) balanceof-plant (BOP) components. It is also relevant to producing a workforce trained in fuel cell technology.
- Published (PEM) fuel cell system data indicate that non-stack components account for about 67% of unplanned system shut-downs/failures. Better understanding of these failures is needed.
- It has been difficult, both in direct discussions and reviewing the presentation, to ascertain what the primary goals of the project are and how the project team intends to meet these goals. The fuel cell BOP can be improved, and educating a potential future workforce for related studies has value; unfortunately, based on the data and approach presented, it is unlikely this project will be effective at addressing either of these areas.

Question 2: Approach to performing the research and development

This project was rated **2.0** on its approach.

- The project has taken the approach of assembling test beds to generate the reliability database, working with a manufacturer to design meaningful tests, and developing statistical models for small sample sizes.
- The BOP components to be evaluated are not listed so it is difficult to fully assess the approach. If the project includes only fittings, tubing, transducers, and gauges, then its usefulness is diminished.
- It is hard to imagine that these test beds would be better or provide more information than the BOP component developer/supplier's in-house testing.
- The barriers and approach are completely unclear. Three test beds have been presented without insight into what they focus on and how the application of them and data obtained will lead to improved understanding or advances. The project represents incompletely formulated ideas without substance. The project seems to focus on test bed design and fabrication without any guidance presented to what this means and how it will be implemented.

<u>Ouestion 3: Technical accomplishments and progress toward project and DOE goals</u></u>

This project was rated 2.0 based on accomplishments.

- The project is just getting started. Turnover in project management has apparently impeded progress.
- Progress is reasonable for the recent start date of August 2008 and low funding to date.
- To date, no progress has been made (except perhaps that a hydrogen safety plan is now in place).

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated **1.3** for technology transfer and collaboration.

- The project team is working with Lockheed Martin to design three test beds, one of which will be located at the partner's site.
- This project desperately needs participation of BOP component developers and system users such as compressor/blower suppliers, humidifier manufacturers, and auto original equipment manufacturers (OEM) to help define operating conditions including cycles.
- Lockheed is a partner and few other institutions are also mentioned, however, their roles aren't clear. At this point no progress has been reported so it is not possible to comment on this aspect of the project.

Question 5: Approach to and relevance of proposed future research

This project was rated 2.0 for proposed future work.

- It appears that the plans for future work are still being refined.
- The future work follows logically.
- Plans have no coherence and it is uncertain what studies will be undertaken and what systems will be designed. From the materials presented, it is extremely unlikely the project will advance the program or address barriers.

Strengths and weaknesses

Strengths

- Collaboration with Lockheed Martin.
- Availability of the student body.

Weaknesses

- The PI is still gaining familiarity with the fuel cell technology, the state of the art, and technology needs.
- This project lacks direction and a clear plan for making any impact.

- DOE needs to redirect this program by closely aligning it with the fuel cell system analysis and cost projects that DOE is sponsoring.
- The project needs better identification of the anode-side BOP components and the needs for performance and reliability data.
- The project should be cut. There is nothing of merit to build on from the work presented.

EDUCATION; SAFETY, CODES AND STANDARDS; AND TECHNOLOGY VALIDATION

In fiscal year 2009, the Education; Safety, Codes and Standards; and Technology Validation subprograms were funded through the DOE Vehicle Technologies Program. Complete detailed reports from the Annual Merit Review and Peer Evaluation meeting for these three subprograms can be found on the DOE Vehicle Technologies Program Web site: <u>http://www1.eere.energy.gov/vehiclesandfuels/resources/fcvt_reports.html</u>.

The following section includes summary overview reports for each of these three subprograms.

EDUCATION; SAFETY, CODES AND STANDARDS; AND TECHNOLOGY VALIDATION

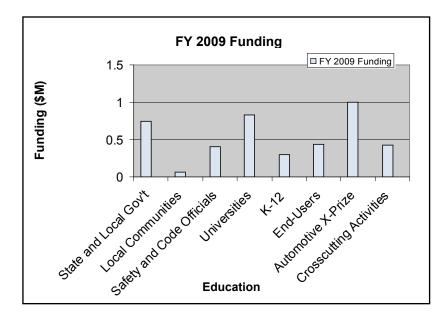
Education Summary of Annual Merit Review Education Subprogram

Summary of Reviewer Comment on Education Subprogram:

Reviewers emphasized the importance of a comprehensive education and outreach effort in advancing the adoption of hydrogen and fuel cell technology. The challenges, goals, and objectives were considered to be well met by the structure of the subprogram; and the target audiences and corresponding outreach activities were considered to be well chosen, well defined, and appropriate to the goals of the program. Comments noted that progress has been demonstrated clearly, but more work is needed to reach out to the safety community and potential adopters. Reviewers underscored the importance of the survey in measuring progress, increased coordination among the different projects and across the country, ongoing communication with principal investigators, and the use of social media and multimedia to reach out to target audiences. The subprogram was commended for the excellent use of limited, inconsistent funding, and reviewers stressed the critical need to sustain education activities in the future.

Hydrogen Education Funding:

The Education subprogram efforts are prioritized to focus on the target audiences involved in facilitating the near-term use of hydrogen and fuel cell technology. With funding at the request level, the FY 2009 budget allowed for support of projects across the education portfolio, including new competitively awarded projects focused on outreach to state and local government officials and potential end users, as well as projects to develop and expand university hydrogen and fuel cell education programs. FY 2009 funds also supported ongoing efforts to educate first responders and code officials, local communities, and teachers and students at the middle and high school levels. The following chart indicates the FY 2009 Education subprogram funding.



Majority of Reviewer Comments and Recommendations:

Education projects scored 3.64, 3.15, and 2.63 for the highest, average, and lowest scores, respectively. Scores reflect progress made over the last year and reported plans for future activity. Key comments and recommendations are summarized below. DOE will act on reviewer recommendations as appropriate to the overall scope, direction, and coherency of the Education effort.

First Responders: Reviewers recognized the need to enhance safety community confidence in hydrogen and fuel cells through training and familiarity as a first step in widespread hydrogen and fuel cell adoption. The use of online learning tools and hands-on training were commended for enhancing learning effectiveness. Reviewers thought that feedback from technical experts and first responders in the steering committee were essential to quality course development and suggested extending collaboration to include more input from energy companies and other Federal agencies. Coverage of stationary and vehicle applications was considered to be comprehensive and reviewers recommended a greater focus on near-term fuel cell applications such as forklifts.

Code Officials: Reviewers felt that educating code and permitting officials is essential and highly relevant to market transition of fuel cell and hydrogen technology. They felt that collaboration and feedback at the national and state level from the codes and standards community and the first responder education program ensured relevancy of course content and recommended extending collaboration to other Federal agencies. Comments commended direct linking to the updated permitting and codes database and suggested adding links to local jurisdiction codes. Reviewers suggested expanding the course to include parking facilities, repair facilities, and indoor fueling.

Universities: Reviewers recognized the need for a well-trained technical professional workforce to support the growing hydrogen and fuel cell industry. The university programs were cited for the breadth and quality of activities including courses, curriculum, textbook chapters, lab activities, internships, seminar series, and programs. They specifically appreciated the integration of real-world research, demonstration, deployment, and hands-on experience into these education programs. Reviewers thought the projects effectively leveraged existing university programs by integrating specialized modules into curriculum and classes for lower- level and upper-level engineers, as well as non-engineers. Collaboration with industry, junior colleges, and other stakeholder groups was viewed as adequate, and

reviewers encouraged several projects to expand their partnerships. Comments underscored the importance of accessibility to the wider student population and called for deployment to other departments, universities, and on-line. Although outreach material development had not yet been completed for most projects, reviewers emphasized the need for outside technical feedback and review. Reviewers stated that projects should be able to continue deployment after funding ends.

End-Users: Reviewers emphasized the importance of using real-world deployments to build the business case for early adoption of hydrogen and fuel cells. They felt that the integration of an education seminar with a trial deployment was especially effective in introducing the technology and showing the benefits of using fuel cell forklifts to potential adopters. Collaborators were considered to be well chosen with representation from many industries. Although the project had just started, reviewers thought that progress was reasonable but future plans were unclear. Reviewers encouraged the continuation of the deployments and workshops and recommended the development of a final business case with aggregate performance results for use as an outreach tool to potential customers.

State and Local Government Officials: Reviewers see education of state and local leaders as essential to the future formation of hydrogen and fuel cell initiatives. Reviewers thought that projects were well chosen to represent states active in hydrogen and fuel cell activities across the nation, and national groups working with all states. Collaboration was considered to be comprehensive with other state groups, industry, the safety community, academia, and government. Reviewers thought that the material developed was audience appropriate and commended the varied delivery mechanisms including workshops, magazine articles, Web sites, Webinars, social media, and train-the-trainer programs. Reviewers underscored the importance of metrics to measure accomplishments and encouraged increased communication among the projects to ensure consistency in content and delivery of information in different regions.

Knowledge and Opinions Assessment: Reviewers noted the importance of the Knowledge and Opinions Assessment for measuring progress. They felt the survey's statistical analysis is proficient and well thought-out, although for the public survey, many viewed the selected methodology of computer assisted telephone interviewing as being limited to a certain segment of the population. To remain statistically valid and adequately compare results over time, the follow-up survey methodology and survey instruments must remain the same as what was used for the baseline survey. Reviewers suggested the use of Web-based surveys, more frequent surveys, and coordinating the survey to align with other outreach projects.

Automotive X Prize: Reviewers stressed the importance of educating students about advanced transportation technologies in ensuring long-term changes in vehicle use and adoption. The Automotive X-Prize was commended for the creative use of a wide-range of outreach tools such as competitions, national events, Web sites, and design competitions in engaging the general public, teachers, students, and industry stakeholders. Reviewers saw the project as an effective campaign to educate and inspire students to learn more about vehicle efficiency and sustainability, and pursue education and careers in the transportation sector. They felt the project was well planned, with appropriately scheduled milestones, and well funded. Reviewers considered collaboration with education providers, science centers, and Discovery Education to be appropriate but questioned the level of funding leverage from partners. Reviewers underscored the importance of metrics in tracking future success.

Safety, Codes and Standards Summary of Annual Merit Review Safety, Codes and Standards Subprogram

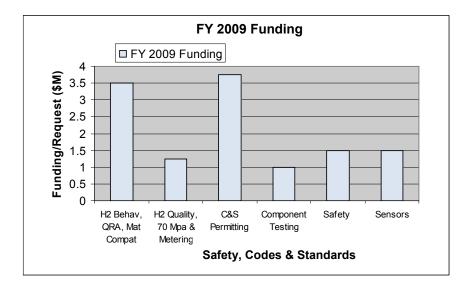
Summary of Reviewer Comments on Safety, Codes and Standards Subprogram:

The Safety, Codes and Standards subprogram reviewers stated that the projects were productive, well coordinated and organized. The reviewers were impressed by the breadth of activities and the ongoing commitment to safety, codes, standards, and information-sharing activities. They stressed that successes in this subprogram touch every other DOE hydrogen-related activity by fostering acceptance, collaboration and communication with critical stakeholders.

Reviewers stressed the importance of continuing efforts in critical areas such as hydrogen materials research, hydrogen codes, standards and permitting coordination efforts, hydrogen fuel quality, the Safety Panel, safety incident reporting and continuous updating of best practices. Reviewers complimented the projects' efforts for maximizing progress including leveraging the efforts of universities, standards development organizations, national laboratories, government agencies, and industry, as well as other subprograms.

Safety, Codes and Standards Funding:

The Safety, Codes & Standards funding for FY 2009 allowed for a strong domestic and international collaboration, as well as national development and coordination between national laboratories, government agencies and standards organizations. With FY 2009 funding at the request level, it allowed for sustained progress on hydrogen release behavior, hydrogen fuel quality, quantitative risk assessment, and leak detection research to continue the development of technically sound codes and standards for hydrogen and fuel cell technologies. The following chart indicates FY 2009 funding for Safety, Codes & Standards.



Majority of Reviewer Comments and Recommendations:

In FY 2009, nine Safety, Codes and Standards projects were reviewed, with good scores from the reviewers for the majority of the projects. The reviewers scored Hydrogen Codes and Standards and Permitting with the highest marks this year. Projects scored a high, low, and average score of 3.9, 3.0, and 3.5 respectively. Scores reflect progress made over the last year and the reported plans for future activity. Key comments and recommendations are summarized below and DOE will act on reviewer recommendations as appropriate to the overall scope, direction, and coherency of the subprogram's efforts.

Hydrogen Codes and Standards and Permitting: Reviewers praised the work for its varied engagement with industry, government, and researchers, particularly national laboratories. This work is seen as essential to the adoption and development of critical codes and standards. However, reviewers felt that a better explanation of the project direction for electric vehicle codes and standards was needed.

Hydrogen Materials Compatibility: This project is focused on materials research to support the development of technically sound codes and standards to ensure the safe design of infrastructure for the storage and transport of high-pressure hydrogen. The project was praised for its highly relevant technical accomplishments and careful planning. The reviewers noted it is an excellent example of how technical expertise and state-of-the-art equipment at DOE national laboratories can be applied to address gaps and obtain critical data needed to develop requirements for hydrogen codes and standards. Reviewers suggested that materials science expertise should be applied to composite materials and that the Technical Reference Manual should be expanded to include chapters on these materials, particularly for hydrogen storage tank standards for portable and vehicular use.

Hydrogen Safety Knowledge Tools: Reviewers considered this project to be valuable in terms of outreach to relevant groups and an excellent source of information for industry. Reviewers noted that both Web sites provide important information in an accessible and searchable way and are valuable tools in making this information available to the hydrogen community and the public. Reviewers also thought as projects mature, more effort should be concentrated on analyzing lessons learned from the Incidents Database and then integrated into the Best Practices Manual.

Hydrogen Fuel Quality: Reviewers said the work should earn praise for its sound approach and progress, rigorous methodology and excellent data exchange between national laboratories, international groups and standard development organizations. Some reviewers wondered how this data was going to be incorporated into hydrogen materials development and engineering.

Hydrogen Safety Panel: Reviewers considered the panel to be an important activity, which is essential to the program and is a key component to the safety, codes and standards work. The reviewers also thought there was an excellent mix of expertise and experience on the panel and were impressed with their accomplishments thus far. Reviewers also stated that the panel should have a method to integrate lessons learned from the plan reviews into an overall guidance document of principles for safety in hydrogen projects. Reviewers commented that the panel should take a more proactive approach when selecting projects to provide its expertise and review.

Safe Detector System for Hydrogen Leaks: Reviewers deemed this project as a critical activity and thought that it aligned well with the program's goals and objectives. They praised it for its technical approach and accomplishments, as well as its potential for developing a low cost and high accuracy sensor. It was suggested that the project should collaborate with national laboratories and other sensor experts.

Hydrogen Release Behavior: Reviewers viewed this project as valuable experimental work with lean ignition limits, auto ignition, and the separation distance work. The reviewers were impressed with the researchers' expertise in experimental design and engineering modeling to increase the understanding of hydrogen behavior. Because of its value, they suggested that this data should be disseminated to the industry when it becomes available.

Hydrogen Safety Sensors: Reviewers thought this project was a valuable contribution to the codes and standards development. The reviewers approved of the project's clear approach to identifying needs and gaps. However, they did suggest that there should be better communication with sensor manufacturers to address the issues of wide area sensing technologies.

Codes and Standards for the Hydrogen Economy: Finally, reviewers thought this project, which is not a research and development activity, played an important management and support role to codes and standards development organizations. The reviewers noted a need to improve its efficiency in delivering funds to projects. Reviewers also felt it would be beneficial to provide more information on how this project plans to overcome its barriers.

Technology Validation Summary of Annual Merit Review Technology Validation Subprogram

Summary of Reviewer Comments on Technology Validation Subprogram:

Reviewers continue to consider the learning demonstration project to be a key element in determining whether the program's hydrogen fuel cell activities are on course to achieve established research and development targets. The comments seemed to be primarily favorable. Reviewers from the auto industry gave the impression that the key players can envision the ability to commercialize these products.

Comments tended to demonstrate consistent themes. Several reviewers mentioned their perception that the subprogram overview was adequately presented with the challenges and focus of work clearly identified. Others mentioned that there do not seem to be any gaps in the project portfolio. Multiple reviewers commented that the subprogram was well-organized, carefully planned, focused, and appeared to be effective in supporting the DOE Program and its goals.

Overall progress was well outlined (total miles traveled, fuel dispensed, etc.), and over a million miles of travel is a significant accomplishment. Progress on durability also appears good (60,000 miles). Progress in the data collection aspect since 2008 is very good. Future projects, including the project at the Volcano National Park were discussed.

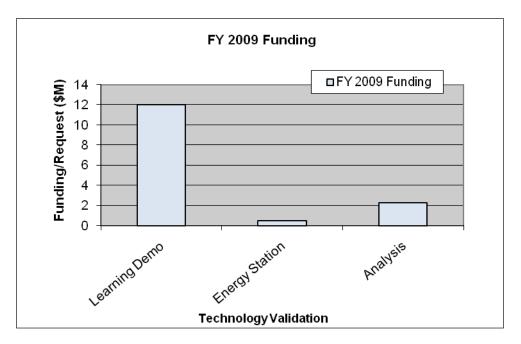
Reviewers commented on the progress that has been made including that the targets are being met with impressive numbers of vehicles/stations, and that the cost is dropping substantially on fuel cell stack and hydrogen cost. Comments noted the performance of fuel cell vehicles under real world conditions, and the documentation and analysis of results are very important activities.

The data collection and analysis portion of the program is very carefully planned, and provides adequate safeguards against distribution of proprietary data while giving more than adequate information for the public to be used in the DOE program activity. Data collection and dissemination is an effective and transparent process. A well-designed data matrix was developed.

The major concern among the reviewers seemed to be that if the 2010 budget holds, and hydrogen fuel cell vehicles are eliminated, future program goals will be abandoned.

Technology Validation Funding:

The funding portfolio for Technology Validation reflects the continuation of the Learning Demonstration project as it enters its fifth and final year. The Technology Validation activity was transferred to the Vehicle Technologies Program for FY 2009 only. The following chart indicates the FY 2009 funding for the Technology Validation subprogram.



Majority of Reviewer Comments and Recommendations:

The reviewer scores for the Technology Validation subprogram were a maximum of 3.78 and minimum of 2.03 with an average score of 3.16. Only three scores were below FY 2008's average score of 2.5. DOE will act on reviewer comments as appropriate for future planning.

Although the reviewers did not provide major redirection recommendations, they did provide key comments in each of the task areas.

- **Learning Demonstration** Although the subprogram is focused on transportation and fuel cell vehicles, one reviewer mentioned he would like to see more effort applied to production and storage infrastructure.
- Energy Station/Power Parks One reviewer asked how the DOE program could justify the cost of continuing data collection in the fleet vehicles and new construction at the Hawaiian power park at this time.
- Analysis Analysis of the greenhouse gas emissions (W-T-W) is a very important addition to address objections, especially regarding hydrogen production via electrolysis.

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Systems Analysis Summary of Annual Merit Review Systems Analysis Subprogram

Summary of Reviewer Comments on Systems Analysis Subprogram:

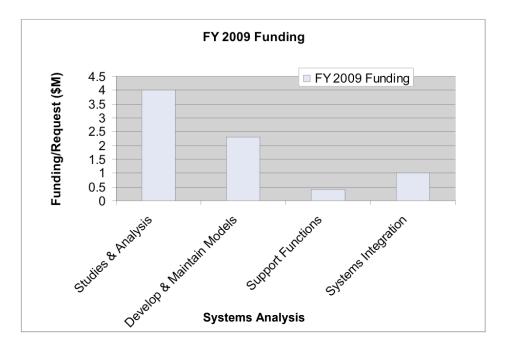
In general, the reviewers commented that useful new insights were gained, and they considered the Systems Analysis subprogram a significant activity of DOE. Reviewers stated that this subprogram is well focused and managed, while playing a critical role in placing hydrogen and fuel cell R&D into perspective. The project portfolio is considered sufficiently diverse, and the suites of models developed are deemed as useful tools for industry and academia.

It was also noted that the Systems Analysis subprogram comprises a very broad range of issues. While this presents a challenge in keeping information up to date, reviewers observed that significant progress was presented and that the evolution of analytical tools has followed a logical path with no significant gaps identified.

The main recommendations identified by the reviewers for Systems Analysis were: 1) the case of a more limited deployment of hydrogen vehicles should also be considered; 2) existing markets for hydrogen (i.e., refinery and agriculture) should be tapped into for central hydrogen generation cases to make use of this vast potential; 3) efforts to more appropriately incorporate hydrogen technologies into national energy models should be considered; 4) interactions between the variety of models should be clarified; 5) early market use of stationary fuel cells should be assessed against competing technologies; and 6) priorities of the subprogram need to be clarified and illustrated, thus allowing the information gleaned from analysis to present clear options for policy decisions. The Systems Analysis subprogram will take these reviewer recommendations into consideration in improving existing efforts and developing appropriate R&D plans.

Systems Analysis Funding:

The funding for Systems Analysis primarily includes emphasis on sustaining a suite of diverse models and conducting in-depth analysis to answer critical cross-cutting questions in meeting the Hydrogen Program's goals. The FY 2010 request-level funding profile, subject to Congressional appropriation, will focus on early market analysis, synergies of transportation and stationary applications, and resolving barriers to hydrogen infrastructure development.



Majority of Reviewer Comments and Recommendations:

In general, the maximum, minimum, and average scores of the reviewers gave for Systems Analysis projects were 3.3, 1.8 and 3.0, respectively. Reviewers commented that a consistent set of analytical tools was developed and various impacts were analyzed utilizing these tools. The main recommendations for the Systems Analysis projects are summarized below. The Systems Analysis subprogram plans to address these recommendations.

Model Development: Projects involved in developing, enhancing, and sustaining models received very favorable reviews, with the highest score given to one of these projects. The majority of the projects were regarded as comprehensive, relevant, and functional tools, developed through appreciable collaboration with a variety of stakeholders. A suggestion emphasized repeatedly by reviewers was that the models be peer reviewed and validated with industry and other stakeholders. It was also pointed out that as these models have become more complex over the years, accumulation of combined errors presents a critical issue that needs addressing. For further expansion of the models, reviewers suggested that factors such as renewable pathways, carbon capture and sequestration, criteria pollutants, and potential new vehicle fuel economy/emissions standards legislation be taken into consideration to enhance analysis results derived from these models.

Program Analysis: Most of the analysis projects reviewed this year are being completed in FY 2009. In general, the reviewers concurred that the analysis projects need to be peer reviewed and validated prior to issue and publication. The reviewers felt that the Argonne National Laboratory hydrogen quality project is an important effort that has shown good progress and suggested the inclusion of renewable fuel sources (e.g., biogas) and consideration of costs associated with analytical requirements (to track if purity is being maintained). The Sandia National Laboratory project on analyzing energy infrastructures was deemed by reviewers as addressing critical questions. Suggestions were made for its scope to be expanded to explore all-electric vehicles and renewable fuels, while recommendations were made to collaborate more closely with stakeholders and employ an iterative approach for supply and demand considerations.

Other Studies: Other studies included in the project portfolio included a "lessons learned" study related to stationary applications by the Missouri University of Science and Technology and an assessment of the commercialization successes of related technologies and studies supported by the Program, conducted by the Pacific Northwest National Laboratory (PNNL). The "lessons learned" study is being completed in FY 2009 and has explored opportunities and strategies for the use of hydrogen in portable and stationary applications based on various national and international strategies of existing applications that were investigated. The commercialization study by PNNL is an ongoing effort that was believed by some reviewers to serve as a good feedback mechanism and a valuable data set, while others raised caution that the project may be premature at this point in time. Reviewers suggested continued updates of findings, development of a user-friendly Web-based access to the information, consideration of market needs/trends, and analysis of the information garnered.

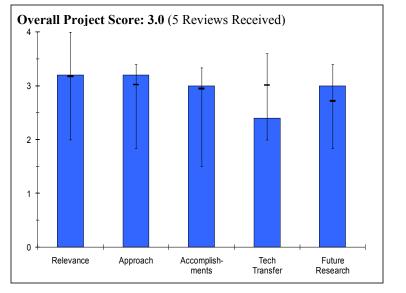
Project # AN-01: HyDRA: Hydrogen Demand and Resource Analysis Tool

Johanna Levene; National Renewable Energy Laboratory

Brief Summary of Project

The objective of this project is to develop a Web-based geographic information system (GIS) tool to allow analysts, decision makers, and general users to view, download, and analyze hydrogen demand, resource, and infrastructure data spatially and dynamically. HyDRA is designed to display and aggregate the results of spatial analyses. It is a repository for spatial data inputs and spatial data results. To access HyDRA, go to http://rpm.nrel.gov and request a login.

<u>**Ouestion 1: Relevance to overall DOE**</u> <u>objectives</u>



This project earned a score of **3.2** for its relevance to DOE objectives.

- It's an interesting program, but it's not clear who is supposed to use it or if it would actually be used by them.
- Very relevant in assessing geographical markets and resource constraints. The Web-based tool allows further development and easy deployment.
- This activity supports Task 2, barriers A, B, C, D, and E to develop and maintain models and tools.
- This project appears to be useful for those involved in hydrogen to evaluate hydrogen demand and resource in a given geographical location.
- It is particularly useful to continually update the model with the latest cost of feedstock (e.g., natural gas, electricity) to have a more realistic picture.
- Conceptually, the relevance is excellent. Practically, gas prices and electrical energy prices are not static but vary tremendously with time as well as location. The same is likely true for real estate, construction costs, capital costs, etc. By the time a composite map is generated, it is likely outdated and might give misleading results.

Question 2: Approach to performing the research and development

This project was rated **3.2** on its approach.

- There is concern that the model is "static" and does not address a dynamic environment of ever changing costs. For example, as the usage of one energy input rises, would the cost remain the same relative to other options? Although a given cost might be "X" today does not mean it will stay that way if there are limits to its production.
- Focus on cross-coordination with other tools and addressing the barriers in maintaining an open structure. Database development is key to the efforts because they will allow data export/import to and from other tools.
- The idea of interactively combining GIS data sets is outstanding. The visual nature of the data will make the information much more accessible to a wider audience and will be particularly useful to government officials who need data at the county resolution.
- While it is useful to know where hydrogen demand and methane wastewater resource co-exist, it is also useful to determine if the methane resource available is enough to satisfy the potential hydrogen demand for the numbers of forecourt commercial hydrogen stations.

- Regarding the Missouri case study, need to specify the scale/capacity factor of the industrial steam methane reformer (SMR) (How much larger is the industrial SMR compared to the commercial SMR?). An "industrial" SMR hydrogen plant at a refinery can produce as much as 50 million standard cubic feet daily of hydrogen and its hydrogen cost is much lower than the industrial SMR (in the Missouri case).
- The approach is a combination of overkill and simplicity.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated **3.0** based on accomplishments.

- Various new analyses done between last year and the current year. Again, acquiring data is the key to these efforts. Didn't quite understand why re-architecture was required; it should have been planned/done from the start.
- Changing architecture is never trivial. Impressive that team redesigned architecture and added more databases.
- The model user interface appears to be friendly and easy to navigate through.
- Analysis and spatial datasets on hydrogen demand appear to be a bit lacking.
- After over three years of effort, the accomplishments can only be considered fair.

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated **2.4** for technology transfer and collaboration.

- Very little comment on collaboration with other organizations, other than integration with other DOE-funded models.
- Interaction with industrial partners would be helpful to validate assumptions and to see if it's really useful in rolling out infrastructure.
- Not too many (industry) partners in this work.
- At this point it would be useful to bring in collaborators from industry and governmental planning.
- It is critical that this model works in conjunction with other models to look at the whole picture (i.e., public acceptance of hydrogen fuel cell vehicles [HFCV], competing technologies, external market forces, right-of-way issues).
- There is the intent to interact with other models and simulations from other organizations, but relatively few interactions to date.

Question 5: Approach to and relevance of proposed future research

This project was rated **3.0** for proposed future work.

- Need to have a plan for dynamic transitions (in time/year).
- Expanding the model past hydrogen will be very useful. Adding a dynamically linked database to keep the model relevant is definitely needed.
- The proposed future work could also take a look at the feasibility of doing carbon capture and storage spatially, specifically the non-renewable and central cases. Given the increasing push to minimize green house gases (GHG), this might be a useful factor to consider for infrastructure installation.
- Future plans would improve the product, especially the dynamic layering and proposed interactions with other software.

Strengths and weaknesses

Strengths

- A useful input into the Macro-System Model (MSM) overall, big picture.
- Strength is its application and relevance to overall hydrogen infrastructure analysis and the creation of the database.
- Interactive GIS is a very powerful tool with wide applicability.
- This is a good concept.

Weaknesses

- It is not clear how the information will get updated over time. For example, natural gas and electricity rates are expected to be volatile. Will the model automatically update pricing or is that manual?
- Decisions on production must assume economics over a 15-20 year period prior to an investment decision, so a look forward on those costs is just as important as today's costs.
- Need to start deploying the tool for transition scenarios; make it dynamic so existing infrastructure need not be ripped up when making transitions.
- Limited to inexpensive databases. There is some more expensive data out there that the DOE should consider purchasing so that the tool can be made as useful as possible.
- A lot of time and effort has been expended for a tool that appears to be only marginally useful as it stands.

- Develop means to address impact of variable pricing due to time-of-day issues.
- Develop a means to address impact of future cost changes as demand from hydrogen production uses more of the given energy input.
- Automate the update of pricing information if this has not already been done.
- Incorporate dynamic behavior to enable playing out a transition.
- More actual studies, at some point the model will contain enough data that it should be validated extensively, especially for the conventional scenarios that exist now.
- Continue as planned.

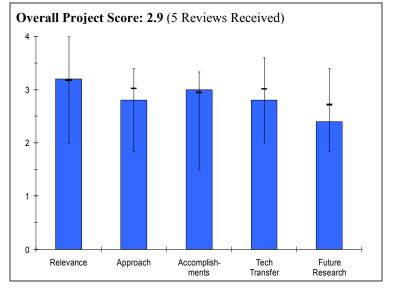
Project # AN-02: Water's Impacts on Hydrogen

A.J. Simon; Lawrence Livermore National Laboratory

Brief Summary of Project

The objective of this project is to quantify the impact of water on a future hydrogen economy, including the economic impact of water prices on hydrogen production and the regional impact of hydrogen production on regional water resources. The project shows 1) how the energy-water nexus affects all future fuels (not just hydrogen), 2) how water impact analysis is fundamentally regional, and 3) how water permitting is likely to be a bigger impediment to hydrogen adoption than water price.

<u>**Ouestion 1: Relevance to overall DOE**</u> <u>objectives</u>



This project earned a score of **3.2** for its relevance to DOE objectives.

- To the extent that this is a problem, it's useful. To the extent that it's not, then it isn't. This ought to be a fairly quick, high-level assessment as a first step. It is likely to only have an impact in certain areas, so only focus on worst case. There is no need to even think about large portions of the country.
- Water is a critical resource and so the role it plays in any future energy infrastructure deployment is an important aspect to look at for intended and unintended consequences.
- Relevant under Tasks 1, Perform Studies and Analysis, and Task 2, Develop and Maintain Models and Tools, in addressing barriers A and B.
- Not certain if this is one of the critical issues for the commercialization of hydrogen fuel cell technologies. Wastewater from reformers and electrolyzes can be captured, treated, and recycled so the net amount of water added to the system is minimized. The total amount of water usage is relatively small.
- Regarding regional impact, it will likely be similar to current gasoline formulation requirements in places like California and the Midwest. These places typically have higher gasoline prices; places with water resource constraint or any other resource constraints will likely have higher hydrogen costs.
- Water availability is already a problem in many areas and is generally expected to become more of a problem. This could certainly be a factor in hydrogen production.

Question 2: Approach to performing the research and development

This project was rated **2.8** on its approach.

- Some of the assumptions are not clear for the use of water. Is it actual process water, and if so, is it electrolysis or reforming? Or, is the larger use as cooling water, in which case there are several options?
- Good overview chart of water source, use and disposal to provide context. Geographical information used to identify water stress areas. The approach overall is based on mass balance at a higher level and is adequate for the current purpose.
- Considering that water supply and demand is critical to hydrogen production from electrolysis, combing energy and water balances again is critical.
- It will be likely that the system developers will have multiple models of hydrogen generators designed to run at certain geographical locations. For water constraint locations, the wastewater recovery and cooling systems would have to be different compared to systems installed at places with less water constraint.

- Data from process modeling and regional analysis will be useful to tailor a system to run at specific locations to maximize efficiency and minimize water usage. Therefore, the model should tell the system developers how to design their systems, not the other way around.
- Generally good, but could be better. Approach neglects possible synergy with existing or possible industrial water users, which seems to be a likely outcome in many instances. It also seems to neglect the effect that hydrogen production, with its water usage, would have on costs.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated **3.0** based on accomplishments.

- It is not clear this is really a barrier to a hydrogen economy. It would be good to show an overall picture of water use compared to a fuel infrastructure. For example, for a worst case (e.g., a desert climate like Los Angeles), what percent of existing water use would be needed to produce hydrogen to supply the existing vehicle fleet? If insignificant, then it's not an issue. Also, some of the existing water use might be available for dual use (e.g., use of water from thermal electricity plants as cooling water and then as process water).
- Unclear in terms of progress made in identifying water resource constraints and high-level implication on hydrogen infrastructure. Accomplishments include model development to date. Focus seems to be resource costs rather than constraints.
- Two different analyses were presented. This approach needs to be much more widely applied.
- Cooling towers most likely fit central SMR and electrolysis cases. They are not typically used at forecourt cases. The cost of treatment could be significant depending on the water purity levels required.
- Not yet complete and relatively few results available to date. Much emphasis on permitting, which seems to be a separate issue.

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated **2.8** for technology transfer and collaboration.

- Some industrial partners would be helpful, as well as support from localities in areas with limited water supply. They would be in the best position to comment on availability of permitting for water supplies, as well as ease (or not) of permitting new applications. Comments on permitting being an issue do not appear founded on actual information.
- No industry partners have vested interest in the development.
- Collaborators are mostly other national labs. This needs industrial input, especially from large utilities that may want to store large amounts of hydrogen via water electrolysis.
- Integration with the DOE Hydrogen Analysis Model (H2A) and Macro-System Model (MSM) is critical to produce any meaningful data.
- Collaborations seem appropriate for the project.

Question 5: Approach to and relevance of proposed future research

This project was rated 2.4 for proposed future work.

- Future work should focus on whether this is even an issue, prior to full integration with MSM. Given the overall uncertainty in hydrogen cost, it appears that water cost really is within the rounding error and not meaningful. There are also numerous technologies around cooling, and it is not clear if the assumptions would be accurate.
- Only a high level description is given; there are no clear milestones.
- Budget is currently zeroed. This is a shame. The project is critical to the DOE mission and should be continued.
- The project should mainly focus on water availability issues and let the system developers design their systems to best "get around" these issues based on the data.
- It might be useful to look at technologies that are/will be competing for the same water resources (especially the significant users).
- Planned work seems very appropriate to make the tool more useful.

Strengths and weaknesses

Strengths

- It is an interesting issue, and one that might not be widely recognized. Good to analyze to see if it truly is an issue.
- Nothing seems to stand out as a strength.
- Interplay of water and energy.
- Fills a need that is not otherwise met.

Weaknesses

- Need to compare to other fuel pathways for comparison. Are they a draw on water resources as well, and/or does water become available as fuel use changes?
- No information was provided (except some vague references during the presentation) on the actual costs of the water and water treatment. Based on the verbal discussions, it appears as if water cost has a minimal impact on overall hydrogen cost. This should be included in the presentation to show overall impact.
- The issue appears to be concerning the "cost" of water more than its actual availability. If so, then other technologies can overcome actual availability issues.
- Focus should be on water resource constraints and not economics.
- Not enough real world analyses have yet been accomplished.

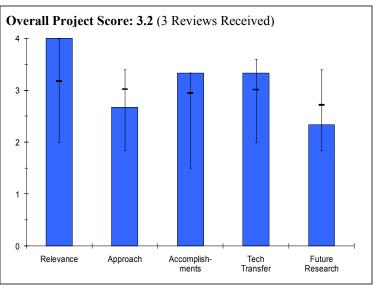
- Develop some conclusions prior to moving any further. This does not appear to be a critical path issue on developing a hydrogen economy. If so, document and move on, with some basic input on costs to H2A.
- Add comparisons of water use/constraints via various energy pathways (e.g., conventional, hydrogen, plug-in hybrid electric vehicles, biofuels) to project scope.
- Continue project.
- Project should be continued with proposed work.

Project # AN-03: Cost Implications of Hydrogen Quality Requirements

S. Ahmed, D. Papadias, and R. Kumar; Argonne National Laboratory

Brief Summary of Project

The objective of this project is to correlate impurity concentrations (in hydrogen) to the cost of hydrogen, as functions of 1) process parameters (e.g., temperature, pressure, and steam to carbon ratio [S/C]) and 2) performance measures (i.e., hydrogen recovery, efficiency). A rigorous model of the pressure swing adsorption (PSA) system has been set up as part of a flexible systems model, and the system model results have been correlated with the cost of hydrogen. The project has concluded that the cost of hydrogen is only slightly affected by the impurity specification guideline in the natural gas-steam reformate PSA system studied.



Question 1: Relevance to overall DOE objectives

This project earned a score of 4.0 for its relevance to DOE objectives.

- Hydrogen purity is a very important topic for the hydrogen economy. This is a continuing debate and needs to be resolved.
- Hydrogen quality represents a key interface between original equipment manufacturers (OEM) and fuel providers, and it is a critical topic of contention/optimization.
- This project supports DOE RD&D objectives under Task 1, Perform Studies and Analysis and Task 2, Develop and Maintain Models and Tools, by addressing barriers A and B.

Question 2: Approach to performing the research and development

This project was rated 2.7 on its approach.

- The approach for this particular pathway is good, but there are several issues. One large issue (other than those mentioned below) is the potential for differences between different manufacturers' equipment.
- Approach is good looking at life cycle analysis and economic impact to determine the optimal purity levels. A reference to SAE J2719 (with current levels) would be good for the audience to look at the context.
- The approach is to analyze the effect of impurities on the cost of hydrogen using reformate from natural gas purified by pressure swing adsorption.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated 3.3 based on accomplishments.

- This is good progress to date, but there is a lot more to do (to broaden to make the program more effective).
- Similar results as the previous year, but including more system types (autothermal reforming [ATR], gasification) and process details. Still no impact of impurity on fuel cell stack included. No progress on canary species establishment/agreement.
- This appears to be a very realistic model that can track realistic impurities. The input seems to be real natural gas and the process appears very relevant.

620 FY 2009 Merit Review and Peer Evaluation Report

<u>Ouestion 4: Technology transfer/collaborations with industry, universities and other laboratories</u>

This project was rated **3.3** for technology transfer and collaboration.

- Several good partners, but should likely add some analytical companies.
- No other working/industry collaborator.
- Good mix of collaboration with other national labs and industry.

Question 5: Approach to and relevance of proposed future research

This project was rated 2.3 for proposed future work.

- The work completed to date covers only a subset of hydrogen production and there are many more to go.
- In addition, it is very important to consider not only actual hydrogen purity, but also the analytical requirements associated with those purities. Cost of production might be small compared to cost of keeping it at that purity, as well as the analysis required.
- Future work does not include identifying fuel cell impacts and costs associated.
- Too much emphasis on fossil fuel inputs.

Strengths and weaknesses

Strengths

- This is an important effort.
- Good industry collaborations.
- Well thought out engineering study.

<u>Weaknesses</u>

- The project team comments on efficiency and recovery, but does not comment on analytical capability and costs. These are very important.
- Does not refer to SAE J2719 and the "full slate" of impurities, especially particulates.
- Looks at "full scale" production, but not impact on lower volumes with initial rollouts.
- Limited data from industry.
- Not enough emphasis on renewable hydrogen. Biomass gasification, methane from fermentation, and a comparison with hydrogen from electrolysis should be included.

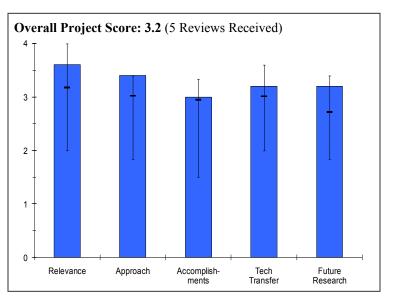
- Continue with other production pathways.
- Add cost for system design (to keep gas at high purity level).
- Add cost for expected analytical requirements.
- Consider a program to analyze if impurity levels do not have to be as low as currently specified.
- Calculate the optimal levels for each impurity species based on fuel cell impacts and purification costs.
- Add more renewable fuel sources.

Project # AN-04: Macro-System Model

Victor Diakov and Mark Ruth; National Renewable Energy Laboratory Mike Goldsby and Tim Sa; Sandia National Laboratories

Brief Summary of Project

The overall objective of this project is to develop a macro-system model (MSM) aimed at 1) performing rapid, cross-cutting analysis by utilizing and linking other models and improving consistency of technology representation (i.e., consistency between models), 2) supporting decisions regarding programmatic investments through analyses and sensitivity runs, and 3) supporting estimates of program outputs and outcomes. Objectives for 2008/2009 are to 1) improve structure of the MSM and expand graphical user interface capabilities, 2) update versions of component models, 3) expand stochastic analysis capability, and 4) build interaction between the MSM and spatial and temporal models.



Question 1: Relevance to overall DOE objectives

This project earned a score of **3.6** for its relevance to DOE objectives.

- Arguably, this is the apex of the DOE modeling and therefore must be important by definition, assuming that modeling is important to DOE goals.
- The idea is to develop an open architecture tool to connect with other tools and build the interaction with those tools. It is quite relevant to deployment and use of other tools being developed as a part of this program.
- This project fully supports the DOE objectives through Task 2, Develop and Maintain Models and Tools, addressing barriers B, C, and D.
- With so many models looking at various areas, having this tool to link the models together to produce meaningful results is important.
- Very relevant since it can tie together several important simulations.

Question 2: Approach to performing the research and development

This project was rated **3.4** on its approach.

- A major barrier to the success of MSM is validation.
- Approach appears to be planned out and has a step-by-step development.
- The approach is to integrate a number of individual models in to an MSM and allow access through a graphical user interface (GUI).
- Appears to be a useful tool for providing critical pieces of information for the assessment of hydrogen technology potential.
- Excellent approach and excellent presentation detailing the approach.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated 3.0 based on accomplishments.

- From an information technology point of view, there appears to be good progress at integrating the models.
- Statements such as the one slide on greenhouse gas (GHG) tax analysis can be very deceiving if shown without the appropriate assumptions. Given the number of assumptions, this can be potentially confusing as well as deceiving. For example, one of the backup slides shows GHG emissions being cut roughly in half with hydrogen, so how can a CO₂ tax have no effect?
- Added risk analysis tool based on expert opinions, which seems like a good addition but I'm not sure how reliable the expert input is (being myself a polled expert).
- Progress towards integrating the component models seems to be on track. It is of concern that the MSM may be beginning to run too slowly. Perhaps more attention should be paid to optimizing code in the integration of the models so that the whole thing doesn't grind to a halt. It would be nice to see more examples of actual analyses run with the model.
- Not able to see much progress based on this year and last year presentations. It appears that most of the activities concentrated on improving the model's user interface. Model needs to be tested and validated by industry for a "sanity check."
- Excellent accomplishments.

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated **3.2** for technology transfer and collaboration.

- Appears to be a number of collaborators. Could use some representatives from hydrogen producers.
- Good long list of collaborators. Need to see industry start using this tool for routine analysis.
- Nice collaborations with national laboratories. Needs collaboration with university computer scientists and government and industrial end users.
- Obviously very good collaboration with other models as they provide critical pieces of information to this tool.
- Combination of national laboratories, industry, and a university is excellent.

Question 5: Approach to and relevance of proposed future research

This project was rated **3.2** for proposed future work.

- There is a need to address the overall "error band" of the results. Each of the input models has an inherent inaccuracy. As these get built up to the MSM, do these potential errors compound to the point where the model results are questionable?
- There is a flowchart showing progress and future work, but we need to see progress in terms of analysis results.
- Adding additional models and improving the GUI are good ideas. MSM needs to allow more comparison with competing non-renewable technologies.
- It is critical that the model is continually updated with the linked updates from other models.
- Proposed future work will make an excellent project even better.

Strengths and weaknesses

Strengths

- MSM provides a means to tie all models together, which otherwise would be very difficult to do independently.
- The project is critical to expanding the use and capability of existing/other tools being developed as part of the systems analysis program.
- Integration of a large number of powerful individual models is a strength.

Weaknesses

- Need to provide a means to validate the model to make sure it provides results that are realistic. For example, if one model was somehow inputting incorrectly, how would it be noticed?
- It seems like much of the effort is spent on programming languages as opposed to real analysis.
- Need to validate the overall results with industry.

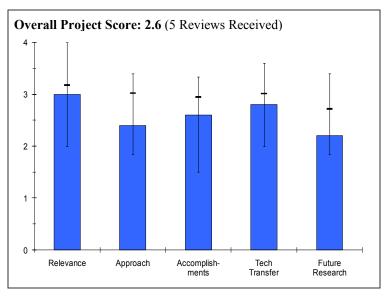
- It may be too cumbersome to deliver analysis tools in real time.
- By combining the other tools, it seems likely that there could be an accumulation of combined errors. It might be prudent to use some type of combined error bands and track possible accumulated error.

- Provide a verification step to demonstrate that the model outputs are realistic.
- Consider performing an industry validation program.
- Add more transparency in what is being calculated. Add more diversity in processes that can be analyzed.
- Continue with proposed work.

Project # AN-05: Discrete Choice Analysis of Consumer Preferences for Refueling Availability *Marc W. Melaina; National Renewable Energy Laboratory*

Brief Summary of Project

The objective of this project is to 1) quantify consumer reluctance to purchase an alternative fuel vehicle due to a lack of refueling availability, 2) compare survey results to comparable results derived from analytic models, and 3) develop a general discrete choice model for major urban areas. The project has developed an improved quantitative representation of the cost penalty for limited refueling availability using discrete choice survey and modeling methodology. Penalties have been estimated for limited coverage at three geographic scales (i.e., metropolitan, regional and national) and for four distinct metropolitan areas (i.e., Los Angeles, Seattle, Atlanta, Minneapolis-St. Paul).



Question 1: Relevance to overall DOE objectives

This project earned a score of **3.0** for its relevance to DOE objectives.

- Very relevant. Understanding the degree of infrastructure needed to enable a reasonably sized hydrogen car fleet determines whether the goals of the overall DOE program are achievable.
- Not critical to the program, but of good relevance to transition scenarios and various possible outcomes (including unintended ones).
- This project supports the DOE objectives under Task 1, Perform Studies and Analysis, addressing barriers A and B.
- It is unclear if this work would be necessary. The interdependency between vehicle and infrastructure availability will largely dependent on both the original equipment manufacturers (OEM) and energy companies and their recognition as to when it is economically viable to enter the "hydrogen economy". There must be a business case for both sides. It is also dependent on government actions. In the end, the single most important factor for the consumer is cost.
- The relevance is good since the types of issues addressed are very important.

Question 2: Approach to performing the research and development

This project was rated **2.4** on its approach.

- Approach defined the difference between alternatively and conventionally fueled vehicles in a mostly neutral manner. However, calling the car an "alternative fuel vehicle" and touting its green benefits may not be the most conservative way to go about it. It is much easier to check a box that says "I would spend another \$2,000 for this" than to actually spend that money.
- It would be interesting to calibrate the survey. To get an idea of the difference in response if people had to put real money on it. The researchers could use the same methodology to attempt to predict consumer preference for the hybrid Honda Civic over the less expensive baseline model to see if reality matches the prediction.
- Not clear how many surveys were completed; with so many variables, a large sample may be required to be able to draw a statistically valid conclusion.
- Discrete choice is a good approach to look at qualitative possibilities, not quantitative. Requires quite a lot of behavioral data, which makes this model all the more inaccurate.

- The approach is to use market survey data in order to predict the essence level of market introduction to achieve a vehicular-based hydrogen economy.
- This study is only looking at one side of the picture. While it is true that the consumers will be reluctant to purchase a hydrogen fuel cell vehicle (HFCV) because of the lack of fueling station availability, the level of reluctance is equally as much for the energy providers since building hydrogen stations represent significant capital investment, especially in the early stage. The old saying "if you build it, they will come" does not necessarily hold true in this case.
- It is useful to eliminate other factors and only include social and environment benefits and limited fuel range factors. This will provide more meaningful survey results based on these limited considerations.
- These types of surveys almost always give unreliable results.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated **2.6** based on accomplishments.

- The approach delivers the right outputs to guide decisions on infrastructure. Per this reviewer's other comments, it needs validation and market input to ensure that the outputs are correct.
- Very well designed survey for consumer acceptance based on refueling availability. The data should be quite useful to fuel providers and OEMs.
- Not convinced that we really learned anything new from extending the study to the new cities studied this year.
- Again, as indicated, the cost barrier for infrastructure is significant and should not be overlooked.
- Better user interface for the survey is a plus.
- Might need to verify for the regional cases whether the number of stations shown is practical from a resource availability standpoint.
- With respect to the charts showing the highest number or percentage of hydrogen station available where there are zero cost penalties, are the hydrogen stations displacing the gas stations or are they in addition to the gas stations? Would a gas station be bulldozed and a hydrogen station built on the same lot?
- The project is complete so the planned work has been accomplished; however, I'm not sure of the value.

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated **2.8** for technology transfer and collaboration.

- Team should consider bringing an automaker on board or another contractor with significant auto marketing experience. Such a partner could provide a lot of insight on how consumers choose which vehicle to buy.
- Quite a few collaborators. Need to get industry validation/approval of this approach.
- Needs collaborations with auto industry and energy companies.
- Good collaborations with various institutions. Consider rolling out the survey to a broader range of the public.
- Some collaboration, but not impressive.

Question 5: Approach to and relevance of proposed future research

This project was rated **2.2** for proposed future work.

- The approach needs to be validated before going forward, for example, by checking the method against a currently available market choice (e.g., regular or hybrid Honda Civic). People want to say they would buy an alternative fuel vehicle if given the choice, but would they really do it?
- Proposed future can include a high level validation of the results from the model.
- The proposed trade-study (scale vs. numbers) is a good one to look at and will be useful for the industry.
- This project appears to have run its course.
- Additional trade-off studies between station capacity and numbers of station will be useful. It is not necessary to have all stations initially be at 1,500-kg/day capacity. This will ease the infrastructure cost penalty pain.
- Proposed additional work seems to be of marginal value.

Strengths and weaknesses

Strengths

- Good methodology and important topic. Examines different strategies and acknowledges the importance of the market driving hydrogen acceptance.
- The project is based on a good theoretical approach.
- Consumer driven surveys allowed real analysis of the market.

Weaknesses

- This project needs validation and specific auto market insight.
- The project team needs to get a thorough validation of the conclusions.
- Not really integrated into other DOE analysis models.
- Too much dependence on an approach that is known to be unreliable.

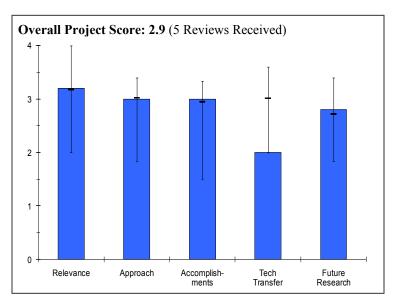
- Add validation tasks.
- Model validation should be a good addition to the project scope.
- The project should end until market conditions change.
- Expansion of scope is not recommended.

Project # AN-06: Analysis of Energy Infrastructures and Potential Impacts from an Emergent Hydrogen Fueling Infrastructure

Andy Lutz and Dave Reichmuth; Sandia National Laboratories

Brief Summary of Project

The objectives of this project are to 1) use dynamic models of interdependent infrastructure systems to analyze the impacts of widespread deployment of a hydrogen fueling infrastructure and 2) identify potential system-wide deficiencies that would otherwise hinder infrastructure evolution, as well as mitigation strategies to avoid collateral effects on supporting systems. Transition to hydrogen fueling is expected to rely on distributed steammethane reforming; we must understand the impact of hydrogen vehicles on the infrastructure.



<u>**Ouestion 1: Relevance to overall DOE**</u> <u>objectives</u>

This project earned a score of **3.2** for its relevance to DOE objectives.

- It is good that this project considers plug-in hybrid electric vehicles (PHEV) and conventional vehicles as competitors to hydrogen vehicles. This is a critical point for the DOE program to understand. The project answers important questions about feedstock supply limits.
- Good relevance to look at the transition in light of other competing vehicles.
- The project is critical to the Hydrogen Program and supports DOE RD&D through Task 1, Perform Studies and Analysis, addressing barriers A, B, and E.
- Not certain how useful this work is since it only looks at one part of the picture (forecourt steam methane reforming [SMR]) regarding infrastructure and only two vehicle technologies [PHEVs and hydrogen fuel cell vehicles [HFCV]).
- Not certain of relevance of looking at plug-in hybrids and other vehicles. They are competing technologies; however, the projected timelines to commercialization are different.
- This project addresses a major issue.

Question 2: Approach to performing the research and development

This project was rated **3.0** on its approach.

- The approach presupposes market share between gasoline, PHEVs, and HFCVs. The prior work that determined the market share does not consider the possibility presented in this project that the increase in natural gas price makes HFCVs expensive to operate and therefore lowers their market share.
- The Energy Information Administration (EIA) projections for gasoline price do not take into account the model's prediction that there will be no gasoline cars on the road.
- An iterative approach should be used to take into account how supply problems affect demand. In the present work, the demand is presupposed and its effect on supply is studied.
- A system dynamics model is a good way to look at the various possible scenarios and the design vs. unintended implications. This is similar to work being done by Massachusetts Institute of Technology (MIT), Shell, and Ford. The teams need to collaborate.

- This project addresses critical questions. In particular, at what HFCV penetration does the demand for naturalgas-derived hydrogen negatively impact natural gas distribution? Also, what conditions affect the competition between HFCVs and PHEVs?
- Night-time-only charging for PHEVs might not be realistic.
- While it is useful to look at competing vehicle technologies (PHEVs and HFCVs), it might also be useful to look at smaller, high efficiency internal combustion engine vehicles and diesel vehicles that can get 30+ mpg.
- It is recognized that the SMR is only an interim technology for hydrogen fueling applications, so looking at SMR out to 2020 and beyond might not be very realistic. Instead, the project should look at renewable hydrogen production technology cases for the long term.
- The approach requires many assumptions, some of which are questionable. Limiting current modeling to California was a good move.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated **3.0** based on accomplishments.

- Work makes a clear case that penetration of hydrogen vehicles will be severely limited by availability of natural gas. This is the most important outcome of the work.
- This is a fair projection of the issues presented. Scope could be much wider in terms of looking at other parameter impacts, policy, geography, regulations, etc.
- This study looks at a very real limitation of the adoption of fuel cell and plug-in hybrid electric vehicles on the existing infrastructure with some very sobering conclusions.
- It is doubtful that oil will be at \$140/barrel if the forecast of PHEV and HFCV rollouts holds true.
- While it is useful to learn about the natural gas supply capacity in the future in anticipation of alternative vehicles, it is also important to understand whether the current natural gas pipeline networks can support the spike in demand in the future.
- It is too early in the program to have significant overall accomplishments, but the California results looked quite promising.

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated **2.0** for technology transfer and collaboration.

- Need to collaborate with industry and other academic entities doing similar work.
- This project needs industrial and governmental collaborators.
- The project could work more with other institutions to review and validate model.
- No collaborations were mentioned except using some results from MIT and ORNL.

Question 5: Approach to and relevance of proposed future research

This project was rated 2.8 for proposed future work.

- The additional work is in the right direction but the primary barrier to overcome is understanding the interaction between supply limit pressures and consumer demand.
- Good description of the proposed future work and milestones.
- Model will be expanded to the production of hydrogen from electrolysis. More renewable inputs should be examined.
- Perhaps the project can look at cost penalties from the infrastructure side for the energy providers (numbers of station and capacities).
- Consider closer look at GHG and other renewable hydrogen production technologies.
- Planned continuation seems appropriate and includes additional collaborations.

Strengths and weaknesses

Strengths

- The project establishes supply limitations on vehicle penetration.
- It is the right approach to look at a very complicated transition scenario.
- This is realistic modeling that looks at limitation of existing infrastructure.

Weaknesses

- The model presupposes market share, which in fact will be affected by the supply limitations predicted by this model.
- Need to validate some of the results.
- There are not enough renewable inputs or scoping for renewable inputs.

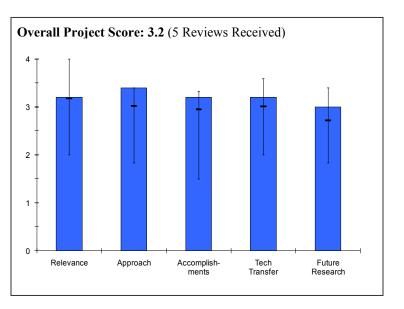
- Consider all-electric vehicles as another competitor.
- Must use iterative approach for supply and demand.
- Propose incorporating biofuels impact as another competitive choice.
- Add more renewable inputs and the effect of additional natural gas pipelines or liquid natural gas terminals in California.
- Continue as planned.

Project # AN-07: Hydrogen Deployment System Modeling Environment (HyDS-ME)

Brian W. Bush; National Renewable Energy Laboratory

Brief Summary of Project

The objectives of this project are to 1) evaluate and update the Hydrogen Deployment System Modeling Environment (HyDS-ME) to assess the state of its tools and to propose and implement enhancements, 2) perform scenario analysis and exercise the enhanced tool on a national case study, 3) expand the interoperability of HyDS-ME with tools such as the Hydrogen Demand and Resource Analysis (HyDRA) Tool, and 4) perform scenario analyses to understand how coal gasification with carbon capture and storage systems might be introduced to serve western markets.



Question 1: Relevance to overall DOE objectives

This project earned a score of 3.2 for its relevance to DOE objectives.

- The project is very well aligned with the analysis barriers, but it is not clear how it is aligned with technical barriers. Does it enable a better or more easily deployable infrastructure? Researchers should consider how to measure their progress against the bottom line.
- Good tool to look at optimized hydrogen infrastructure rollout possibilities. It is quite critical that reliable manufacturing, supply, and retail data are used for doing the analysis.
- This project is critical to the DOE objectives under Task 1, Perform Studies and Analysis, and Task 2, Develop and Maintain Models and Tools, addressing barriers, B, D, and E.
- Relevant to assist energy providers in deciding the best location to install hydrogen fueling stations at a regional level.
- It is more relevant for the model to integrate well with other models in order to provide valuable data on resource availability, hydrogen demand, costs, etc.
- Generally very relevant, but does not (and probably could not) include many intangible factors that will influence production sites.

<u>Ouestion 2: Approach to performing the research and development</u>

This project was rated **3.4** on its approach.

- Project used the DOE Hydrogen Analysis Model (H2A) to build empirical correlations for infrastructure deployment. It is demand-driven and takes most important market forces into account.
- Good approach to use existing/other tools and not recreate something. Tool integration planned to be seamless and scalable. Flowchart displayed showing various interactions.
- The model integrates production, transmission, demand, and feedstock costs to predict the delivered cost of hydrogen. The model is transparent, flexible, scalable, and maintainable.
- Model optimization approach is useful to decide on production and transmission technologies based on demand and feedstock price forecasts (temporal and spatial).
- Model appears to have some flexibility for continual updates to reflect the latest changes.
- Given the fact that the model incorporates inputs/information from various models, it is critical to closely examine key assumptions of the models to avoid overlap and conflict information (too many assumptions could lead to erroneous output).
- Generally good, but requires many assumptions which limit the value of any specific numbers.

FY 2009 Merit Review and Peer Evaluation Report

Ouestion 3: Technical accomplishments and progress toward project and DOE goals

This project was rated 3.2 based on accomplishments.

- Nice, iterative approach that simulates the market-driven deployment of hydrogen infrastructure. Will be very useful in making decisions on future infrastructure programs.
- Clear presentation of milestones and status; it is quite useful to look at progress in that format.
- Simulation results presented only at a very high level; need to look at them in further detail.
- Need to look at the existing infrastructure and possibility of adding on to or taking out from the base state.
- Accomplishments included optimizing 20,000 lines of code and completion of several studies. It would have been nice to see these published in the peer-reviewed literature.
- Appears to have generated quite a bit of data. Need to focus more effort on carbon capture and sequestration and scenarios for places outside of California. Need to also consider the logistics, geopolitical aspect, and feasibility of installing hydrogen pipeline within a regional area. Perhaps this area is being looked at by other models.
- Apparently, a great deal has been accomplished relative to the original planned work.

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated **3.2** for technology transfer and collaboration.

- This project unifies several analysis efforts.
- There are a good number of collaborators. Need to involve other industry partners.
- Several national laboratories and an engineering company, but the project needs more industrial collaborators.
- Good collaborations with H2A and Macro-System Model. Perhaps the model needs to be looked at and validated by industry experts in the area.
- Several good collaborations noted.

Question 5: Approach to and relevance of proposed future research

This project was rated **3.0** for proposed future work.

- It is the right idea to look harder at feedstock availability effects.
- The proposed future work should include the timeline for when it will be completed. Also, need to validate the assumptions from an infrastructure industry player.
- Model will be applied to more elaborate scenario analysis.
- Consider expanding model study to outside of California. Looking at additional key constraints will be useful.
- Proposed work seems appropriate based on material presented.

Strengths and weaknesses

Strengths

- The model is market-driven, iterative, and connects a suite of predictive analysis tools.
- The approach of geographic infrastructure optimization is nice and can be useful.
- Optimized code for powerful transparent analysis is a strength.

Weaknesses

- Unclear connection to technical and market barriers.
- Need to involve an industry collaborator for validation and feedback.
- Need more comparison with renewable resources.
- There are so many assumptions that isolated results could be questionable. Best use is probably for trends and first comparisons.

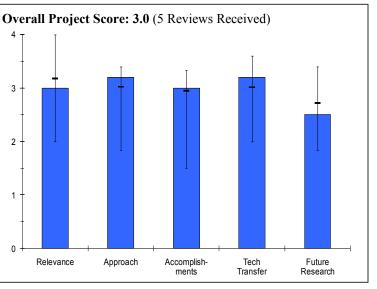
- Include a model validation step.
- None.
- Not clear that program should be expanded after current planned work is completed.

Project # AN-08: Analysis of Hydrogen Production and Delivery Infrastructure as a Complex Adaptive System

George S. Tolley; RCF Economic and Financial Consulting, Inc.

Brief Summary of Project

The purpose of this project is to use agentbased modeling to address the "chicken or egg" problem between the supply of hydrogen fuel and the purchase of hydrogen vehicles. The overall aim is to answer two questions: 1) Will the private sector invest in hydrogen infrastructure, and 2) What, if any, policy assistance is needed? Objectives for 2008-2009 are to 1) add finishing touches to the model, 2) carry out parameter sensitivity analysis, 3) conduct policy analyses, 4) do model validation, and 5) write the final report.



Question 1: Relevance to overall DOE objectives

This project earned a score of 3.0 for its relevance to DOE objectives.

- The analysis on issues of hydrogen-fueled vehicles competing with/replacing gasoline vehicles is in the interest of the DOE program. A would-be investor can use this report as a decision making tool and understand market behavior.
- The Hydrogen Production and Delivery scenario reports financial indicators as the individual investor's risk and decision analysis tools. The model appears to assume that there is no issue with hydrogen availability at cost and convenience similar to gasoline (failures are stated in the Policy scenario analysis). It is assumed in the final report that issues with hydrogen availability scenarios at costs competitive with gasoline will be discussed. Hydrogen availability at costs and convenience competitive with gasoline along with the financial predictors will make the analysis more complete.
- Evaluating market is critical for infrastructure deployment strategy. However, while the project predicts the choices, different "agents" might make it is unclear exactly what is to be done with this information. The project should lead to one or more strategic recommendations.
- Good premise. This is a very real issue. This is needed to best understand what incentives might be needed to spur development.
- The project is critical to the DOE RD&D objectives under Task 1, Perform Studies and Analysis, addressing barriers A, B, and C.
- Understanding of the parameters affecting market development is certainly important. The model addresses most questions.

Question 2: Approach to performing the research and development

This project was rated **3.2** on its approach.

- The work focuses on predictive financial models, competition from other investors, and parametric sensitivity; it also provides information for potential investors to make go/no-go decision.
- There are three drivers: legislation, market forces, and technical barriers. Hydrogen production technology cost, on-board storage, pumping stations, feedstock (renewable or fossil), and many other safety, emission, and environmental issues remain for commercial maturity of hydrogen production technology at quantities needed for the successful introduction of hydrogen vehicles. The study isolates these issues, although the issues are not mutually exclusive, and therefore the usefulness of the predictive models cannot be objectively ascertained.

- This is an intriguing approach. This project addresses motivations and is an important complement to other projects that take a purely mathematical approach to predicting market choices. Not clear how this approach addresses the barrier "lack of consistent data, assumptions and guidelines"; it seems to be more about performing a better analysis on the assumptions that exist.
- A comment was made that it does not consider alternative pathways to infrastructure, such as home fueling.
- The uncertainty is broad, and it's not clear that there are specific recommendations at this point.
- Project analyzes complex interplay of consumers, investors, geography and companies and assesses whether or not policy intervention is needed.
- Agent-based modeling is a good approach for studying this problem.
- This project has mostly been geared toward developing a model. But what about the continued use of the model, with the associated upgrading and stewardship of it? If the project is not continued in some fashion, the model will be relegated to past work.
- Unfortunately, this project was hard-wired for hydrogen, and therefore cannot easily be used to study other energy systems. This limits the way that the model can be used to evaluate hydrogen within the context of other energy options, or if hydrogen is not the only answer.
- Early transition is important, and solves the "chicken or egg" problem, but what about full commercial deployment or half-hearted adoption of hydrogen? Won't agents behave very differently at a mid- or end-point?

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated **3.0** based on accomplishments.

- The question is how an individual investor can and needs to be educated. The study results are based on 140 parameters (from the DOE Hydrogen Analysis Model [H2A]) and a variety of sensitivity analyses. The terms and analysis methodology may not readily comprehensible to an investor.
- The near-to-mid term negative discounted cash flow rates of return as reported in the financial indicator analysis results study does not suggest how best to interpret the information and may simply be a deterrent to a potential investor. The analysis reports the barriers, but could have discussed alternative assumptions and scenarios to overcome the barriers.
- The project takes into account sensitivities to many important factors, and concludes that "if parameters are right," there will be investment in hydrogen. It is not clear what those parameters need to be in order to overcome barriers.
- As presented, the graphs are somewhat confusing and not easy to understand. Presumably, they are truly reflective of reality. It is not clear what inputs were used for assumptions for the graphs shown, such as hydrogen storage pressure (350 or 700 bar), cost of hydrogen, which source (i.e., reformer, liquid, gas), etc. Making the assumption that H2A is accurate enough to eliminate the need for a sensitivity analysis might not be a good assumption.
- A sensitivity analysis for various factors has been completed, and it appears to be useful.
- It is hard to tell what was accomplished this last year. However, this is an excellent set of results and a very useful model.
- It seems unreasonable to assume that all stations will grow in capacity utilization at the same rate.
- Very interesting use of comparative technology adoption scenarios. What would happen if the decision to adopt a technology were based on a real or perceived need (e.g., gasoline not available or way too expensive), rather than just an item to own (e.g., color television)?
- Why does a higher familiarity premium result in slower adoption?
- This is an excellent set of sensitivity analyses. What are the boundaries of the analysis, i.e., best case of all parameters tested and worst case of all parameters tested?

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated **3.2** for technology transfer and collaboration.

- A national laboratory, auto manufacturing company, and oil producer are team members in addition to other hydrogen technology industries and industry advisors.
- Not clear how this fits in with other analysis projects in the program.

FY 2009 Merit Review and Peer Evaluation Report

- Good list of partners from pertinent functions, provided that they were involved heavily. This was not clear.
- Excellent collaboration with a national laboratory and energy and automotive companies.
- Good team, but would like to know who the industry advisors were and what advice they provided.

Question 5: Approach to and relevance of proposed future research

This project was rated 2.5 for proposed future work.

- The project is fully funded and ends in June 2009.
- Future work is aimed at providing a specific set of scenarios that would enable hydrogen investment. It is not clear that a comprehensive and actionable picture will follow from the work presented here.
- Project is effectively complete except for the report, so this future work proposed is not applicable. It was stated that there would be more recommendations in the report; if so, then that would be key to its effectiveness? It is difficult to comment without the report.
- Project is ending.
- Yes, the project is ending, but a slide should have been provided just in case additional funding is available for analysis activities. Or, if someone else (e.g., DOD) has money to continue this model, what would be your suggestions? How will the model live on, even if its development is not continued?

Strengths and weaknesses

Strengths

- Includes important sensitivity factors and an agent-based approach.
- Provides some realistic expectations for market penetration to start discussions.
- It will be a strength if specific recommendations are in the report that can further the rollout.
- Great model with lots of capability.

Weaknesses

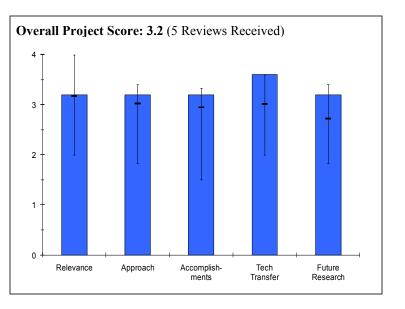
- The project needs a more specific path to conclusions.
- This has been an expensive analysis compared to other programs.
- The conclusions and answers to previous questions are very broad and generic they are somewhat obvious and not surprising.
- The model is only relevant to hydrogen. No plans for continued use of model.

- The potential fuel economy and emission regulation of gasoline vehicles may change hydrogen energy economy scenario. It is suggested that this scenario be included in the final report.
- The project is complete except for the final report.

Project # AN-09: Adapting the H2A Hydrogen Production Cost Analysis Model to Stationary Applications *Michael Penev; National Renewable Energy Laboratory*

Brief Summary of Project

The DOE Hydrogen Analysis (H2A) Power Model allows for transparent and consistent analysis of new transition strategies. The H2A model's discounted cash flow model has been modified to perform distributed generation analysis. Hydrogen infrastructure costs for an early transition phase are large, and are relatively high risk due to the uncertainty of demand. Combining hydrogen production with combined heat and power (CHP) capability may reduce upfront costs and reduce investment risks. Hydrogen can be generated by electrolysis and fuel cell co-generation.



Question 1: Relevance to overall DOE objectives

This project earned a score of 3.2 for its relevance to DOE objectives.

- The predictive model reports cost information related to phased transition to hydrogen energy and, therefore, relevant to DOE Hydrogen Program objectives.
- One purpose of systems analysis is research guidance. In the hydrogen community, it appears the two groups are not communicating with each other and not using each other's results for advancing hydrogen energy technology overall. The audience pretty much gets to hear the same story each year at the Annual Merit Review, from either side, mutually exclusive.
- CHP is not going to make or break hydrogen infrastructure. This project considers the idea that CHP would make facility owners want to invest in tri-generation. There are still very significant compression and storage capital costs: the classic barriers to infrastructure adoption still exist, but they are lessened.
- This type of analysis showing an integrated infrastructure is very useful to maximize efficiency. Need to prove value (or not), which is the purpose of the model.
- Project has good alignment with the goals and objectives of the Hydrogen Analysis Subprogram as evidenced by its focus on evaluating transition strategies needed to introduce co-production of hydrogen for transportation applications at stationary fuel cell sites.
- Excellent description of how the project relates to meet DOE objectives.

Question 2: Approach to performing the research and development

This project was rated **3.2** on its approach.

- The models predicting transition to hydrogen energy economy are based on highly idealized assumptions and have not changed in the past few years to more realistic scenarios based on emerging new experimental, market, technology, or legislative information.
- The approach involves approximately \$3,000/kWe capital and suggests that without Federal incentive, market diffusion of the technology is not an option. This is somewhat understood, and a detailed modeling effort may be redundant.
- The highly competent team does not address the assumption that a CHP plant capital of \$3,000/kWe is not costcompetitive; it is ~3 times more than today's proven, rapidly environmentally progressing coal-fired plants.
- The system analyses results are informative but do not seem to help to really move the hydrogen energy technology potential forward along the program's defined technology development road map.

- There are a lot of factors in the model: electrolysis, CHP, etc. The question to answer is simple: does CHP enable a hydrogen infrastructure?
- Seems to have addressed major variables.
- Good approach to the "chicken or egg" issue for introducing hydrogen sites and hydrogen vehicles in a timely, well-coordinated time frame. Co-production of hydrogen coupled with CHP would accelerate the introduction of hydrogen stations with minimal risk.
- All aspects of co-production of hydrogen and power are included.
- The modeling assumptions are consistent and practical.
- Connecting with industry for input and review is very productive.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated **3.2** based on accomplishments.

- The analysis is very well done and well presented. Hydrogen co-production is claimed to be practical and economical, but compared to utility industry economics, is not clear. If CO₂ capture and sequestration cost is added, even though lower CO₂ emission is predicted under ideal production cases, the reported options become cost-intensive.
- The model accomplishments predicting greenhouse gas (GHG) emissions, etc. do not address the adoption barriers. The work should focus on the factors that influence deployment of fuel cell CHP systems and the case for CHP system owners making the additional capital investment required to co-produce hydrogen.
- The analysis seems complete and was well presented. It is in a clearly understood format.
- Tri-generation of hydrogen by utilizing waste heat from high temperature fuel cell systems is an interesting approach to not only generate electricity, but also process heat and hydrogen. Good analysis of the need to optimize mix of applications at different times of the day. Good example model output for the U. S. Postal Service (USPS) site in San Francisco.
- Excellent results.
- Very good parametric analysis.
- Good application to real life applications such as the post office.
- Good recommendations on how to apply their work and results.

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated **3.6** for technology transfer and collaboration.

- NREL, appropriate DOE offices, and Directed Technologies, Inc., are team members. Fuel Cell Energy, UTC Power, Plug Power, ANL, and SNL are also partners/reviewers.
- Works with existing fuel cell companies and includes relevant case studies.
- A good cross-section of partners was included.
- Good list of collaborators, but little detail on collaborations except for USPS.
- Excellent coordination with industry and other laboratories.

Question 5: Approach to and relevance of proposed future research

This project was rated **3.2** for proposed future work.

- Future work is a legitimate extension of current work.
- The future work as presented makes sense. Building in CO₂ reduction with the Macro-System Model will be a key with future regulation.
- Would like to see more discussion on the USPS project. Aside from the analysis, is the USPS moving forward on this project and will they be privy to data to validate their model?
- The proposed plans are very useful and will produce helpful results for DOE and industry.

Strengths and weaknesses

Strengths

- Good collaboration and an interesting deployment model.
- This might have good applicability as a tool for customers to assess their suitability for fuel cell systems. It will be very useful to prove the value to people who otherwise would struggle with the complexity.
- Modeling co-production of hydrogen for transportation this is an important approach to overcome the "chicken or egg" issue for HFCVs.
- This is a comprehensive model.
- Engaging all stakeholders is great.
- Good return on DOE funds with 85% work done at <50% funds spent.

Weaknesses

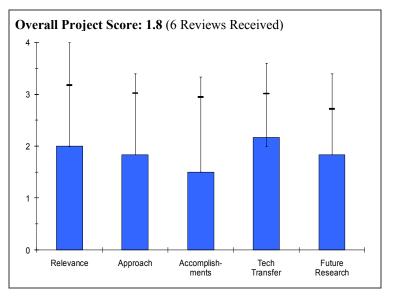
- The model does not focus on what this reviewer believes to be the primary barriers to hydrogen adoption.
- The output needs to be validated compared to a real-life installation.
- None.

- The future work should also consider the impact of potential fuel economy and emission standard legislation of gasoline-powered cars.
- A model for renewable supply would be very useful.
- Can you include effects of NO_x, SO_x, CO₂, and VOC emissions and monetize them?
- Include universities and national laboratories as possible demonstration sites.

Project # AN-10: Hydrogen and Fuel Cell Analysis: Lessons Learned from Stationary Power Generation S.E. Grasman; Missouri University of Science and Technology

Brief Summary of Project

The objective of this project is to collect and articulate lessons learned from past experiences that can improve future decisions related to hydrogen fueling infrastructure development. Project objectives are to 1) to consider opportunities for hydrogen in stationary and portable applications in order to make recommendations related to research, development, and demonstration strategies and 2) analyze the different national and international strategies utilized in existing systems and identify the different challenges and opportunities for producing and using hydrogen as an energy carrier.



<u>**Ouestion 1: Relevance to overall DOE**</u> <u>objectives</u>

This project earned a score of 2.0 for its relevance to DOE objectives.

- The project objectives are relevant to DOE Hydrogen Program goals. The approach-milestone checklist is quite informative.
- A stated objective is R&D guidance based on system analysis results; however, no such recommendation can be gleaned from the presentation.
- The presentation is mostly a checklist of activities, ongoing or past. A member of the audience new to this presentation cannot have many "take home" messages.
- The project is a survey of existing fuel cell users and manufacturers. The researcher states that this will give important market knowledge and lessons learned.
- The objectives are too broad for the amount of analysis. The intent is good, but it is difficult to grasp how this study, for example, can "model and analyze the hydrogen supply network" among several other equally broad objectives.
- Project is reported to be a "lessons learned project" to assess the issues that stationary fuel cell developers are experiencing, which if properly carried out, could have an impact to identify critical issues that need to be rectified. However, no substantive details were provided on critical issues.
- Lessons learned from stationary fuel cell experience are of good relevance, in principle, to apply to other programs.
- This is a typical market research type study approach, but it is unclear exactly know how it fits within the prescribed R&D scope of DOE.
- Some description of relevance in the presentation.
- Not quite clear how it meets DOE goals or which barriers it overcomes.

Question 2: Approach to performing the research and development

This project was rated **1.8** on its approach.

- Well-defined approach, consistent with achieving intended results. Approach is relevant to diffusion of early market entrance of hydrogen technologies.
- The survey, as presented, appears simplistic. It is not clear about how it will contribute to overcoming the stated barriers of technology validation and predicting future market behavior.

640 FY 2009 Merit Review and Peer Evaluation Report

- This appears to be a qualitative "survey" as opposed to a quantitative, scientific process. It also appears to be subject to "self-selection," both in selecting the sample population as well as getting the responses. Too many variables for the amount of data. The results are not likely to be meaningful or conclusive, and there is risk that false conclusions cold be drawn.
- Approach appears to involve development of a Web-based survey, literature reviews, and site visits. No discussion of the types of questions and level/details of responses was presented.
- Data collection is based on survey rather than a more methodical approach of collecting inputs from industry. General survey does not necessarily reveal key lessons learned. Milestones are activity-based rather than meeting some key targets.
- The approach portion of the presentation is inadequate.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated 1.5 based on accomplishments.

- Technical objectives and barriers were not addressed in a manner comprehensible to the reader. The value and applications of the technical accomplishments are not clear; it is difficult to interpret the information. What problem needs to solved for early market penetration of hydrogen energy is not understood, nor does the study identify what challenges and opportunities exist in order to produce and use hydrogen as an energy carrier in a market-competitive scenario.
- The results presented are unspecific and not really actionable. The insights gained from the work, as presented, do not seem to tell us anything we do not already know about fuel cells.
- The survey is likely to be somewhat subjective. There were also comments from previous years about manufacturer input, but that perspective on the applicability of various markets and technologies (e.g., PEM vs. SOFC vs. MCFC) can skew this survey. It is also not clear how survey results could be affected by one particular manufacturer's good (or bad) equipment.
- Progress presented appears to be a list of the number of respondents, sites visited, and reports analyzed. Details on typical responses are lacking.
- So far, the project team has created a Web-based survey with 100 respondents. Don't know how/why this is called a "technical accomplishment"?
- The presentation included only general learnings, nothing new or surprising.
- Relevance of survey results not adequately presented.

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated **2.2** for technology transfer and collaboration.

- Missouri University of Science and Technology is the lead. Other team members, if any, are not listed.
- Collaboration consisted of site visits and meetings with manufacturers.
- This activity does not seem to interact well with the other DOE analysis programs. Not sure how it would tie in. Some contacts with manufacturers, but report could have made this participation more clear.
- The fact that they had numerous responses and site visits shows a good degree of collaboration, but the collaboration appears to be one-sided. No indication of how the responses and analysis are being used as feedback to collaborators to share experiences and solutions.
- No collaborators to assess.
- Not clear how this was achieved.

Question 5: Approach to and relevance of proposed future research

This project was rated 1.8 for proposed future work.

- Future work is listed.
- Scope of future work is not specified.
- This is not really applicable since the program is finalizing its report at this stage.
- No follow-on work proposed.

- Proposed future work mostly includes sharing learning.
- No clear path related to DOE goals.

Strengths and weaknesses

Strengths

- None.
- The idea is very good.

Weaknesses

- The two slides on Technical Accomplishments & Progress are not comprehensible. What an investor should interpret from the information presented is not clear.
- This project does not appear to lead to a useful conclusion.
- The span of types of fuel cells, applications, and time (e.g., widely varying usage history) makes the data too sparse in any one area and not easily comparable.
- This project appears to be a literature search of limited value to fuel cell industry. It is unclear how results/findings are of sufficient detail to be useful.
- Survey-type project that is non-technical; not clear why DOE is funding this.
- The data analysis appears to be inadequate.

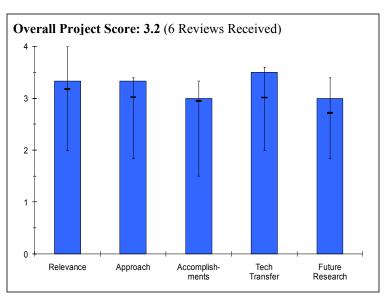
- A statement like, "The role and use of hydrogen fuel cells in stationary and portable applications can be significant," is difficult to interpret. Market is not yet ready to quite accept this inference, although similar statements have been made during the last several years.
- The presenter needs to interpret the model results for the reader and audience. The PI needs to use more realistic assumptions in system analysis studies.
- Project cost seems very high given the scope as presented.
- Too late at this point, but if meaningful input is desired, then narrow the scope to a specific type of fuel cell and applications.
- It is not likely worth gathering any additional data (unless a more precise methodology is established and a there is a greater sample to draw from) or pursuing any further activity past the project conclusion.
- Terminate project.
- This project should not be within the DOE Systems Analysis scope.
- Better presentation of data by customer-choice parameters would help better interpret the data.

Project # AN-11: Modeling the Transition to Hydrogen

Paul N. Leiby, David L. Greene, Zhenhong Lin, David Bowman, and Sujit Das; Oak Ridge National Laboratory

Brief Summary of Project

This project addresses the need for transformational and long run analysis of hydrogen and fuel cell vehicle market potential, using valid and consistent data from the program. The project supports benefits analysis and greenhouse gas/energy security impacts analysis. By updating and improving the HyTrans (hydrogen transition) integrated market model, the approach is to develop a dynamic market simulation model integrating fuel production and delivery pathways, vehicle technologies and production costs, and consumer choice. In FY 2009, ORNL will 1) complete analysis of storage technology cases, 2) develop model-capability and scenarios to integrate early hydrogen



transportation and stationary power in early market, and 3) incorporate global trends and explicit representation of uncertainty.

Question 1: Relevance to overall DOE objectives

This project earned a score of **3.3** for its relevance to DOE objectives.

- The work aims to determine the true potential and possibility of hydrogen vehicles using credible transition scenario analysis, and it is highly relevant to program objectives.
- This work provides an important insight on quantifying the effect of performance to target parameters on the market penetration of hydrogen vehicles.
- The intent is excellent, provided that it is done correctly.
- The project is well aligned to meet DOE goals and to develop an analytical tool to model the transition to a hydrogen-based transportation economy and the impact of achieving critical DOE technical goals on the timing of the transition.
- Good relevance to determine the scenarios for transition to the hydrogen economy.
- Analysis emphasizes estimation of different scenarios, including if partial goals of DOE Storage Technology are met.
- Exploring synergy between stationary and transportation applications is quite useful.

Question 2: Approach to performing the research and development

This project was rated **3.3** on its approach.

- The intended results are bulleted and comprehensible to the reader.
- The attempt to develop an integrated model of all major components of hydrogen fleet addressing market and technical issues fully supports the DOE Hydrogen Program goals.
- The project team realizes what information the analysis should provide to the appropriate stakeholders, and attempts to accordingly fill the knowledge and information gaps.
- An integrated approach is so much more comprehensible; discreet approaches seem to contradict one result with another.
- One of the few projects in this field that includes all the relevant vehicle choices in the model.

- As discussed even in the report, input assumptions are key to the validity of the model. It will be difficult to look at all the potential combinations and permutations, although that is the effectiveness of the model. It is also subject to being manipulated to show the "desired" outcome. For example, the inputs shown in the presentation for battery and fuel cell costs seem very aggressive.
- Good analysis in that it includes competing technologies (i.e., advanced gasoline, gasoline hybrids, and hydrogen fuel cells). There does not appear to be any evidence that hydrogen internal combustion engine vehicles are modeled.
- Good approach to make use of existing models/data and project the transition. It is quite critical to have the right policy inputs/scenario and use the correct data from industry regarding current status of vehicles and infrastructure.
- The market simulation and coordination with Europeans is very useful.
- Focusing the tool on the "chicken or egg" problem to help transition to hydrogen economy is very relevant and productive.

Ouestion 3: Technical accomplishments and progress toward project and DOE goals

This project was rated **3.0** based on accomplishments.

- Results are insightful. However, there is now a third driver, and the project team needs to consider that. The driver is the potential legislation of fuel economy and emission standards of gasoline-powered vehicles. This new factor is highly inclusive for studies on market acceptability and technical barrier issues for hydrogen vehicles that need to be overcome. Crude prices may fluctuate some, but perhaps will not impact fuel-cell-powered car production to any significant extent, and there is competition from all electric cars. The growth projection for the hydrogen fuel cell vehicles (HFCV) from 2015 (only 6 years from now) may not apply. The scenario analysis presents impact for not meeting DOE high-tech goals for storage costs, and the information tends to indicate that HFCV is more of a "no-go." The work presents more "what if" analysis results. Decision makers cannot rely on speculative information as decision tools.
- This project synthesized a large number of existing models, provided a lot of unique functions, and demonstrated relevant outputs.
- Barriers are vague and somewhat general. This year it seems most effort is on software-related issues and not "real analysis."
- A lot of cautionary interpretations/incomplete results are reported suggesting the progress is slow.
- Would like to have a more structured view of the technical accomplishments. What were the proposed milestones and how/when were they accomplished?
- The transition analysis published in FY 2008 is clearly a major accomplishment. Not sure if the shared results today represent new learnings beyond that publication.
- The three-dimensional plots of delivery costs presented were not very clear. Two-dimensional plots may be better.
- The addition of PHEV types is a good improvement to the existing model.
- Results shown compare the cost of hydrogen storage (current vs. goal) and the impact. This is quite useful.
- The result presentations showed that PHEVs and HFCVs are very comparable. Does this mean HFCVs may face a serious challenge in successful commercialization?

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated **3.5** for technology transfer and collaboration.

- Coordinated collaboration with relevant stakeholders including U.S. auto manufacturers, other national laboratories, university, and fuel cell manufacturer and marketer will generate credible information acceptable to decision makers.
- Incorporates existing models and provides a good framework.
- There appear to be a number of partners and collaborators across a wide range of specialties, including government, industry, and academia. Assuming that they are actively involved, this is encouraging.
- Excellent coordination and collaboration with other modeling efforts at sister laboratories as evidenced by future incorporation of results from the Powertrain Systems Analysis Toolkit; DOE Hydrogen Analysis Model;

and Greenhouse Gases, Regulated Emissions, and Energy Use in Transportation Model into the Hydrogen Transition Model.

- Why were there no collaborations with the energy industry?
- Very good coordination with NREL, ANL, and University of California-Davis.
- Getting input from auto and fuel cell suppliers is very productive.

<u>Question 5: Approach to and relevance of proposed future research</u>

This project was rated **3.0** for proposed future work.

- Legitimate future work proposed by extending scope, including sensitivity analysis and benefits assessment.
- In addition to storage cases, the project should also consider feedstock supply scenarios as potential limiting factors to deployment.
- Given the task at hand, the approach forward seems logical.
- Effort will include co-production of hydrogen at stationary fuel cell sites.
- No mention of transition scenarios with PHEVs, biofuels, etc. in the proposed future work. Otherwise, seems like a good list.
- Shared fueling structure concept offers a fresh option to help transition to hydrogen economy.
- Hydrogen CHP system evaluation is timely and useful.

Strengths and weaknesses

Strengths

- This is a very comprehensive market model. It unifies other good analysis work.
- If done correctly, the tool can be very useful to understand sensitivity of various inputs. A "roll-up" of the models is really needed to understand the bigger picture.
- Prediction of market share of competing technologies into the future is a strength.
- Good skill set of people involved in the project.
- ORNL experience in model development is a plus.

Weaknesses

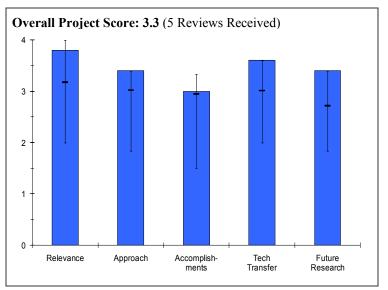
- This is the integration of multiple models, each of which having their own potential errors or inaccuracies. These may be compounded as the individual models are connected.
- Lack of buy-in from energy industry and the government.

- Future work should consider three drivers: market, technology, and regulation.
- Consider effect of supply pressures on feedstock cost in vehicle choice model as studied by Lutz (Project Number AN-06).
- A method to validate that the results are "accurate" will be important to trust the results.

Project # AN-12: Fuel-Cycle Analysis of Fuel-Cell Vehicles and Fuel-Cell Systems with the GREET Model *Michael Wang, Amgad Elgowainy, and Jeongwoo Han; Argonne National Laboratory*

Brief Summary of Project

The objectives of this project are to 1) expand and update the Greenhouse Gases, Regulated Emissions, and Energy Use in Transportation Model (GREET) model for hydrogen production pathways and for applications of fuel cell vehicles (FCVs) and other fuel cell systems, 2) conduct well-towheels (WTW) analysis of hydrogen FCVs with various hydrogen production pathways, 3) conduct life-cycle analysis of hydrogenpowered fuel cell systems, 4) provide WTW results for Hydrogen efforts on the Hydrogen Posture Plan and the Multi-Year Program Plan, and 5) engage in discussions and dissemination of energy and environmental benefits of hydrogen FCVs and other fuel cell systems. Data were



obtained for hydrogen production pathways (from open literature, DOE Hydrogen Analysis Model (H2A) simulation results, process engineering simulations) as well as hydrogen FCVs and other systems (from open literature, Powertrain Systems Analysis Toolkit simulations, data from industry).

Question 1: Relevance to overall DOE objectives

This project earned a score of **3.8** for its relevance to DOE objectives.

- The project objectives, especially the WTW analysis of hydrogen FCVs with various hydrogen production pathways, are consistent with DOE Hydrogen Program objectives.
- Development of this model is critical to understanding production pathways.
- The GREET model has been extremely relevant and useful in doing WTW analysis of various pathways. It is a critical enabler for the hydrogen economy.
- This project seeks to expand and update the GREET model, which enables WTW analysis of unwanted atmospheric emissions under different scenarios.
- Environmental modeling tools of this sort provide confidence in the ability of the fuel cell program to deliver intended environmental benefits.
- This work is essential for the quantification and comparison of energy use and emission reduction benefits for alternative technologies.

Question 2: Approach to performing the research and development

This project was rated **3.4** on its approach.

- The approach is fairly general, obtaining data from known, available, and public-domain sources. The project team uses the tools to analyze, validate models, and present WTW results. A variety of scenarios on vehicle types, fuel options, power generation mixes, and hydrogen production pathways were considered, and the presented results are insightful.
- Recommend a consistent figure of merit to compare different pathways. This could be minimization of kilowatt -hours of fossil fuels or minimization of kilowatt-hours of imported energy, for example.
- Detailed analysis of various pathways with good background knowledge serves the project well and offers good credibility to this program.

- The investigators obtained the necessary data from appropriate sources, programmed it into the GREET workbook (Microsoft Excel), and demonstrated its application.
- Data collection, which is from multiple sources, is an important aspect of the ongoing effort to validate data sets and to verify results.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated **3.0** based on accomplishments.

- The predictive models present results that appear consistent with conventional wisdom. PHEVs based on steammethane reforming (SMR) or electrolytic hydrogen will reduce petroleum use. What is missing is costcompetitive and environmentally acceptable hydrogen availability and hydrogen infrastructure. It is not clear if such parameters are considered in the model assumptions.
- Conventional hydrogen production technologies are CO₂-intensive. Advancements are not yet mature in the areas of hydrogen production technologies, feed stock availabilities, product recovery, storage, use, and distribution in a cost-effective, environmentally acceptable manner. How these factors affect the study results and conclusions are not clear.
- Carbon dioxide management approaches in a distributed power generation scenario are not discussed and could be cost intensive. Results do not indicate if this factor was considered in analysis.
- Cannot evaluate progress since the project is "ongoing" and does not appear to have performance milestones at specific times.
- Plug-in hybrid electric vehicles (PHEV) are now included in the GREET model, which is a good and relevant addition.
- Combined heat, hydrogen and power (CHHP) is also useful addition and a positive technical accomplishment.
- Need to look a structured progress update (progress vs. proposed milestones).
- A new version of GREET (v. 1.8c) was released.
- Fuel-cycle studies of forklifts and distributed power generation (prime early-adopter markets) were published just last week. (These data were in last year's review.)
- Preliminary results for a hypothetical CHP system address another prime early-adopter market.
- The principal results on slides 9 and 10 demonstrate the use of the GREET model to compare petroleum use and greenhouse gas emissions under different (mostly PHEV) scenarios. However, the data of the last three bullets would be a lot more meaningful if some form of uncertainty analysis was provided in each case. Its absence over multiple studies indicates a systemic weakness that can be improved.
- The incorporation of the evaluation of forklifts and distributed power generation are important additions to the public version.
- The ongoing PHEV and CHHP work will also be important additions to the public version.

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated **3.6** for technology transfer and collaboration.

- A team of several national laboratories and industry partners are involved. The contribution(s) of each team member is not described.
- Very good coordination with academia and industry. The model is widely accepted and used as the benchmark tool for WTW analysis.
- There is a high level of collaboration in the acquisition of the data to build the GREET model.
- The GREET model is publicly available on the project website, which encourages its wide adoption and use.
- Excellent collaboration with industry to obtain data.

Question 5: Approach to and relevance of proposed future research

This project was rated 3.4 for proposed future work.

• Landfill gas is not carbon neutral or negative. Many analyses over years have worked on "early market applications," but a market transformative technology scenario has not evolved yet.

- Consideration of PHEV and electric grid is very important.
- Biogas/landfill gas would be a good addition to GREET; so would an expansion on PHEV and CHHP capabilities.
- The proposed future work evidences a commitment to keep the GREET model relevant, broad-based, and user friendly.
- I encourage future work to quantify the uncertainty of the model parameters within GREET and to facilitate the propagation of those uncertainties through calculations.
- Good plan that builds on past success and future modeling needs, particularly related to improving ease of use.

Strengths and weaknesses

Strengths

- Technical expertise and background knowledge of people involved is a strength.
- Compilation of modeling data in publicly and easily accessible format is a strength.
- The model provides credibility for environmental benefit claims of the Fuel Cell Program.
- Continued relevance to evolving interests of the fuel cell program, e.g., early market opportunities such as forklifts, premium power, and CHHP systems.
- A strong team contributes to the continued success of this work.
- The addition of new technologies or new configurations in a timely manner is strength.

Weaknesses

- Need to increase collaboration with the energy industry.
- The lack of uncertainty/sensitivity analysis makes it impossible to distinguish precision of predictions, e.g., accurate to within a percent or two or simply a coarse estimate.

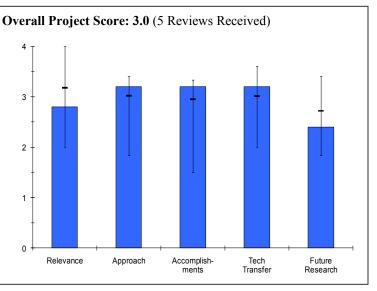
- New potential fuel economy and emission standard regulations need to be considered in future studies.
- All possible pathways for hydrogen production should be included.

Project # AN-13: Evaluation of the Potential Environmental Impacts from Large-Scale Use and Production of Hydrogen in Energy and Transportation Applications

Don Wuebbles; University of Illinois at Urbana-Champaign

Brief Summary of Project

The purpose of this project is to systematically identify and examine possible ecological and environmental effects from the production and use of hydrogen from various energy sources based on the DOE production strategy and use of that hydrogen in transportation and power applications. This project uses stateof-the-art numerical models of the environment and energy system emissions in combination with relevant new and prior measurements and other analyses to assess the understanding of the potential ecological and environmental impacts from hydrogen market penetration. In the process, DOE will be provided with a capability for further assessing current understanding and



remaining uncertainties for addressing the potential environmental impacts from hydrogen technologies.

Question 1: Relevance to overall DOE objectives

This project earned a score of **2.8** for its relevance to DOE objectives.

- This is an important study of potential impacts of large-scale hydrogen production.
- This project is an amalgam of modeling projects to assess environmental benefits and consequences of largescale adoption of production and use of hydrogen fuel.
- Environmental impact studies of this sort provide confidence in the ability of the fuel cell program to deliver intended environmental benefits.
- The objective of this project is to assess the potential ecological and environmental effect of large-scale production and use of hydrogen in transportation and stationary applications out to the year 2050.
- With the hydrogen technologies of interest to this program still being in their formative stages, such a study appears to be premature at this time.
- Ground-level changes in air quality pollutants are important to study, but focus should be on show-stopping concerns regarding stratospheric ozone.

Question 2: Approach to performing the research and development

This project was rated **3.2** on its approach.

- In part, the project uses standard models such as Community Atmosphere Climate Model with Chemistry (CAMChem) and Community Multiscale Air Quality Model (CMAQ) to compute the effects on the atmosphere from emissions under various scenarios.
- Other aspects of this project have tailored approaches that were not described in detail.
- The project uses a combination of measurements, modeling, and analyses. They use global effects models for air quality, ozone, climate effects, etc., and they are trying to assess sensitivity to hydrogen leaks and embrittlement effects on materials. These are important questions, but focus on troposphere seems to miss the point. From basic chemistry, you would expect regional air quality to improve with increased hydrogen availability. Need to move more quickly to stratospheric impacts. Ozone reduction in the stratosphere could be catastrophic to hydrogen future. And what about indirect greenhouse gas (GHG) formation? Why has team

spent so much time on troposphere? Should have started at the top of the atmosphere. Seems like you answered the obvious questions first.

• Are the right climate/atmospheric models being used?

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated 3.2 based on accomplishments.

- The project is very comprehensive. Estimate changes in concentration of all atmospheric species are likely to be affected.
- Project reports progress in several areas: a conclusion that atmospheric hydrogen is not a threat to metal structures; a conclusion that oxygen discharge from hydrogen production is probably not a problem; a model of hydrogen uptake by soil; and atmospheric impact analysis of emissions under certain scenarios for 2050. However, the results in all these areas would be a lot more meaningful if some form of uncertainty analysis was provided in each case. Its absence over multiple studies indicates a systemic weakness that can be improved.
- LANL partner is unfunded in FY 2009. They were at an impasse in gathering actual data of hydrogen emissions from typical industrial plants. There were also unspecified "setbacks in laboratory studies at LANL relating to equipment suitability."
- The project determined that hydrogen embrittlement and oxygen plumes from centralized hydrogen production by electrolysis would not be of concern.
- Hydrogen uptake by soils was difficult to understand from the way it was presented and discussed.
- Only the extreme case of all transportation conversion to hydrogen was considered for assessment of emissions changes for hydrogen, CO, NO_x, etc. The resulting ambient concentrations of O₃, CO, NO_x, etc. showed only minor changes; even the 25% to 40% increase in the ambient hydrogen concentration still led to less than 1 ppm hydrogen or so.
- It was not clear whether the analysis considered a static global fleet of vehicles or if it assumed the global vehicle fleet to grow at a certain rate.
- The global pollutant concentration maps shown were interesting, but the significance of the indicated changes was not clear. Also, the speaker could not explain certain features, such as why the summertime CO concentrations showed a decrease by two-thirds over the New York City area.
- The rate of progress on this project appears to be slow. The soil hydrogen uptake study interesting, but not worthy of focus. The oxygen plume study is also interesting. The leak measurement study very useful and important; it is good to spend future work on understanding leaks from other systems. Graph on slide 16 has way too much information to digest in a presentation. Suggest a breakout, different format, or interpretation at the bottom of the slide.

<u>Ouestion 4: Technology transfer/collaborations with industry, universities and other laboratories</u>

This project was rated **3.2** for technology transfer and collaboration.

- This is a joint project of University of Illinois at Urbana-Champaign, LANL, PNNL, University of Calgary, and Stanford University. While this is a nice, diverse set of institutions, the synergies are not clear. The institution reported the results, not the team as a whole.
- Even within UIUC, the two departments reported separately.
- The project collaborates with three other universities and two national laboratories, although at least one of those collaborations (with LANL) has not yet been successful due to external considerations.
- Lots of good partners; not clear what role each played. Not sure that coordination is tight because presenter actually said, "Someone else made this slide on our team, and I'm not quite sure what it's saying; I haven't talked to him directly."

Question 5: Approach to and relevance of proposed future research

This project was rated 2.4 for proposed future work.

- Complete switchover to hydrogen would result in less than 1 ppm of hydrogen in the atmosphere. Any future work should begin with an estimate of the effect on stratospheric ozone in the most extreme case. If this is not a cause for concern, then no additional work to refine the case is required.
- The future work is largely connected with studying hydrogen uptake by soil.
- Future work should be more clearly linked to specific issues that need resolving, relevant questions that need answers, or technology decisions that need be made.
- They propose to complete the ongoing analyses, incorporate new soil uptake measurements, and refine regional air quality models.
- Based on the overall very minor effects observed so far for even the extreme case of all transportation switching to hydrogen, such refinements are not likely to provide any additional meaningful insights.
- Consider the project done when it comes to the troposphere. It is time to move to the stratosphere. Soil uptake study is complete. Oxygen plume study is complete.

Strengths and weaknesses

Strengths

- Comprehensive study of the effects of a full-scale hydrogen economy.
- The strength of the project is the extent to which it seeks new measurements to serve modeling (e.g., soil effects and hydrogen emission studies).
- The project's major strength is the involvement of multiple disciplines in the study.
- Nice tropospheric modeling and mapping of regional air quality impacts.

Weaknesses

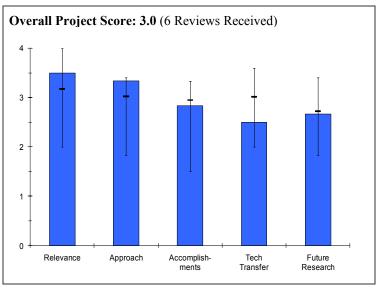
- Project appears to be a disjointed collection of efforts, only loosely grouped around the common theme of assessing environmental impacts.
- Lack of uncertainty/sensitivity analysis makes it impossible to distinguish precision of predictions, e.g., accurate to within a percent or two or simply a coarse estimate.
- The major weakness is that the hydrogen technologies are still maturing, and the results of this study may be only a very preliminary first cut at the resulting assessments.
- Need to move above the troposphere.

- The project should not consider multiple scenarios: take the maximum case for hydrogen in the atmosphere and confirm that there are no ill effects.
- Reconcile overlaps with Project Number AN-14.
- The project is due to be completed in September 2009.
- It might be useful to assess the uncertainties in the different results obtained to date, rather than derive new ones, in the remaining months of the study.

Project # AN-14: Potential Environmental Impacts of Hydrogen-Based Transportation & Power Systems *Mark Z. Jacobson; Stanford University*

Brief Summary of Project

The objectives of the project are to 1) compare emissions of hydrogen, the six criteria pollutants (CO, SO_x, NO₂, PM, ozone, and lead), and greenhouse gases (GHG) from near and long-term methods of generating hydrogen for vehicles and stationary power systems and 2) evaluate the effects of emissions on climate, human health, ecosystem and structures. The following will be developed: 1) market penetration scenarios for vehicles, 2) market penetration scenarios for electricity generation, 3) emission-profile databases, and 4) a soil uptake model. Changes in hydrogen and other atmospheric gases and aerosols in the troposphere and stratosphere will be predicted. Effects due to the



implementation of two market penetration scenarios will be quantified.

Question 1: Relevance to overall DOE objectives

This project earned a score of **3.5** for its relevance to DOE objectives.

- The project seeks to determine the environmental benefits and consequences of hydrogen fuel production (and use) both by different methods of production and by comparison to fossil fuel production (and use).
- Environmental impact studies of this sort provide confidence in the ability of the Fuel Cell Program to deliver its intended environmental benefits.
- The project objectives could be clarified. Slide 3 gives an objective of evaluating effects of emissions on human health something that would require an epidemiological study, which this is not. Likewise, this is not a study that directly evaluates effects of emissions on ecosystems and structures. The present study estimates atmospheric changes that result from predicted emissions as determined by atmospheric chemistry and physics. It also predicts certain climatic changes that may result.
- Assessing emissions of hydrogen and criteria pollutants for a technology that is still in its formative stages appears to be premature.
- This analysis is absolutely needed to explore showstoppers for hydrogen future.
- The study of the impacts of hydrogen concentrations in the troposphere and stratosphere address questions raised about the potential and unintended consequences of increased hydrogen use.
- The majority of the tropospheric impacts are from decreased criteria pollutants due to displacement of fossilderived fuels.

Question 2: Approach to performing the research and development

This project was rated **3.3** on its approach.

- The most useful output would be to show pollution reduction benefits for a reasonable market penetration case and estimate stratospheric ozone effect of maximum hydrogen penetration.
- The investigators use the Argonne Greenhouse Gases, Regulated Emissions, and Energy Use in Transportation Model (GREET) to estimate emissions under various scenarios and then use the highly detailed and computationally intensive Gas, Aerosol, Transport, Radiation General Circulation, Mesoscale, Ocean Model (GATOR-GCMOM) model to predict the effect of these emissions on atmospheric composition and climate.

The results, detailed global maps of the characteristics of interest, are then differenced to demonstrate the difference in outcomes of the scenarios.

- They are analyzing components of the simplified hydrogen cycle (i.e., soil uptake, emissions, and concentrations of hydrogen and other gases in the atmosphere).
- They have defined the market penetration scenarios for vehicles and electricity generation.
- They are assessing quantitative effects of two different market penetration schemes.
- Excellent work in studying both the troposphere and stratosphere. Expansion of system to include status quo of fossil fuel vehicles excellent. Suggest looking at fossil-based hydrogen production transitioning to renewable hydrogen. Also, what about high-atmospheric loss of hydrogen to space? How will this change the balance of gases in the atmospheres? Need to look at secondary GHG formation and destruction. How does increasing cloud formation affect global albedo and, thus, temperature?
- Explicit modeling approach eliminates the parameterization issue, although this results in a large complex simulation that requires very long computer run times.

Ouestion 3: Technical accomplishments and progress toward project and DOE goals

This project was rated 2.8 based on accomplishments.

- The addition of a soil-uptake model to GATOR-GCMOM provides added refinement.
- The complexity of the GATOR-GCMOM model makes some results difficult to interpret. The effort the presenter took to explain slide 16, "Effects of Wind-HFCV on Global Climate and the Ozone Layer," illustrates this.
- The complexity of the GATOR-GCMOM model also makes uncertainty and sensitivity analysis difficult; nevertheless, results such as slide 16 would be a lot more meaningful if some form of such analysis was to be performed.
- There was a slight drift in study purpose from comparing effects of different methods of hydrogen production (slide 3) to comparing two 2050 scenarios, one with hydrogen (wind generated via electrolysis) and one without (slides 19-24). Again, uncertainty analysis would make these results much more meaningful and would calibrate expectations of how precise these results might be.
- They have shown reasonably good agreement between model predictions and several atmospheric parameters, concluding that the model is, thereby, validated.
- They then used this validated model to assess the hydrogen deposition flux, surface concentrations of hydrogen, and global changes in temperatures and ozone concentrations using the Intergovernmental Panel on Climate Change (IPCC) 2050 scenarios "A1B" and "A1B with hydrogen fuel cell vehicle penetration."
- Several global maps were shown as the results from 18-month-long simulations, but the significance of the relatively small changes in the various values was not made clear. Furthermore, the significance of the study so far was not readily apparent.
- Getting a better understanding on leak rates is needed. What about large accidental releases? How would sudden hydrogen plumes affect regional atmospheric chemistry?
- Good use of existing models and validating models. Good scenario setup and set of runs made in models.
- Test model predictions show excellent comparison to data.

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated **2.5** for technology transfer and collaboration.

- The level of collaboration seems appropriate to the task.
- The researchers are aligning their work to Argonne's GREET model.
- The only collaborations identified were among Tetra Tech, Inc., Stanford University, and Hudson Engineering, Inc.
- Would be interesting to collaborate with atmospheric scientists at the National Center for Atmospheric Research and the National Oceanic and Atmospheric Administration. The contributions of the partners were not clear from the presentation.

- No collaboration with another funded effort (Project Number AN-13) that is performing very similar studies.
- The difference in the results is significant and should have been discussed prior to the review meeting and on a regular basis.

Question 5: Approach to and relevance of proposed future research

This project was rated 2.7 for proposed future work.

- Recommend completing the study after the estimate of ozone in the maximum hydrogen case is complete.
- The proposed future work in modeling and effects will complete the project within scope.
- The proposed future work is necessary to compare the two 2050 scenarios to the 2000 baseline.
- The proposed future work returns to the objective of comparing impacts of different methods of hydrogen generation.
- The capability of high resolution and a fine computational grid within the GATOR-GCMOM model yields nice graphics. However, it is not clear what actual decisions would be dependent on this level of detail or the level of precision to which the results are meaningful and/or necessary.
- This project is scheduled to end by September 2009. As such, the only future work identified was to complete the ongoing model simulations and to further quantify the effects of market penetration of hydrogen vehicles.
- The study of impact of hydrogen on structures does not seem very compelling; suggest skipping this work and focusing on increased use of models in your domain. Do not dilute this modeling work and expertise with work on structures. Similarly, work on environmental effects from mining, etc., will only dilute the outstanding work you are doing on climate modeling. The name of project needs to be changed from "Environmental Effects of Hydrogen" to "Effects of Hydrogen on the Troposphere and Stratosphere." Seems like the future work is being written generally to keep the funding flowing rather than digging into the very important topic that you've started to address.
- Completion of the current plan is appropriate.

Strengths and weaknesses

Strengths

- There is a huge amount of information embedded in the GATOR-GCMOM model. Applying it to this problem has the potential for revealing outcomes that would not otherwise be obvious.
- Several simulation results of GATOR-GCMOM have been published over the past two decades, which is offered as confirmation of the validity and value of the model.
- Excellent use of climate models and study of the two first layers of the atmosphere.
- The detailed model can be used to evaluate effects at a global scale.

Weaknesses

- Absent an uncertainty and confidence analysis, one cannot distinguish between a precise prediction and a coarse estimate. The more detailed the figures produced, the easier it is to forget this point.
- Last year, a reviewer asked how to determine confidence levels for the model outputs, and the response was that the GATOR-GCMOM model had been widely published (45 publications) over 19 years. This answer could be made much more responsive by the investigators demonstrating how this historical information might be applied to their work to quantify its level of uncertainty.
- The results of the hydrogen effects that were shown took 18 months of model run, and the results were still listed as preliminary! This suggests that trying to examine the effects of varying any of the parameters or assumptions (for a sensitivity analysis, for example) would require a prohibitively long effort.
- There is the potential to dilute the effectiveness of work with study of other environmental effects. Recommend that researchers focus their work where their strengths lie and their reputation is strong. This work is needed and should not be diluted to all environmental effects.
- Complex model requires enormous computation resources and is not likely to be useable by many other groups.

- Reconcile overlaps with Project Number AN-13.
- I encourage future work to quantify the uncertainty of the results as derived from the uncertainties of the fundamental processes making up the model (slide 9) and the sensitivity of the results to the input conditions. This could be done, of course, at lower resolution.
- This project is scheduled to end in a few months (by the end of September 2009), so no specific recommendations are appropriate.
- For similar studies in the future, it would appear that the DOE Hydrogen Program is, perhaps, not the appropriate sponsor.

Project # ANP-01: Pathways to Commercial Success: Technologies and Products Supported by the HFCIT Program

Steve Weakley and Marylynn Placet; Pacific Northwest National Laboratory

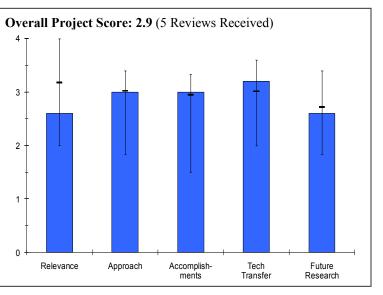
Brief Summary of Project

The objective of this project is to provide an assessment of retrospective HFCIT Program benefits by tracking the commercial success of HFCIT-developed technologies (and technologies developed by HFCIT predecessor programs) and estimating their impacts/benefits.

<u>Question 1: Relevance to overall DOE</u> <u>objectives</u>

This project earned a score of **2.6** for its relevance to DOE objectives.

• This survey of the HFCIT-supported technology R&D products is a good feedback mechanism to analyze the



- program success and its contributions to achieving the overall DOE RD&D objectives.
- The database would help future technology developers and program officials to obtain necessary background information, both knowledge and technical know-how, in order to formulate R&D plans and technical strategies to further advance and/or commercialize the technology products.
- This project attempts to provide a quantitative measure of the outcomes of DOE-sponsored projects that can promote the commercialization of the related technologies. Such a "measure" is of benefit to the DOE management.
- As hydrogen is not a commercial success yet, this project seems a little premature.
- If the purpose is to develop marketing materials to justify past and future funding (see slide 22), then the barrier being addressed is not, "Inconsistent data, assumptions, and guidelines."
- Not sure if this project adds much value. It is very likely that various companies and venture capitalists are already doing this type of monitoring/tracking work.
- The collection of "corporate" knowledge is important. Analysis of the information could be more effective.

Question 2: Approach to performing the research and development

This project was rated **3.0** on its approach.

- This is a rational approach to creating a database on HFCIT-sponsored technology, R&D activities, and products for systematic feedback and forward planning of R&D needs and programs.
- Starting with a patent search, and following through with the inventors and the HFCIT Program managers, is a good way to initiate this study.
- One concern that could lead to under-counting, is that the appropriate HFCIT technology development managers (TDMs) may have moved on to other positions, thereby making it difficult to resurrect the "corporate history" of the technology developments in the program over the years.
- Such a study is best done in retrospect, after a market develops and there are actually products being sold. However, the resulting success stories are quite interesting (maybe not analysis, but interesting). The database of previous research efforts could also be useful.
- Tracking product offering for sales and patent issues in hydrogen and fuel cell areas might be worthwhile; however, initial offering of a product for sales (a few units) does not necessarily make it a "commercial success."

- Patents typically get granted 3 to 5 years after they were initially filed. By this time, the idea might or might not have turned into a commercial product. The commercial product and patent timelines need to be properly tracked.
- It is not clear how the process of going from patents to licensing and commercial products is being effectively tracked.
- The information that is most needed seems to be difficult to collect from corporations and some labs.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated **3.0** based on accomplishments.

- Examples of accomplishments regarding hydrogen storage tanks, distributed hydrogen production systems, etc. have been listed; however, what continued improvements may be necessary for industrial competitiveness is not discussed (perhaps delegated to future researchers to determine).
- It is certainly OK to accentuate success, but issues such as hydrogen leaks from the high-pressure storage tanks (and thus, issues on materials and seals) are not addressed. The success of high-pressure hydrogen tanks may solve one problem, but create another.
- The project has prepared a quantitative listing of the patents issued in the three different categories along with the current status of these patents, i.e., commercialized, part of emerging technology, being used in research, or abandoned.
- Some examples given are a bit of a stretch. For example, it would be difficult to qualify two units sold as a "commercialized technology." The other major example given, that of Quantum compressed gas tanks, appears to predate the technology assessment period of 2002 onwards.
- In the poster presentation, there was no mention of software being trademarked and licensed, which is a significant component of the DOE Hydrogen Program. The poster presenter, Steve Weakly, assured me, however, that the software commercialization is included in the draft report that has been prepared.
- To say that, "Of the 118 patents reviewed, 48% are being used in commercial products, are part of emerging technology development, or are still being used in research," implies that these three categories are equally representative of how successful the patent-generating research is. These three categories are not equally representative.
- This study only represents R&D that resulted in patents, not all HFCIT R&D. Would like to know what percentage of HFCIT R&D money led to patents or emerging technologies.
- The cumulative number of commercial technologies (slide 12) is less than 25! Project "success stories" seems a little enthusiastic given this small number.
- Having a tracking database might be useful to the HFCIT. It is unclear how the HFCIT plans to use the data.
- Completed a draft report as required.

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated **3.2** for technology transfer and collaboration.

- The team is working closely with HFCIT partners, laboratory/contractor researchers, and private sector vendors to establish the database.
- This project has involved developing contacts and relationships with the wide spectrum of researchers sponsored by HFCIT. In terms of sheer numbers, this project has most likely "worked with" more individuals and organizations than any other HFCIT-sponsored project.
- Excellent contacts with hydrogen technology developers. The list of projects and researchers is, in itself, a valuable data set.
- It is difficult to understand how the benefit of this database/report will be realized.
- Have obtained information through cooperation with a number of players, but not all.

Question 5: Approach to and relevance of proposed future research

This project was rated **2.6** for proposed future work.

- It is an ongoing project, and the project personnel will continuously update the database as new information becomes available.
- Finalizing and publishing the annual report, which is presently in draft stage, will be a useful documentation of the technologies identified in the project.
- Also useful will be providing Web-based access to the project's findings and updating these findings in an ongoing manner.
- Not sure that future work is warranted.
- Future work also needs to make the database and other information widely available to those involved in hydrogen research.
- No plans to address the difficulty in getting complete information. Important to keep this database up to date.

Strengths and weaknesses

Strengths

- A database on the current technology state-of-the-art and currently available commercial hydrogen energy technology products would benefit technology developers, vendors, and program analysts to legitimize future work.
- They have set up a comprehensive database that should prove to be a good resource of information for HFCIT and other interested organizations.
- Interesting data set.
- Good starting point for the database.

Weaknesses

- The success of the project is limited by the combined "memory" of the program office TDMs. As such, some of the older projects may not have been covered adequately.
- Seems really premature and of little value in setting up R&D priorities and "pathways to commercial success." However, in providing marketing material for the Hydrogen Program, some very interesting stories emerged.
- Very little in-depth analysis of the information. Limited utility as a tool to assess the success or failure of the program.

- The database should be widely available in the public domain. Combining this work with market needs and trends for future diffusion of hydrogen energy knowledge and technical know-how would be of much benefit.
- Once the draft report has been approved for release, the information should be made readily available.
- Any database is only as current as the date of the last entry for each item. To be meaningful, the database would need to be continually updated (even if there is new information for a particular item in it).
- Perhaps one additional piece of information to track is the change in the number of employees of these companies from year to year. If a company in the hydrogen and fuel cell areas has workforce reduction, it would most likely imply that any new commercial products or their current product(s) are not doing too well.

Project # ANP-03: Thermodynamic, Economic, and Environmental Modeling of Hydrogen (H₂) Co-Production Integrated with Stationary Fuel Cell Systems (FCS)

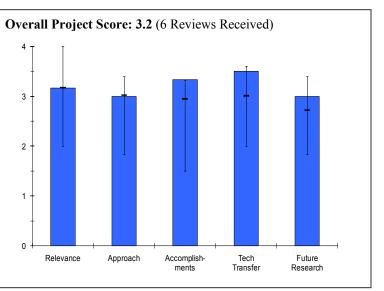
Whitney Colella, Aerel Rankin, and Amy Sun; Sandia National Laboratories Pere Margalef and Jack Brouwer; University of California at Irvine

Brief Summary of Project

The objective of this project is to analyze the potential for hydrogen co-production within high-temperature stationary fuel cell systems (H₂-FCS) and identify novel designs with minimum CO₂ and cost. Specific objectives are to 1) develop novel H₂-FCS designs that release low greenhouse gas emissions; and 2) develop novel H₂-FCS designs with low hydrogen production cost.

<u>Question 1: Relevance to overall DOE</u> <u>objectives</u>

This project earned a score of **3.2** for its relevance to DOE objectives.



- This project is highly relevant to the existing technical challenges of stationary fuel cells and their integration with hydrogen production and/or cogeneration.
- The project supports the DOE Hydrogen Program objectives.
- Hydrogen co-production integrated with fuel cell systems is an interesting technology idea, although its viability is uncertain. Distributed hydrogen production facility management, maintenance, safety aspects, product recovery, and CO₂ management are not expected to be cost-effective and may be operationally difficult. Without adequate analysis and information of relevant parameters, an objective evaluation of the concept is difficult.
- The project focuses on thermodynamic, economic, and environmental models to analyze recouping waste heat from high-temperature stationary fuel cell systems to enhance steam-methane reforming to co-produce hydrogen for transportation and/or industrial applications. Interesting approach to build stationary fuel cells, and then utilize waste heat to produce distributed sources of hydrogen that can be used to power mobile fuel cell applications. Project addresses key issues facing introduction of hydrogen fuel cell vehicles (HFCV) and hydrogen infrastructure: which comes first? By introducing the use of stationary fuel cells (powered by steam reforming of natural gas), one can switch over to using waste heat to produce hydrogen for transportation.
- This project has the objective of investigating options for combined hydrogen, heat, and power production using high-temperature fuel cells that have the potential to lower the overall costs and lower the CO₂ emissions (as compared to generating the three separately and independently).
- This project addresses the multiple elements of the overall Hydrogen Program to produce hydrogen (e.g., for fuel cell vehicles) and to commercialize fuel cells for distributed power production. Being able to use the fuel cell waste heat effectively is an added bonus.
- The scenario of co-producing electricity and hydrogen in a high-temperature fuel cell from natural gas would only be attractive in places where there is a wide price spread of natural gas purchased to electricity sold (back to grid). It might be more relevant to look at a forecourt case where the electricity is used for charging hybrid batteries and hydrogen for HFCV. There is a time-of-day issue that needs to be worked out.
- Hydrogen at 350-bar would not necessarily be liquid.
- The modeling approach/tool is quite useful in developing a value proposition for stationary fuel cells to produce power, heat, and hydrogen. The lower cost hydrogen will enable HFCV deployment.

<u>Ouestion 2: Approach to performing the research and development</u>

This project was rated **3.0** on its approach.

- A good combination of a simpler model for preliminary details plus a more detailed Aspen model for improved estimates.
- The diverse team is more than qualified and capable to execute the intended tasks successfully. However, it appears that the work scope and objectives are too broad, varied, and unfocused. It is not clear what specific technical issues and barriers the research team is addressing and intends to overcome. Without a focused approach that is comprehensible to the audience other researchers, analysts, and program managers, the work and its conclusions may not be meaningful. For example, what technology R&D product is intended and what is its value and application for improving science, technology, commerce, etc.?
- A good approach that first models the thermodynamic requirements (although the models assume all waste heat is converted to hydrogen). My only hope is that subsequent versions include realistic assumptions on waste heat utilization and actual (not ideal) component efficiencies.
- This is an analytical rather than an experimental project. In the system models they are developing and analyzing, they are attempting to identify opportunities for close thermal integration.
- They have analyzed solid oxide fuel cells (SOFCs) and molten carbonate fuel cells.
- They have also investigated other options, such as a network of such systems to provide for load following and other benefits, even if some of these options may be rather difficult to implement (at least, until the technology is much more fully developed and mature).
- While the concept of using the excess heat from a SOFC for a reforming reaction to produce hydrogen is straightforward, the controls complexity of this system should not be understated, especially when additional heat is generated through capturing and burning of tail-gas stream from the pressure swing adsorption (PSA).
- The system might not be running robustly due to the degree of interdependency of the fuel cell, the internal reformer, the external reformer, the combustor, and the PSA. This concept offers operating flexibility, increased efficiency and lower greenhouse gases (GHG), but also adds complexity and capital cost (potentially).
- A high-temperature fuel cell and PSA might not be the best match. The fuel cell runs at high temperature and low pressure, whereas PSA likes low temperature and high pressure.
- Thermodynamic analysis and modeling activity is well organized for high temperature fuel cells. The hydrogen purification approach is also theoretically sound. The team is well qualified.
- Involving fuel cell manufacturers in proactive planning and review of results has led to useful work based on realistic assumptions.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated 3.3 based on accomplishments.

- Really good value. A lot of work for very little funding.
- Significant results have been presented. However, the PI has presented an enormous amount of material with excessive narratives, thereby making it difficult for the reader to comprehend the real story. The coherence and continuity of the subject matter is soon lost. The slides are extremely busy with so much text, tables, figures, and mathematical derivations that a reader cannot understand the message of what (i.e., the issue, what problem needs to be solved), why (i.e., why and how solving the problem would advance the current status of science in support of DOE program goals), how (i.e., the technical strategy for achieving the intended results) and, finally, the so what (i.e., benefits of the study results).
- Simple statements of technical approach, results, and how the results advance the state-of-the-art generally interest a broad audience. This presentation is suitable only for a specific audience.
- Considering the project just started in January 2009, the progress has been remarkable. Three scenarios have been developed and modeled with increasing levels of complexities.
- The accomplishments were illustrated by describing a case study of networked systems that could provide variable heat-to-power and hydrogen-to-heat ratios for load following of either heat or hydrogen, respectively.
- The case study presented analyzed thirteen different system configurations, showing that different configurations would be optimum, depending on whether the manufacturer revenues, CO₂ emissions, or cost to the consumer is the major driving factor.

- Many of the results of their analyses appeared to be affected significantly by external factors, such as fuel prices. With such interconnected relationships, it is difficult to assess the usefulness of the results.
- It was difficult to understand the major outcomes or implications of the studies conducted.
- Project started recently. Appears to have done quite a bit of work and be on the right track.
- 1 MW(e) is too large for forecourt electricity while 450 kg per day of hydrogen is too small for hydrogen (1,500 kg/day for commercial station). A few hundred kW(e) for forecourt might be more practical and run the fuel cell less efficiently to produce more hydrogen as demand dictates.
- Results of tri-generation system look reasonable. Load following analysis for power, hydrogen, or heat is interesting. Value-based prioritizing of co-products will help to focus the tool better for a majority of applications.

<u>Ouestion 4: Technology transfer/collaborations with industry, universities and other laboratories</u>

This project was rated **3.5** for technology transfer and collaboration.

- Great consortium of national labs, academia, and industry.
- A highly competent team of six national laboratories, University of California-Irvine (UC-I), and industry (e.g., Fuel Cell Energy, Inc.; Technology Management, Inc.) are conducting the tasks, and major industries (e.g., ExxonMobil, Shell, ConocoPhillips, and Chevron) are evaluating models. This is truly an exemplary collaborative R&D effort.
- There appears to be a large degree of collaboration. Not quite sure how detailed interaction with such a large number of collaborators can be. Would it be better to focus on fewer collaborators with a higher level of interaction with select partners?
- The project has a good breadth of collaborators from universities, national laboratories, and the high-temperature fuel cell industry. In principle, this collaboration offers the model developers good access to realistic fuel cell data.
- Very good collaborations with fuel cell industry partners and national labs.
- Suggest the team talk to reformer developer to confirm numbers and validate key assumptions.
- The PI and team come from SNL and UCI. Both have very good experience in the stationary fuel cells and hydrogen systems. Strategy to solicit input and share results is very well focused. Good coordination between team members.

Question 5: Approach to and relevance of proposed future research

This project was rated **3.0** for proposed future work.

- A good plan for future research. Hope the project can continue.
- This section is missing. However, only 12% work has been completed since the project started in January 2009. It is expected the competent team will continue the work per established technical baselines and a planned development path.
- Future efforts focus on continued model development/enhancement, which is appropriate for a project at this stage (6-9 months). The project indicates it will include more realistic assumptions for the input, which will temper the predicted advantages and hydrogen production to values below the 150 to 450 kg/day.
- They will develop more detailed Aspen models to validate the potential for hydrogen co-production with heat and power. This would offer a good comparison with their modeling results, particularly with regard to variable hydrogen, heat, and electricity production.
- Suggest the team verify key assumptions in the model.
- The future work plan is logically organized. Creating a value proposition for a potential consumer to maximize the benefits is very useful. Techno-economic-environmental analysis is good.

Strengths and weaknesses

Strengths

- Good collaborations with multiple partners.
- Good skills and expertise from the PI.

- Results are important for the future of stationary fuel cells.
- Super accomplishments within a limited time. Analysis of an innovative H₂-FCS integrated concept, which can potentially make enough hydrogen cost-effectively and can power 660 fuel cell cars per day with no additional CO₂ emissions.
- Interesting approach to introduce hydrogen production (distributed) through by recouping waste heat from stationary FC systems. Could provide a route to produce the levels of hydrogen needed for early introduction of FC vehicles.
- Defining and analyzing of innovative system and network configurations is a strength.
- Analyzing systems from different perspectives, such as whether the highest priority is electricity production or GHG emissions reduction, is a strength.
- Thermodynamic analysis is based on good electrochemical principles and chemical system analysis. Use of realistic assumptions derived from fuel cell experience is very good.

Weaknesses

- Presentation is hard to read and follow. It is understandable that they want to show the extensive work conducted, but they should reduce the number of slides and focus on the key points.
- The PI has not addressed how CO₂ emissions can be managed (i.e., captured, transported, and stored) in a distributed scenario. Also, how easy or difficult it is to pump hydrogen in vehicles, and the associated safety and hydrogen emission concerns, has not been addressed.
- The use of ideal efficiencies is unrealistic and oversells the concept. More realistic thermal and mechanical efficiencies should be used to provide more realistic predictions.
- Project should indicate how the models and codes will be used to demonstrate the co-production aspects. Are they working with an actual demonstration or is this still in the concept development stage?
- The models have a large number of parameters that have significant influence on the analysis outcomes (i.e., costs, GHG emissions, relative amounts of electricity, heat, and hydrogen). It is difficult to understand the main messages from the study.
- It is difficult to understand how to use the results from such analyses to guide future R&D or future analyses.
- Focusing on practical aspects and realistic data will help improve the benefits of the study.

- Continue detailed analysis of optimum stationary fuel cells.
- Suggest the team present each focus or barrier area, one at a time. Present an analysis of what problems need to be solved so that audience has a comprehension of what results are expected.
- Use realistic efficiencies to bracket the projected benefits.
- Should consider how we get from the present situation (conventional stand-alone systems for electricity, heat, and hydrogen) to the intermediate scenario of combined heat and power, and then to the ultimate situation envisaged in this study (combined hydrogen, heat, and power) without discarding or stranding the earlier investments i.e. how should the near-term systems be configured so that they are flexible enough to add heat recovery at a later time, with the capability of then adding hydrogen production (initially small amounts and then subsequently larger amounts) at an even later stage.
- Please include effect of financial incentives related to emission trading-NO_x, SO_x, VOC, PM-2.5, etc.
- Apply the model to university sites and national laboratory sites.
- Include renewable fuels in the analysis.
- Use of photovoltaic and wind in a smart grid may be helpful.

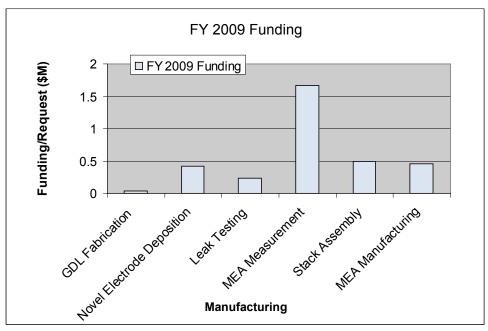
Manufacturing R&D Summary of Annual Merit Review Manufacturing Subprogram

Summary of Reviewer Comments on Manufacturing R&D Subprogram:

The Manufacturing R&D subprogram develops and demonstrates technologies and processes that will reduce the cost of components and systems for fuel cells, hydrogen storage, and hydrogen production to enable the growth of a strong domestic supplier base. The activities focus on near-term cost goals for early market applications. In FY 2009 six new manufacturing projects, started in late FY 2008, were reviewed along with two continuing projects. The continuing projects addressed fuel cell membrane electrode assembly (MEA) manufacturing and fabrication of catalyst-coated membranes. In addition to new manufacturing R&D on low-cost, durable MEAs, the subprogram added work on gas diffusion layer production and fuel cell stack in-line testing. Two of the new projects addressed lower cost manufacture of high-pressure containment vessels for hydrogen storage.

Manufacturing R&D Funding:

Funding for the Manufacturing R&D subprogram was level for FY 2008 and FY 2009 at approximately \$5M per year. All current projects are scheduled to continue through FY 2009 with future efforts subject to appropriations.



Reviewer Comments and Recommendations:

The manufacturing projects were rated high to average with six individual projects rated at 3.2 or higher. Overall ratings ranged from 3.5 to 2.4. All projects were judged to be relevant to the DOE hydrogen and fuel cell activities with good or adequate technical approaches employed in the R&D. In most cases, project progress and accomplishments were judged as satisfactory; however in several projects it was difficult to judge progress since the work had been underway for only six months or less. Project teams were judged to be strong for most projects with partners having demonstrated experience and expertise in the required technical disciplines. In general, reviewers felt that, particularly early in the project, more

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effort should be devoted to quantifying and validating potential cost reductions. Lower manufacturing costs were judged to be an important rationale for continuation of the projects in the future.

The highest ranked (3.5) projects were:

- "Reduction of Fabrication Cost of Gas Diffusion Layers," Ballard Material Products. Reviewers considered this new project to be highly relevant, with an excellent approach, progress, and strong technology transfer and collaborations.
- "Digital Fabrication of Catalyst Coated Membranes," Pacific Northwest National Laboratory. Reviewers also considered this continuing project to be highly relevant with a strong approach to complete the proposed research and project objectives on schedule in FY 2009.

The lowest ranked (2.4) project was "Inexpensive Pressure Vessel Production through Fast Dry Winding Manufacture," Lawrence Livermore National Laboratory. This project was judged to be relevant but lacked sufficient discussion of technical and cost details due to disclosure restrictions of propriety information.

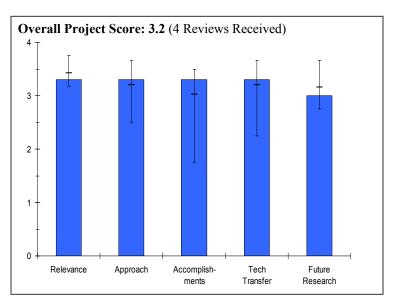
In summary, manufacturing was considered to be an important key element for fuel cell and hydrogen technology commercialization. The Manufacturing R&D subprogram was judged to be well-managed, organized, and focused on addressing programmatic performance targets.

Project # MF-01: Fuel Cell MEA Manufacturing R&D

Michael Ulsh and Huyen Dinh; National Renewable Energy Laboratory Adam Weber; Lawrence Berkeley National Laboratory

Brief Summary of Project

The objectives for this project are to 1) evaluate and develop in-line diagnostics for membrane electrode assembly (MEA) component quality control and validate inline, 2) investigate the effects of manufacturing defects on MEA performance and durability, and 3) further develop and validate models to predict the effects of local variations in MEA component properties. Fuel cell system cost targets are based on a projection of 500,000 units per year. The supplier base needs highspeed manufacturing methods – and quality control methods to support them – to achieve these volumes.



Question 1: Relevance to overall DOE objectives

This project earned a score of 3.3 for its relevance to DOE objectives.

- The objective of this project is to evaluate membrane diagnostics for various types of defects.
- If these in-line, 2-D, image-based diagnostic methods can be reliably used for most or all in-line evaluation of proton exchange membrane (PEM) roll stock production quality assurance, it would have a significant impact on fuel cell costs and reliability.
- An understanding of defect thresholds is important in the identification and development of diagnostic methods.
- MEAs represent a significant opportunity for PEM fuel cell cost reduction, and the project is attempting to address program cost reduction goals.
- The relationship between MEA dimensional defect detection and part/stack/system cost needs to be developed to better understand the cost reduction potential of this effort.

Question 2: Approach to performing the research and development

This project was rated **3.3** on its approach.

- This is a good approach.
- This appears to be a logical approach in establishing relationships between various defects and effects in cell/stack assemblies, then applying specifications to measurement methods.
- The approach towards identifying the means to identify certain defects and the defects' impact on performance and durability is sound.
- It is not yet clear what cost savings can be realized by reducing defect frequency or severity. Additionally, while identifying defective components before delivery is an important aspect of quality control, potentially greater cost savings could be achieved by working towards defect reduction (maybe this is a step left to the component manufacturers).
- Milestones beyond September 2009 could be more clearly identified.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated 3.3 based on accomplishments.

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- This project established a development platform in addition to standard industry practices for membrane samples.
- This is a good use of test methods across single cells and multiple/segmented cells.
- Progression of NREL diagnostic from concept to in-practice since 2008 is good.
- In the segmented cell experiments, the ability to potentially locate a defect in an assembly doesn't translate into in-line membrane and MEA production, but it would be valuable for sub-assemblies and assemblies *if* it works with single and multiple defects.
- Defect identification effort has made appreciable progress but the overall value of the project relies on the successful establishment of defect threshold values through modeling/experimental work and collaboration with industry partners.

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated **3.3** for technology transfer and collaboration.

- This is a good mix of universities, small business, national labs, but no industry partner. Collaborations are mostly universities, but the team should consider an industry partner for guidance.
- An impressive set of collaborators, including Nafion[®]-like and would-be polybenzimidazole membrane suppliers.
- Appropriate collaborators have been identified, but it is not clear to what degree some are contributing. This may be somewhat an artifact of the progression of the overall effort.

Question 5: Approach to and relevance of proposed future research

This project was rated **3.0** for proposed future work.

- The team should add industry partners to validate future work. Is there any way to get additional industry partners (in addition to the two) to participate? The program appears to be limited to just these; it would be good to get additional feedback/testing methods from others.
- Proposed work looks good. Maintaining a close relationship among test/diagnostic/model developers and manufacturers will be critical as the project proceeds.
- Future technical efforts are clearly described, but neither decision points nor possible risk mitigation approaches are delineated.
- Future work needs to characterize the cost implications of reductions in deliveries of defective components.

Strengths and weaknesses

Strengths

- Strong base of industry and academic contributors.
- There is good collaboration among the team. Developing procedures and hardware that can have a positive impact on a broad segment of fuel cell industry.
- Good overall technical approach and progress.

Weaknesses

- Should have additional industry partners.
- Critical information, particularly defect thresholds, has not yet been ascertained. This effort should have preceded the identification effort as knowing what you need to find is important in identifying how to find it.
- Cost implications of defects need to be identified.

- The scope appears correct. I look forward to future progress reports.
- Since 2-D image data is used in full-area diagnostics, there may be value in adding the software for a 2-D autocorrelation routine for identifying non-random defect sources in a real manufacturing environment.
- It would be valuable to be able to model a relationship between the measurements of defects in MEA production runs vs. final cell/stack costs in \$/cm² or \$/kW. Presenter stated that they hope to do this. The model needs to be capable of adapting to different manufacturers' processes.
- Are developers looking at other fuel cell types besides PEM? Solid oxide fuel cell may be amenable to transmission diagnostics.

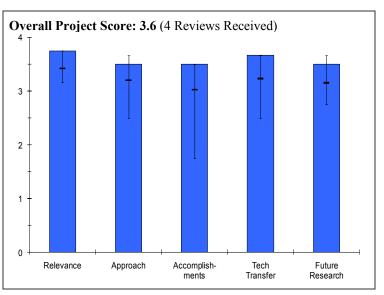
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Project # MF-02: Reduction in Fabrication Costs of Gas Diffusion Layers

Colleen Legzdins; Ballard Material Products

Brief Summary of Project

The objectives for this project are to 1) reduce the fabrication costs of gas diffusion layer (GDL) products and demonstrate the means of achieving six sigma quality standards at high-volume manufacturing, 2) produce high-performance GDLs at lower cost in the near term, and 3) verify the design of a new production facility incorporating new GDL process technologies to meet automotive volume requirements at the DOE 2015 cost target of \$30/kW for the fuel cell system (GDL cost target = \$4/kW).



<u>Question 1: Relevance to overall DOE</u> <u>objectives</u>

This project earned a score of 3.8 for its relevance to DOE objectives.

- The methods outlined to reduce GDL costs and develop online quality control are very important; if successful, they will immediately feed and expand parent company's markets.
- It was not entirely clear whether the manufacturing improvement processes being looked at were scalable to commercial levels. Some discussion of manufacturing volume range would be helpful.
- The presentation was well laid out to identify various processes being targeted.

Question 2: Approach to performing the research and development

This project was rated **3.5** on its approach.

- This reviewer would have appreciated more details on the online tests.
- What metrics are being used to measure improvement? Without revealing manufacturing details, could frame the measurement as percent reduction in number of coats, increase throughput by X%, etc.
- How are the online tests being used for quality control? Are they being related to actual performance data?
- Good discussion on involvement of manufacturing personnel and integration with existing processes /
- techniques.
- Good review of processes being identified for cost improvements.
- A process flow diagram of the GDL manufacturing process that identifies the process steps that have the greatest impact on overall cost would have been helpful.
- It was difficult to understand the relative benefits of the various process steps being discussed. Does ink-mixing impact cost more than ex situ testing? It probably does not.

Ouestion 3: Technical accomplishments and progress toward project and DOE goals

This project was rated 3.5 based on accomplishments.

- Without a reference of numerical improvement (e.g., X% decrease in time to make ink), it is harder to gauge actual progress.
- This reviewer would like to know what, if any problems were encountered during the tasks and how they were overcome. Otherwise, the project appears to be on track.
- The coating weight scan is a great advance.

- While this is the first year of the project, it appears many key components are ahead of schedule.
- Outstanding progress relative to being a new project.
- The team has isolated two key manufacturing line processes elements whose improvement has the potential to significantly reduce costs.
- In-line measurement and product property variation versus performance study is an excellent plan as feedback to optimize key manufacturing line process elements under investigation.
- Accuracy evaluation relative to international standards for surface topography measurements shows good understanding of metrology.
- Excellent overall consideration of the vast array of measurement technologies available in all aspects of the manufacturing process. Great understanding of the factors that affect measurement performance.
- Since it is early in the project, few results can be expected yet.

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated **3.7** for technology transfer and collaboration.

- The main partner appears to be parent company Ballard Power Systems.
- Good addition to now include NREL/M. Ulsh in addition to Pennsylvania State University.
- It appears that Pennsylvania State University is the only substantive partner external to Ballard Material Products. To be successful in this project, Ballard is very dependent upon its ability to apply established inhouse processes and protocols for other Ballard product lines to the new GDL product.
- It appears that collaboration teams are identified and apparently working well.
- This reviewer is not entirely clear what the different roles are for each collaborator.

Question 5: Approach to and relevance of proposed future research

This project was rated **3.5** for proposed future work.

- The project is "on plan," and future actions are appropriate to achieve objectives.
- Again, Ballard's progress will be predicated on its ability to transfer protocols and processes for other Ballard products to the new GDL product.
- Future research is very aggressive. This is great.
- Most of the project is yet to be performed. "Future Work" beyond this project should be easier to identify once more results start coming out of this project.

Strengths and weaknesses

Strengths

- This program covers a full line of coating processes (i.e., ink delivery, reduction of steps) and online measurement of various parameters.
- The project has full control of web (carbon paper) manufacture.
- Ballard's good track record as a manufacturer of products using similar materials and processes is a strength.
- The manufacturing process element improvement is good.
- Online, in situ measurement is a strength.
- Structure and manufacturing processes are identified well.

Weaknesses

- This reviewer would like to see more metrics on improvement for the various tasks and subtasks, even if they are relative or normalized.
- The relative impact on the cost of each process step is not clear. They are probably clear to the PI, but they were not communicated during the presentation.

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Specific recommendations and additions or deletions to the work scope

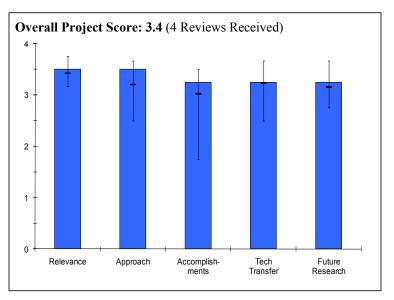
• Is there room to add modeling of the impact of defects on MEA performance to determine what value of a defect is critical? For example, how would you relate the roughness scan to performance and a specification?

Project # MF-03: Modular, High-Volume Fuel Cell Leak-Test Suite and Process

Ian Kaye, Ru Chen, and Matt Mendez; UltraCell Corporation Peter Rieke and Dale King; Pacific Northwest National Laboratory Gordon Splete; Cincinnati Test Systems

Brief Summary of Project

The objectives for this project are to 1) design a modular, high-volume fuel cell leak-test suite capable of testing in excess of 100,000 fuel cell stacks per year (i.e., 50 fuel cell stacks per hour), 2) perform leak tests inline during assembly and break-in steps, 3) demonstrate fuel cell stack vield rate to 95%, 4) reduce labor content to 6 minutes, and 5) reduce fuel cell stack manufacturing cost by 80%. Phase I of the project will focus on analysis of the manufacturing process, stack failure modes, and leak-test methods; prototype design and fabrication; and leak-test suite design. Phase II will include pilot production line modification; leak-test suit fabrication, integration, and verification; and a limited production test run.



Question 1: Relevance to overall DOE objectives

This project earned a score of 3.5 for its relevance to DOE objectives.

- This was a good presentation, and it appears to have good progress at 20% level.
- This is a key area in terms of fuel cell performance and durability.
- This project is very relevant to the fuel cell manufacturing initiative at DOE. A means of quickly determining whether or not an assembled stack is leak-free would be a significant contribution. The as-assembled UltraCell fuel cells have inconsistent quality with significant variations in yield from batch to batch. This test fixture appears to be designed specifically for UltraCell; therefore, even if it is successfully developed, it may not be universally applicable.
- This is very relevant to the DOE objectives for cost and reliability improvements in fuel cell power systems as they are evolving in the early portable market.

Question 2: Approach to performing the research and development

This project was rated **3.5** on its approach.

- This is a good use of the flexo-tiltometer, particularly in the identification of the use of bolts. The material costs seem expensive.
- I have been impressed with the manufacturing expertise of the people that UltraCell has brought into the program. Great background and understanding of how to interject quality control principles into the manufacturing process, first with Deming and then with Six Sigma.
- The approach is to use the manufactured stack as part of the sensor network. The presentation indicates that the yield for finished stacks is quite variable. This being the case, testing finished products may result in considerable wastage. Testing materials and/or stacks during assembly, rather than after, would appear to be a better approach. If this is not possible, use the resources to improve the yield of the fuel cell stacks to begin with. However, the project would have more significance if a test fixture could be developed to check the health of stacks before they are completely assembled. Once the yields become more consistent, the approach of

developing a test fixture appears sound. The specifications for the test sensor are being continually refined as defects and/or leaks in assembled stacks are discovered. This is a good thing.

- Combining manufacturing process analysis, stack failure modes and effects analysis (FMEA), and leak test development is a good mix for leveraging investment into improvements in system cost, reliability, and production rates.
- For high-rate stack leak checking, investigator's approach provides what appears to be a robust set of methods to do the job. From a presentation answer, it looks like the diagnostics of pressure distribution, compression, and leak current is, or will be, implemented on every cell during assembly. This is great, if true.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated 3.3 based on accomplishments.

- This is a good use of partners and evaluation of technologies.
- The potential of the learnings from this project to successfully transfer to other fuel cell technologies is uncertain.
- Progress is pretty good for roughly six months of work completed before the presentation needed to be submitted. A greater discussion of the analysis of the manufacturing process would be beneficial, particularly since the analysis could show the path to better yields.
- Good test results that translate into good test hardware and protocols for testing as-built stacks.

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated **3.3** for technology transfer and collaboration.

- Very well done.
- UltraCell has brought together a good team.
- Collaboration appears to be going well, particularly between UltraCell and PNNL.
- Project lead is a significant fuel cell system provider. The collaboration with PNNL will benefit from their background in fuel cells and systems.

Question 5: Approach to and relevance of proposed future research

This project was rated **3.3** for proposed future work.

- On track for go/no-go decision.
- The future work plan is good and builds on past successes while learning from failures.
- The leak-test prototype brassboard planned for FY 2009 should quickly show the value of an ultimate 50 pph (i.e., 50 fuel cell stacks per hour) test system from this project.

Strengths and weaknesses

Strengths

- UltraCell's focus on quality control in the manufacturing process is a strength.
- Very well thought out and organized project.
- The implementation of test methods into company's production line as they are developed provides a rapid translation of a DOE project into a realistic industry benefit.

Weaknesses

- The potential of the solution from this project to transfer to other fuel cell technologies seems weak.
- It is not clear how the development of this test suite will be used to improve stack yield. The process analysis needs to be explored.

Specific recommendations and additions or deletions to the work scope

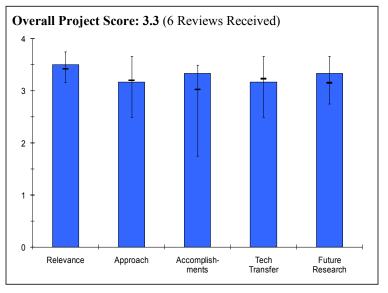
• Perhaps some interaction with an organization with expertise in improving the manufacturing process would be helpful.

Project # MF-04: Manufacturing of Low-Cost, Durable Membrane Electrode Assemblies Engineered for Rapid Conditioning

F. Colin Busby; W.L Gore and Associates, Inc.

Brief Summary of Project

The overall objective of this project is to develop unique, high-volume manufacturing processes that will produce low-cost, durable, high-power density 3L (3-layer) membrane electrode assemblies (MEAs) that require little or no stack conditioning. Objectives include 1) developing a manufacturing process scalable to fuel cell industry MEA volumes of at least 500,000 systems per year, 2) developing a manufacturing process consistent with achieving the \$15/kWe DOE 2015 transportation stack cost target, 3) the product made in the manufacturing process should be at least as durable as the MEA made in the current process for relevant automotive duty cycling test protocols, 4)



the product developed using the new process must demonstrate a power density greater or equal to that of the MEA made by the current process for relevant automotive operating conditions, and 5) the stack break-in time should be reduced by at least 50% compared to the product made in today's process, and break-in strategies employed must be consistent with cost targets.

Question 1: Relevance to overall DOE objectives

This project earned a score of **3.5** for its relevance to DOE objectives.

- This project addresses the lack of high-rate manufacturing processes for MEA fabrication. It is very relevant to the DOE Fuel Cells Subprogram objectives and is important to enable the cost of MEAs to meet the DOE targets.
- Project goals are laudable and relevant to DOE goals for improving proton exchange membrane (PEM) MEA production. If the remaining tasks for this phase can be accomplished, there should be a valuable lab-scale production prototype for lower-cost production.
- The project is addressing cost issues associated with MEAs, but there is conflicting information regarding whether durability is to be improved or simply maintained.
- Relevance to overall program was well defined in the presentation. There was an obvious attempt to tie the project goals to DOE's overall goals.

Question 2: Approach to performing the research and development

This project was rated **3.2** on its approach.

- The approach is logical and has identified the areas in which improvements are sought. Reduction in materials (e.g., eliminating the backing layer and direct coating) and wastage is key, as is understanding MEA failure mechanisms during fabrication and conditioning. Gore plans to address both issues in this project. W.L. Gore & Associates is anticipating a 25% reduction in material cost; reductions in conditioning cost will also be considered.
- There are numerous diverse subtasks related to reducing cost and improving durability. All are worthy of doing, but not sure if the project plan is an optimization of these activities.

- Phase 1 cost modeling nearly completely relies on a thinner membrane (still with ePTFE [expanded polytetrafluoroethylene] reinforcement?), direct coating for one electrode, and removal of backers in process. Will this be demonstrable in any of the production prototypes supposedly developed and built in the remainder of CY 2009?
- The approaches for both mechanical property and conditioning modeling are appropriate.
- More details concerning the cost modeling approach should have been provided.
- The approach is well formulated.
- The approach seems well thought out. More detail on the downselect of cost-reduction processes that will be modeled would be nice; however, there was not enough time in the presentation or room on the submitted materials to cover all the material. This was not the presenter's fault.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated 3.3 based on accomplishments.

- Progress on this project is reasonable. It is scheduled to end in December 2009. The schedule appears to be quite aggressive and may need to be extended. Preliminary results from the cost model indicate the possibility to reduce 3-layer MEA manufacturing cost by 25%. However, it is not clear if this reduction will meet the DOE MEA cost target because a baseline cost was not presented.
- The mechanical testing and property data generation is valuable to the remainder of the project.
- The integration of modeling and data for a new conditioning model should prove very useful in designing a new MEA and manufacturing method.
- The cost model indicates the potential for 25% MEA materials cost reduction, which when added to potentially reduced conditioning costs, would help in meeting DOE goals.
- Membrane durability testing shows good progress although it is unclear if continuous and cyclic testing were performed within one test sequence or separately (either consecutively or in parallel).
- More details concerning the cost reduction effort should have been presented. It could be clearer how the potential cost savings will be realized.
- There is some risk that modifications to production processes to reduce cost will not maintain performance or durability relative to the baseline. Risk mitigation approaches should be examined.
- This is early in the project, so accomplishments are understandably "slim" so far.
- More definition on the "failure criteria" baseline would be helpful. The benchmarks and the trade-offs between cost and quality were not clear. Would slightly less quality yield higher cost savings, but still be acceptable? It probably just needs a bit more explaining.

<u>Ouestion 4: Technology transfer/collaborations with industry, universities and other laboratories</u>

This project was rated **3.2** for technology transfer and collaboration.

- Collaboration is strong between Gore, UTC Power, and the University of Connecticut. Each brings appropriate skills to bear on the problem.
- This looks like an appropriate and good collaboration.
- The team incorporates experienced partners, but the overall effort does not seem to be terribly integrated. (It almost seems like three separate projects under one umbrella).
- The responsibilities of each team member were clearly spelled out.

Question 5: Approach to and relevance of proposed future research

This project was rated **3.3** for proposed future work.

- The work plan is well laid out and focuses the remaining resources on the appropriate activities, such as on the conditioning model development and on the installation of continuous lab-scale equipment.
- The planned future work on completing and testing the models is important in meeting goals for future MEA and process designs. The prototype design, build, and test phases for lab-scale production equipment will be the

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ultimate validation for the designs and modeling. There should be some iteration and contingency time included in the plan.

- The planned work for new production processes/cost reduction seems appropriate.
- In other areas, the future work needs more detail concerning decision points and the relationships/interactions between different project aspects.
- Since it is early in the project, there was understandably not a lot of detail on future work. Program plans, however, were clearly explained.

Strengths and weaknesses

Strengths

- Very good team that includes industry leaders. Baseline MEA meets the DOE durability targets (9,000 hours with no sign of failure) so that membrane development will not consume resources that can be spent on the manufacturing process development.
- Good planning for the modeling and experiments required to make decisions on new MEA manufacturing processes. The resulting models and database will be helpful in other future projects regarding improved cell designs and manufacturing.
- An experienced team working on important potential MEA cost reduction avenues is a strength.
- Key collaborators are in place for research, modeling, and testing, which is a strength.
- Rapid conditioning emphasis is excellent.
- Good team and well planned project. The concept of modeling before implementation is the way to go.

Weaknesses

- The schedule may be too aggressive. It is hard to know if a 25% reduction in MEA cost will meet the DOE cost targets.
- The project scope is probably more ambitious than remaining schedule allows.
- Weak (or unclear) interaction and coordination of seemingly disparate team member efforts is a weakness.
- Nothing really problematic was identified in this project.

Specific recommendations and additions or deletions to the work scope

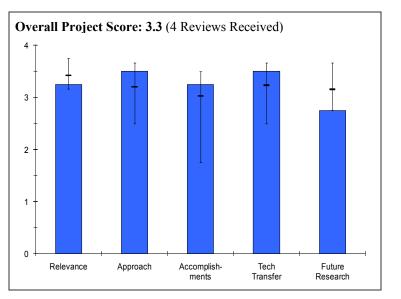
- Regardless of proprietary considerations, some indication of the cost of the baseline MEA should be provided.
- Consider a change of scope or extending the remainder of this project.
- Make an addition to the project to develop/evaluate, integrate, and demonstrate process control strategies.

Project # MF-05: Adaptive Process Controls and Ultrasonics for High Temperature PEM MEA Manufacture *Raymond Puffer; Rensselaer Polytechnic Institute*

Brief Summary of Project

The overall objectives of this project are to 1) achieve greater uniformity and performance of high-temperature membrane electrode assemblies (MEA) by the application of adaptive real-time process controls (APC) combined with effective in situ property sensing to the MEA pressing process and 2) greatly reduce MEA pressing cycle time through the development of novel, robust ultrasonic bonding processes for high-temperature (160-180°C) proton exchange membrane (PEM) MEAs.

<u>**Ouestion 1: Relevance to overall DOE**</u> <u>objectives</u>



This project earned a score of **3.3** for its relevance to DOE objectives.

- The project is relevant to the DOE Fuel Cells Subprogram.
- High temperature PEM MEAs will likely play a major role in fuel cell system commercialization, and adapting manufacturing and quality assurance methods relevant to PA-PBI (phosphoric-acid-doped polybenzimidazole) membranes and MEAs will provide an important contribution to DOE's and industry's commercialization goals.
- Adaptive process control has the potential to markedly increase MEA manufacturing quality and therefore reduce costs.
- The project would have more relevance if it was not limited to high-temperature MEAs, and there is some uncertainty regarding the ability to scale up the ultrasonic process to larger cells.

Question 2: Approach to performing the research and development

This project was rated **3.5** on its approach.

- The project hopes to improve the uniformity and performance of UltraCell's high-temperature MEAs through adaptive process control over the hot pressing cycle. A second objective is to reduce the cycle time for the pressing operation through the use of ultrasonic welding techniques. UltraCell has had difficulty in achieving consistent performance from its fuel cells as seen in Project MF-03. It is not clear that this effort will improve the consistency of the fuel cells. A better understanding of the cause of the performance variability is needed.
- Adaptive process control and design-of-experiments strategies are well thought out.
- Model validation using miniature thermocouples in ultrasonic (U/S) and thermal pressing may be a challenge.
- U/S welding and sealing of MEAs would be a major improvement for production of PBI MEAs. This looks very promising.
- Design of experiments is an excellent approach for determining the influence of various fabrication parameters.
- Potential cost savings analyses should be performed earlier in the overall project.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated 3.3 based on accomplishments.

MANUFACTURING R&D

- The project is new and demonstrated the feasibility of ultrasonic welding with a cycle time of less than one second as compared to about one minute for thermal bonding. Details on the modeling task are lacking in the presentation.
- U/S welding and sealing of MEAs prior to the use of APC looks promising.
- It will be important to identify the reasons for the slight departure of the ohmic region of the polarization curve. It looks like either a resistive change from interfacial or bulk resistivity, mass transfer reduction from diffusion layer compression, or both. Good that there will be extensive experimentation for optimization of U/S processing and identification of process control parameters.
- This early-stage project is showing promising early results.
- No indication yet of potential cost savings from ultrasonic fabrication process. Also, performance and durability of MEAs made with an ultrasonic process needs to be confirmed.
- Not clear if adaptive process control can be successfully implemented in fabrication process if cycle time drops to less than one second.

<u>Ouestion 4: Technology transfer/collaborations with industry, universities and other laboratories</u></u>

This project was rated **3.5** for technology transfer and collaboration.

- Solid list of industry and academic partners are on this team.
- The partners appear to have effective collaboration. BASF Fuel Cells is an important team member because they supply the high-temperature MEAs for UltraCell.
- An outstanding, complementary list of collaborators.
- For an early stage project, the level of team collaboration and coordination is adequate.

<u>Ouestion 5: Approach to and relevance of proposed future research</u>

This project was rated 2.8 for proposed future work.

- While this seems like a strong team, the long intervals between future milestones are of concern more than one year between the second and third phase. The time plan does not explain why this interval needs to be greater than a year.
- The project appears to be long when considering the hoped for results.
- The future research looks good. In Phase III, the APC work could require significant iterative development and should be planned for.
- The scope of future work is appropriate, but there is little indication of the timing of and interaction between future work elements. Decision points are not clearly defined.

Strengths and weaknesses

Strengths

- Good team organization. The ultrasonic welding technique could be applied to low-temperature MEAs if it proves successful at reducing cost.
- Very good organization and collaboration.
- Excellent approach to the work plan.
- This early-stage project is showing promising results.

Weaknesses

• The project needs additional effort in assessing potential cost reductions

Specific recommendations and additions or deletions to the work scope

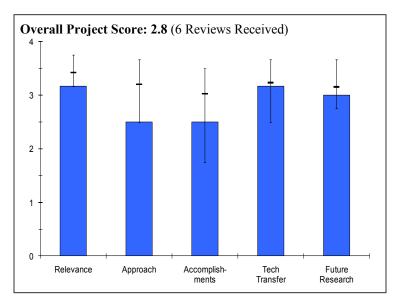
• Concentrate more on UltraCell's lack of consistent performance. Perhaps add scope or reduce project duration.

Project # MF-06: Development of Advanced Manufacturing Technologies for Low Cost Hydrogen Storage Vessels

Carter Liu; Quantum Fuel Systems Technologies Worldwide Inc. Bruce A. Johnson; The Boeing Company

Brief Summary of Project

The overall objective of this project is to manufacture Type IV hydrogen storage pressure vessels, utilizing a new hybrid process with the following features: 1) optimal elements of flexible fiber placement and commercial filament winding and 2) reduced production cycle times by adaptations of high-speed "dry winding" methodology. The aim is to achieve a manufacturing process with lower composite material usage, lower cost, and higher efficiency.



Question 1: Relevance to overall DOE objectives

This project earned a score of **3.2** for its relevance to DOE objectives.

- High-pressure compressed hydrogen is one of the primary methods of transport and storage of hydrogen, and economically acceptable methods of manufacture need to be pursued.
- The project is very relevant to the DOE Fuel Cells Subprogram as it seeks to reduce the cost of high-pressure hydrogen storage tanks, which is the only technology currently available for storing hydrogen on board a vehicle. Reductions in cost and weight are important even if the volumetric storage density will not be improved much.
- Uncertain valuation of combined processes of fiber winding and advanced fiber placement. The significance of weight savings may not warrant the additional process costs.
- Tank improvements employing advanced fiber placement and fiber winding are apparently an incremental improvement from the existing composite tanks used in vehicles.
- The project is relevant to DOE objectives but there is little indication that cost reductions can be realized from the somewhat varied efforts within the project.
- This is borderline "Good/Fair." It looks as much like a product development/research project as it does a manufacturing process project. Fiber placement and dome design, plus evaluation of liner polymers, does not seem as related to manufacturing as to product improvement.
- Cost goals were not clearly defined. There was discussion of reduction of the fiber required, but it was not clear what cost that represents.

Question 2: Approach to performing the research and development

This project was rated **2.5** on its approach.

- A number of significant weaknesses in the program description are evident.
- Little attention is paid to test evaluation of the composite structures fabricated. Specifically, how will they be tested? What instrumentation will be employed? Will the tanks be tested to operating pressure, burst or cycles?
- No evidence of stress analysis was given to assure the new winding patterns will be practical and give sufficient safety factors. The contributing organizations are experts in these areas; however, no evidence of addressing these deficiencies was given in this presentation, and the PI did not adequately address questions posed at the end of the presentation.

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- The approach brings together leaders in the field of fabrication with composite material sets. Fiber placement has been thought to be a viable approach to reducing the amount of expensive carbon fiber in filament-wound storage tanks. Developing a cost model is absolutely necessary to determine whether or not this approach makes sense. The project will also examine a long-shot approach to tank fabrication being developed by LLNL.
- The hybrid fiber winding and advanced fiber placement process effort and tape fabrication processes seem to be significantly different from each other enough, that they may have been better served in separate projects.
- The approach to performing the work is generally rational and appropriate for addressing barriers.
- The liner work could provide assistance in mitigating cylinder thermal limitations due largely to fueling thermodynamics.
- The LLNL work is insufficiently characterized, and it is not clear how it integrates into the overall project.
- It almost seemed like three separate projects under one umbrella. Possibly, it is just because there was limited time for the presentation, but the interdependence between the three partners' work was not clearly demonstrated.
- There was little discussion of testing protocols for assuring that structural integrity is maintained with new fiber wrap placements (except for dome area).

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated 2.5 based on accomplishments.

- The program is in the very early stages, and significant accomplishment would not be anticipated.
- The project was about six months old when the presentation materials were due, so progress has not been great. At the time the presentation was due, the cost model should have been largely developed according to the schedule provided. If this was so, some details of the model and any preliminary results should have been presented – at least a baseline against which to compare reductions achieved through this project. Reaching the go/no-go decision point with adequate data upon which to make the decision is key to the project.
- The assessment of scalability for fiber placement is important for project, but it is not evident how much of an assessment there is to the capability for scaling for dome-end fiber placement.
- Quantum's filament winding accomplishments listed (slides 7, 8) look like their traditional winding process. Was there an additional accomplishment during this reporting period?
- For an early-stage project, some progress is being made.
- The combination of filament winding and fiber placement trades material cost for capital and processing cost, and it is not clear if any cost savings can be realized. Additionally, the filament winding process is characterized as having high repeatability, a high level of automation, low labor cost, high accuracy, and a relatively fast process cycle time. What precisely is going to be improved?
- It is too early to tell. Even with modeling it is hard to see if material and weight savings will exceed equipment investment (the inclusion of the cost model is excellent consideration but needs figures to ascertain the benefit).
- This is early in the project so a lack of demonstrable progress is understandable.

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated **3.2** for technology transfer and collaboration.

- The team assembled has the technological expertise to carry out the program adequately.
- This is a good team. Boeing has tremendous experience in fabricating composite structures for the airline industry. They are attempting to adapt and scale down the processes to tank fabrication requirements. The LLNL work could provide a large payoff if successful.
- The hybridization of Quantum's history in filament winding with Boeing's fiber placement looks like an opportunity to develop a new standard for composite tank design. LLNL's contribution with a high-risk, high-payoff approach of tape fabrication can increase the project's likelihood for success. PNNL's modeling and compatibility studies are helpful.
- Boeing is an experienced and knowledgeable partner that appears to be fully engaged.
- The LLNL work does not seem well coordinated.
- Each of the partners' roles in the project was described adequately. The interdependence of the work (as mentioned above), however, was not entirely clear.

<u>Ouestion 5: Approach to and relevance of proposed future research</u>

This project was rated **3.0** for proposed future work.

- The future plans need to be adjusted, such as to clarify stress analysis, safety margin, and test methodology.
- Most of the work in this project is yet to come. The plans going forward look reasonable and logical.
- It would be very helpful to the DOE program if the "Go/No-Go decision → demonstrate process can reduce material usage and cost" step was moved ahead of the June 2010 Merit review. At least some qualitative assessment of the potential for weight and cost reduction using the hybrid process should be completed by then.
- While the elements of future work are identified and seem appropriate, there is little indication of the interaction between some of the elements, and timing is unclear. Decision points are not clearly defined.
- Most of the project has not yet occurred. Future work/milestones were described sufficiently.

Strengths and weaknesses

Strengths

- Demonstration of advanced composite tank winding manufacturing methods is a strength.
- Good team makeup.
- Teaming is strong. Good and relevant histories for composites and tanks with Quantum, Boeing, and LLNL.
- PNNL hydrogen compatibility study can translate to other polymer/composite hydrogen pipeline development done elsewhere.
- A solid team with good interaction and coordination.
- This project could provide incremental improvements in cost and manufacturing of Type IV pressure vessels.

Weaknesses

- Demonstration of understanding of analysis of stresses, safety factor, and required testing protocols is weak.
- Investigators need to demonstrate that there can be a significant value to the DOE Hydrogen Storage Subprogram that can result from the addition of advanced fiber placement process to the filament winding method.
- It is not clear that costs can be reduced (and therefore barriers be addressed).
- Is this project correctly categorized as manufacturing, or should it be product development research?

Specific recommendations and additions or deletions to the work scope

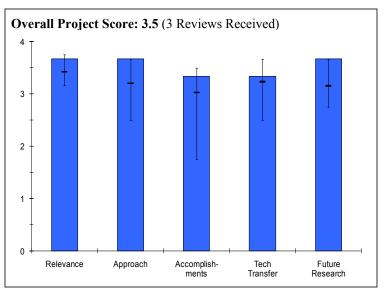
- Detailed stress analysis in dome and transition areas to compliment advanced manufacturing method development should be added to the project.
- Quantum should be required to provide a true baseline cost estimate and accurate projections regarding the advancements possible in this program.
- If there is a significant increase in safety factor at constant weight using the hybrid process, would that have a greater value than a reduction in weight at constant pressure? (Are they helping improve real or perceived safety of 700 bar automotive tanks?)

Project # MF-07: Digital Fabrication of Catalyst Coated Membranes

Peter C. Rieke and Silas A. Towne; Pacific Northwest National Laboratory

Brief Summary of Project

The overall objectives of this project are to 1) demonstrate basic process steps in the digital fabrication of catalyst-coated membranes (CCMs) and membrane electrode assemblies (MEAs), including ink formulation and delivery with industry standard print heads, catalyst layer quality and mechanical durability, and electrochemical utility; 2) define advantages and disadvantages of digital fabrication including the reduction of large run MEA fabrication cost, versatile and agile process line, and the integration of new technology; and 3) identify the unique advantages of digitally fabricated CCMs, including Z gradation in composition.



Question 1: Relevance to overall DOE objectives

This project earned a score of 3.7 for its relevance to DOE objectives.

• The effort is relevant to program goals and has the potential to be a significant process improvement and cost reduction.

Question 2: Approach to performing the research and development

This project was rated **3.7** on its approach.

- The approach to the work is generally appropriate and should address identified barriers.
- An initial assessment of economics is needed.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated 3.3 based on accomplishments.

- Early results are promising, but the need for multiple passes/layers to achieve desired deposition thicknesses could impact potential cost reduction.
- The potential ability to control layer deposition in three dimensions has significant implications for MEA optimization.
- The ability to sustain or improve operational performance and durability of MEAs using new fabrication processes needs to be demonstrated.
- The technical barrier relating to low levels of quality control, specifically "Adaptation of print industry quality control process to MEA fabrication." was not achieved. It was not the fault of the PI, but rather an underfunding of the effort. The intent to address this barrier was on target, and the plan was appropriate.
- The presenter admitted that performance data of printed CCM product versus conventional product was suspect for numerous reasons. Without a reputable validation, the final product cannot necessarily be declared a success. It would not cost much, if anything, to send the CCM product to a well-validated testing lab like General Motors, Hawaii Natural Energy Institute, or LANL.

<u>Ouestion 4: Technology transfer/collaborations with industry, universities and other laboratories</u>

This project was rated **3.3** for technology transfer and collaboration.

- The project team is balanced and seems reasonably well coordinated.
- Given current business conditions, General Motors' commitment to the project could be a risk factor, and the team should investigate potential alternate team members.
- Collaborators chosen were right on target. General Motors could have been more involved especially in performance testing.

Question 5: Approach to and relevance of proposed future research

This project was rated 3.7 for proposed future work.

• The proposed future work is largely appropriate, but more emphasis needs to be placed on potential cost reduction.

Strengths and weaknesses

Strengths

- There are early promising results, and this is a solid team.
- All the right players are involved in this project.
- This is a great plan and results show a potentially great outcome.

Weaknesses

• More emphasis on estimates of potential cost reduction is needed.

Specific recommendations and additions or deletions to the work scope

- The inkjet process could have application to solid oxide fuel cell fabrication as well, and at least a preliminary assessment should be incorporated.
- The results look very promising. Funding should be secured to bring the project to closure.

Project # MFP-01: Inexpensive Pressure Vessel Production through Fast Dry Winding Manufacture

Andrew Weisberg, Salvador Aceves, Blake Myers, and Tim Ross; Lawrence Livermore National Laboratory

Brief Summary of Project

The overall objective of this project is to reduce long-term hydrogen vessel cost to \$4/kWh (\$800 for 6 kg vessel) through innovative winding technology. LLNL has a patent pending tape fabrication technology that retains high fiber strength through continuous fiber path control. LLNL can reduce costs through high-speed dry winding operations.

<u>**Ouestion 1: Relevance to overall DOE**</u> <u>**objectives**</u>

This project earned a score of **3.3** for its relevance to DOE objectives.

- Finding methods to reduce the overall cost of carbon fiber wound vessels will
- Overall Project Score: 2.4 (4 Reviews Received)
- cost of carbon fiber wound vessels will contribute tremendously towards achieving DOE objectives.
- Significant increases in winding speed are projected from the dry wind method, but no evidence supporting the supposition are given to support this claim due to proprietary information.
- This was a very good presentation with good analysis and identification of return on investment (ROI) from an invention.
- Assuming the loosely described effort yields feasible results, the project could provide some cost reduction; though at this time, it is not clear how significant the reduction could be.

Question 2: Approach to performing the research and development

This project was rated **2.5** on its approach.

- The concept of using tape versus a cumbersome curing method is intriguing. This approach could eliminate the costly winding and curing process and improve the overall repeatability and quality of the winding process.
- Due to proprietary information limitations, sufficient information to evaluate the approach to be taken for this program could not be given.
- The project is well done and on track.
- The approach is not clearly defined, possibly due to intellectual property (IP) concerns at the time of review.

Question 3: Technical accomplishments and progress toward project and DOE goals

This project was rated 1.8 based on accomplishments.

- The PI did not answer critical questions such as the following:
 - How does the adhesion process work? Is it complicated? Is it costly?
 - Does this process change the way the vessels will be wrapped in the future? Will it require more or less fiber?
- Since a calorimeter is used to determine the enthalpy change of the bonding process, is there still a curing process similar to that of contact cement? Is he using the same resins? Is he using self-setting resins? What is the cost? What are the material interactions?
- The PI should be able to tell us the high-level process procedure without revealing the recipe specifics.
- This program has just started, and little progress could be made. The preliminary development of a calorimeter to assess dry tape bonding has been made.

- The project team has made good progress.
- Accomplishments are not identified, possibly due to IP concerns at the time of review.

Question 4: Technology transfer/collaborations with industry, universities and other laboratories

This project was rated 2.3 for technology transfer and collaboration.

- Quantum, Boeing, and PNNL are good partners. The first two are big consumers of carbon fiber technologies in varied industries.
- While part of a well-rounded team, there is little demonstrated evidence of collaboration with team partners.
- A good evaluation of the project.
- This effort seems to be operating in isolation at the moment.

Question 5: Approach to and relevance of proposed future research

This project was rated 2.8 for proposed future work.

- This project is non-responsive due not revealing the basic premise of the process.
- Demonstration of IP-protected technology will determine utility of the proposed process. Comparison testing of conventional composite layups with the dry tape method needs to be more clearly detailed.
- The future work is not adequately described, nor is there much confidence that the effort will address identified barriers.
- "Exotic procurement efforts" are identified, but without any contingencies or risk mitigation.

Strengths and weaknesses

Strengths

• The potential high-speed composite lay up method proposed may significantly reduce manufacturing cost.

Weaknesses

- Secrecy of the high-level process makes it difficult to judge strengths or weaknesses.
- Technical description of methods could not be given due to IP limitations.
- An evaluation of the proposed method was not clearly demonstrated.
- Due to IP concerns, insufficient details were available to adequately review this project. In the future, please consider withholding from review projects in similar circumstances.

Specific recommendations and additions or deletions to the work scope

- Even without IP in place, the PI must discuss the high-level process idea of how this tape is to work. He must establish a gap chart and a set of metrics against traditional winding techniques and track his progress against that.
- The PI should clearly define comparison methodology for dry tape vs. conventional methodologies to determine utility of the proposed technology.
- The team should define a pathway for implementation into large-scale articles with team members.

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APPENDIX A: ATTENDEE LIST

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APPENDIX B: SUBPROGRAM COMMENTS PROVIDED BY REVIEWERS

Production and Delivery Subprogram Comments

Hydrogen Production Element

1. Was the Subprogram area adequately covered? Were important issues and challenges identified? Was progress clearly presented in comparison to the previous year? (Include information presented in the Plenary presentation of the Subprogram if appropriate.)

- Yes, the broad goals of the program, as well as quantitative targets, were discussed. Critical issues and challenges were specifically identified for each of the key production approaches being pursued in this program. Progress for each of the production approaches relative to last year was clearly addressed.
- The program was adequately covered. All programs were mentioned, but there was only intermittent mention of primary contributors. Consistency in attribution of programs should be adhered to.
- The progress was adequately covered; however, the challenges—specifically with regard to cost targets and market barriers, equipment reliability, and the tie-in with the infrastructure validation program were not discussed.
- The subprogram was covered well.
- Some progress was highlighted, but it is difficult to tell how close the future technologies are to cost targets.
- Hydrogen production was covered OK. There was too little emphasis on coal, natural gas, and wood; there was too much emphasis on ethanol and other high-cost, low-value offerings (nuclear heat, in particular). It was nice to see some compressor work. It is very important, and there could be more. There was little emphasis on competitive costs, life cycle (durability), and purity needs. These points would have helped us see progress from the standpoint of where we want to go, not only from the point of what was done.
- Would have liked to have a good talk on the zeroing out of the mobile hydrogen program. It's awfully relevant to all those here.
- Good summary presentation. Key issues were identified and progress was delineated. Some targets were more qualitative than quantitative.
- The Hydrogen Production Subprogram was adequately presented considering the limited time available. The scope of the subprogram (i.e., various aspects from budgetary to technical) and relevant information were nicely illustrated and were very informative.
- The subprogram area was adequately covered and progress was clearly presented given the time frame of the presentation. I particularly appreciated the fact that the subprogram's manager referred to DOE's zero request for FY 2010 (which not all managers did in their presentations).
- The subprogram area was thoroughly covered, and all important issues and challenges were identified. Progress against the previous year was discussed.
- The subprogram was adequately covered during the review. Gaps were clearly identified and progress was highlighted.
- The subprogram needs to present a specific/numeric [progress towards multi-year program plan (MYPP) targets] chart showing year-by-year progress.
- The Hydrogen Production kick-off session provided a clear and concise overview of its challenges, direction, and accomplishments.
- Yes to all. The team leader covered highlights of the 2009 program accomplishments and covered 2009 budget in the context of 2008 and 2010 proposals.
- Yes. The rationale of 2010 was explained well.

- Yes, the subprogram area was adequately covered and challenges and barriers of respective areas were identified. The presentation also addressed progress highlights of selective projects compared to the previous year.
- The subprogram was well presented in the overview presentation, giving an update on the status of research in each area of hydrogen production. Progress compared with last year was strong considering the 80% budget cut.
- The subprogram area was broken down into past accomplishes, budget, and successes. The subprogram area was adequately covered with important issues and challenges identified. Progress was clearly presented in comparison to past years.
- Important issue: The FY 2010 budget is set at zero for production and delivery of hydrogen. This is based on a balanced budget and the fact that DOE sees the plug-in hybrids as a near-term solution.
- Challenges: Capital cost for hydrogen production is a critical barrier, and the next cost targets are set at \$2-3/kg.
- A very good overview was given of the Hydrogen Production Subprogram.
- Goals were clear and highlights were clearly presented:
- The presentation was a good overall review of the Hydrogen Production Subprogram.
- The important issues and challenges for the various options for hydrogen production were clearly and concisely presented.
- The presentation included a very good overview of the progress of the subprogram in terms of technical achievements and advancements. However, it was not apparent how these technical achievements were moving these production technologies towards the overall cost goal of \$2-3/kg for delivered hydrogen.
- Several important processes were not discussed; however, presentation time was insufficient to permit comprehensive presentation of all the important work in the subprogram. Progress in thermochemical production did not address well-reviewed cost estimates, some of which seem competitive with other production processes. Comparison of progress with previous year's work was limited to only a few of the many processes. For example, no mention of the Integrated Lab Scale testing of the nuclear-driven sulfur-iodine cycle was mentioned. Furthermore, no mention of cross-agency collaboration between nuclear and solar thermochemical work was evident, missing an important element of this work in contrast to many DOE stove-piped activities.
- The subprogram on hydrogen production was presented and outlined. The presentation focused on past research accomplishments and on the budgetary plans of DOE's Offices of Energy Efficiency & Renewable Energy (EERE), Fossil Energy (FE), and Nuclear Energy (NE) for the near future. The goal of \$2-3/gge was mentioned, but it was not clear from the presentation what production means have the most promise to achieve it. It was mentioned that DOE recommended zero participation from NE and EERE programs for FY 2010, but there was no justification given on why such a decision was reached. In other words, there were no underlying technical reasons listed for the non-participation of these specific components of DOE over the next year. It was mentioned that biofuels were to continue to be explored, but it was not clear why. This reviewer believes that biofuels is an approach that has no traction within the citizenry as a long-term solution. In addition, it is an approach not given very high marks by the National Research Council review of the Hydrogen Program.
- "Yes" to all questions.
- Yes, within the allotted time, the subprogram area was adequately covered. Not enough information was presented with regard to the important issues and challenges that still remain and need resolution. This may be due to the fact that each component of the subprogram area was covered extensively at regular meetings that take place in the course of the year. However, it would be nice to provide a detailed matrix showing progress made in each project, from year to year, and DOE's programmatic targets. It would be nice to have all hydrogen production and

delivery technologies rated using the same yardstick. For example, slides 8 and 9, give a very wide range of hydrogen production costs for photoelectrochemical (PEC)- and polyborazylene (PB)-based technologies?! While at the same time, no estimated cost figures are given for other technologies.

- Given the short amount of time for the presenter, the subprogram was covered succinctly and in sufficient detail.
- This presentation also should have been 30 minutes long. The subprogram could not be adequately covered in 15 minutes. Hence, important issues were only briefly covered, which left more questions than answers. For example, I would have liked to have seen more side-by-side comparisons among the various hydrogen production technologies. Also, no time was left to ask questions.
- The subprogram area was adequately covered. Important issues and challenges were identified, and progress was clearly presented and highlighted.

2. Are plans identified for addressing issues and challenges? Are there gaps in the project portfolio?

- The current portfolio addresses the major issues and challenges.
- No technology gaps were mentioned and no plans defined to meet these challenges.
- The state of the art and the contrast with the actual field data need to be improved.
- In view of program termination or lack of 2010 budget, what are the plans to capture and consolidate the lessons learned, if any?
- The program has both near-term technologies and longer-term technologies covered. Emphasis for longer-term production should be on renewable hydrogen production.
- Electrolysis is focused on low-temperature technologies; however both low-temperature and high-temperature electrolysis technologies should be covered.
- There were some gaps, I thought, in particular when considering the customer for hydrogen. There was no sense that cost or convenience was an issue. Rather, there was an emphasis on meeting various targets despite that some approaches probably would not find real-world customers, even if they worked.
- Plans were identified. No large gaps were identified.
- It appears that several major issues and challenges regarding the Hydrogen Production Subprogram have been identified, and the DOE-funded projects presented here, reflect the diversity of the approaches.
- Technical barriers and plans for addressing the barriers were correctly identified.
- Issues and challenges were fully identified, and there were no gaps in the project portfolio.
- A gap resolution plan was identified through various technology pathways. There are gaps in the project portfolio but it is possible that funding limitations would not allow adequate coverage. Portfolio gaps include more focus on delivery of feedstock to the forecourt and focus on hydrogen quality/purity.
- The largest gap moving forward is our inability to produce near-zero, carbon-emitting hydrogen.
- Are plans identified for addressing issues and challenges? Plans are not mentioned in the subprogram presentation.
- Are there gaps in the project portfolio?
- By-product hydrogen is not mentioned in the subprogram presentation. Is it only covered as a "delivery item"?
- Coal without carbon capture and sequestration (CCS) is not explicitly mentioned in the longerterm goals.

APPENDIX B: SUBPROGRAM COMMENTS

- The presenter did not discuss plans, but >90% of projects did. The plans broadly address issues, but frequently lack focus on the key information needs for the present state of the technology.
- In terms of portfolio, two gaps among the areas I reviewed are as follows:
 - The delivered hydrogen cost target is \$3/kg (which is already high), but many solar nuclear programs are allowed to target much higher cost by using the same value without adding in delivery.
 - Making hydrogen fuel from an already useable liquid fuel (e.g., ethanol) has limited incentive.
- Good summary was provided of various technologies being developed under the DOE umbrella.
- Yes, plans were identified for addressing issues, challenges, and technical barriers, which at present, constitute advances needed for the success of the project. There are no gaps in the project portfolio.
- Given the current budget, there are no plans to address the challenge of hydrogen production in a hydrogen economy. The only gap in the project portfolio is funding to address the gaps already identified.
- The biggest issue is that the funds for delivery are being reduced. However, Congress appears set to re-establish the budget at the requested rate. This year, they plan to down-select a single nuclear technology to scale up. The program designed to produce hydrogen from the hydrogen generation module (HGM) is focused on E-85. However, the availability of E-85 is not sustainable in today's market. E-20 to E-30 maybe more realistic to obtain.
- Very good and clear description of production issues and challenges, both for near-term and long-term technologies.
- With a zero budget, plans are obviously not there.
- The plan is focused solely on distributed production for the transition. There are people in the hydrogen community, including Energy and Industrial Gas companies who believe that semicentral production, or taking some hydrogen off existing and expanding production units at or near a city gate combined with tube trailer (or liquid) hydrogen delivery, presents an "as good" or better approach for the transition to hydrogen fuel cell vehicles. This line of thinking and appropriate associated research should be added to the DOE Hydrogen Production Subprogram.
- There was very little discussion about the future of the Hydrogen Production Subprogram relative to the very small FY 2009 budget and \$0 request for FY 2010. The remaining un-obligated and un-costed funding could have been discussed. It was stated that DOE's Office of Basic Energy Sciences (BES) had \$50M that would be used toward research that could benefit hydrogen production. There were no slides on what research was being done by BES to support this statement.
- Plans were not presented in light of the DOE decision to terminate this activity.
- Yes, the Delivery Subprogram team leader cited the key items for work on delivery. Pipelines, compression, and storage are several of these key areas.
- The program seems to have identified natural gas reformation, renewable liquid reformation, and electrolysis as the most attainable production means for the near future and a number of other means such as biomass gasification, solar, nuclear, etc. as long-term plans. It was identified that the hydrogen-from-coal approach is capable of achieving the 2010 target and that electrolysis is also approaching the relevant target. However, no specifics were given with regard to the specific challenges and directions that need to be followed. The results of the various approaches were not compared, and a message to take home with regard to what can be achieved in the near future was not given.
- Yes.
- This is a difficult question. No doubt, DOE has spent considerable time and effort to identify challenges and issues that need to be addressed in each project activity of the subprogram areas. However, it is not obvious how one compares hydrogen production and delivery costs in one

technology area that is renewable to another that utilizes non-renewable resources (e.g., coal). Likewise, how can you really compare hydrogen production by solar to hydrogen production based on nuclear energy use. The choice of the resource affects the choice of technology for generating hydrogen. One major gap in the project portfolio is complete lack of accounting of greenhouse gas production in each technology area. Another gap is the apparent DOE decoupling of technologies' hydrogen production costs from their efficiency.

- Reformation should still be included in the program for the future (if funded again). While there are a couple of commercial, small-scale reformers on the market, there is still research to be conducted in controls systems, catalyst development, and multiple fuels capabilities.
- Again, due to the time limitation, it was unclear if plans are in place to address issues and challenges. One potential gap is the apparent rush to downselect technologies. It's one thing to cancel funding for technologies that are not meeting milestones, but it is shortsighted to downselect among technologies that are meeting milestones.
- Yes, plans are well identified. There are no gaps in the project portfolio.

3. Does the Subprogram area appear to be focused, well-managed, and effective in addressing the DOE Hydrogen Program R&D needs?

- Yes. There is no clear near- or long-term technical solution to hydrogen production, and this program provides a well-balanced portfolio to aggressively pursue the most promising avenues for each of the production approaches to enable meeting the DOE targets.
- The subprogram spans three DOE offices: EERE, NE and FE. This is a wide-ranging effort, requiring extensive coordination across DOE and its contractors. Good coordination of efforts was presented, and objectives and results were clearly defined.
- The subprogram could improve by changing focus, sharpening the need for the termination phase, capturing the lessons learned, and developing a path forward.
- The subprogram is focused on hydrogen production. It covers a span of technologies for hydrogen production, both in the near term and long term. It is premature to focus the subprogram further, especially as concerned with hydrogen production from renewables.
- Focus on hydrogen is less broad than for most meetings. This was a good-sized meeting with a good variety and appropriate length.
- The subprogram is highly focused, yet it presents several viable options. The current pivot in DOE's Hydrogen Program direction could impact progress and meeting needs.
- The subprogram on Hydrogen Production is well managed with a number of very good projects on relevant key areas and for addressing the R&D needs of hydrogen production. The progress reported for these projects is substantial.
- The subprogram area is well focused and managed, given the constraints of the Hydrogen Program.
- The subprogram area is well focused, well managed, and apparently effective in addressing DOE Hydrogen Program R&D needs.
- It is quite well focused, covering most of the important pathways, and it is indeed well managed. Focused execution of the subprogram plans should lead to good results and address the R&D goals.
- The hydrogen production team has a strong work ethic and management style. The challenges to reduce the cost of sustainable hydrogen production are significant. The production team effectively manages a wide spectrum of production technologies and implementation timeframes.
- Yes, it does.
- The subprogram itself is divided into several sub-subprograms (e.g., biological hydrogen or solar thermochemical). As a whole, these sub-subprograms are fairly well focused on their appropriate critical issues, which may differ from one to the next. Some have defined flow sheets, and are

doing proof-of-concept experiments and economic analysis; some are much longer term and are engaging in knowledge-build activities. By and large, it is a reasonably well-managed portfolio.

- The team leader is doing a good job managing the subprogram. However, in 2009, hydrogen production was zeroed out. Some work continued with carry-over funds, and DOE supported further effort. However, this question is no longer relevant. In 2010, there is no Hydrogen Program. The go-stop pattern associated with government-sponsored research is not productive. The subprogram area is focused and well-managed. Provided all the research subjects were adequately funded, it will overcome the technical barriers and meet the technical targets according to the DOE MYPP and the DOE Hydrogen Program R&D goals.
- The subprogram is extremely well focused and managed. This last year, they did quite a bit with next to nothing.
- It appears that the subprogram is on target to meet its goals and objectives.
- The subprogram appears to be very well focused and well managed, with a strong portfolio of diverse near- and long-term pathways.
- The subprogram has done well with minimal resources.
- The program does appear to be well managed in terms of using the available funding for projects that address the critical issues to reduce the cost of hydrogen production from a wide variety of clean, domestically resourced production pathways.
- It is not clear why so much funding is going into coal gasification in FY 2009 (\$25M) while little went to the EERE Hydrogen Production efforts (\$10M). Coal gasification hydrogen production is fairly well understood. The key to this approach is being able to sequester the carbon. Carbon sequestration is funded independently. There is a great deal of research needed for the production options being researched by EERE, as clearly stated in the presentation.
- The Production and Delivery Subprogram has engaged most of the management and decision tools essential to effective progress to meet established goals. Inherent in the subprogram, however, are necessary R&D investments to permit decisions that would better focus resources to "winning" concepts. Funding has been consistently inadequate to allow program management to move quickly toward decision milestones. This should be seen as critical of DOE and its consistent reluctance to request a budget adequate to the stated task and schedule.
- The subprogram is focused and well managed but underfunded for two years now.
- The subprogram appears to have a balanced portfolio. But since there was no comparison between the various production approaches, I cannot state whether the subprogram is focused as far as technical approaches and corresponding advantages are concerned. It was not clear as to what the objectives of the subprogram are: Is the objective toward massive hydrogen production that meets the needs of the country for vehicular transport in the long term, or does the subprogram aim at exploring distributed hydrogen production capabilities using whatever means are available? The subprogram is lacking such a focus.
- The subprogram area is all-inclusive, but not focused. It can be made more focused by, among others, incorporating the propensity to release GHG and other environmental emissions (air and water) as a factor for consideration in all hydrogen production and delivery technologies funded by DOE.
- The DOE team is doing a great job.
- The portfolio of projects seems good. Again though, I question the management decision to prematurely downselect among good, competing technologies.
- The subprogram area is focused, well managed, and effective in addressing the DOE Hydrogen Program R&D needs in the out years.

4. Other Comments:

- Economical hydrogen production is clearly one the most important areas in the entire Hydrogen Program. The customer will ultimately demand the most economic means of transportable energy, and this will ultimately be hydrogen. Even in the event that all other EERE and NE hydrogen programs are eliminated, this program element (Hydrogen Production) should be continued. No plans were offered to move this effort along, and this will lamely be seen as short sighted.
- The subprogram needs to quickly develop and plan for the next phase and capture its findings and lessons.
- This subprogram does not appear to have funding in the administration request. This subprogram is critical to the long-term success for fuel cell technology. It does not make sense how hydrogen will be available without funding for Hydrogen Production and Delivery. This area needs to be funded.
- I would not mind seeing high-temperature nuclear hydrogen dropped (there are sufficient safety concerns without having to run at 1000°C). Ethanol to hydrogen seems equally mysterious— why? I would have liked to hear a good talk on the zeroing out of the mobile hydrogen program. It's extremely relevant to all those here.
- The Hydrogen Delivery Scenario Analysis Model (HDSAM) work was especially valuable in understanding/anticipating how various hydrogen delivery scenarios impact the cost/capacity/delivery method.
- For peer review and progress evaluations, it would be helpful if reviewers have access to the original proposal.
- The Peer Review Meeting had a number of parallel sessions (oral presentations) on important and closely related subjects. It will be helpful to most attendees and reviewers if oral presentations for closely related subjects can be scheduled so they do not overlap.
- The overview was complete and thorough. The presentation was the right amount of detail and the presentation itself was excellent.
- In light of constrained funding, should the program portfolio be narrowed? (i.e., maybe focus more on near-term technologies to bring them to market and leave out the long-term ones till there is a sustainable budget for those.)
- This presentation was not available before the review.
- My biggest concern is that portfolio is comprised mostly of technologies that have the potential to provide hydrogen at costs that are significantly more costly than petroleum-based fuels or hydrogen. The cost differential infers a cost of carbon, and the inferred carbon cost represented by these technologies is well above anything that rational people are talking about. So I don't see how a consumer or commercial interestor would ever be able to make the decision to choose to use or commercialize any of these technologies. There may not be a solution to this problem that includes hydrogen as an energy distribution means. It may just be too expensive to be worth the trip.
- The team leader is a great manager.
- None.
- Membrane technology efficiency is approaching targets.
- This was a nice presentation giving a good overview of the status of hydrogen production, both technologically and economically.
- It is interesting to note that both Europe and Japan spend more on production and delivery than they spend on storage, whereas this trend is reversed in the United States.
- Need to address questions of how the subprogram might proceed with minimal funding.
- The overall production cost goal of \$2-3/kg for delivered hydrogen was established in 2005. This important goal should be reassessed considering how much the cost of oil has changed/fluctuated

FY 2009 Merit Review and Peer Evaluation Report

since then and relative to how the U.S. now perceives the importance of global warming and potential carbon policy.

- There was no time for questions.
- The notion that production and delivery work is "deferred" while other more near-term technologies are brought to maturation is essentially unrealistic, and it is overly optimistic to think that the work could be picked up in the future and moved forward. The teams of experts who do know what has been done will dissipate and much of what has been accomplished will have to be re-done before further progress can be achieved.
- The program needs to be focused given the recent remarks by the Secretary of Energy that hydrogen does not provide a near-term solution to our energy needs. The program seems to be more balanced than spearheading the most effective solution. In a 2004 report titled "The Hydrogen Economy," the National Research Council (NRC) identified coal and nuclear energy as the most promising means for hydrogen production. I did not see the NRC's view weighing in the subprogram elements and objectives. For instance, biomass-related approaches do not provide the solution to hydrogen production, do not serve the technical demand for massive production, and most importantly, using farmland for fuel production does not resonate well with the public. The subprogram needs to become more relevant toward the strategic needs for getting the hydrogen economy up and running with regard to the most urgent problem, that is, the need for a green transportation vehicle fleet.
- With the impression on the requested DOE FY 2010 budget allocation, it is unclear what the DOE long-term goal/strategy of Hydrogen Production Subprogram is.
- The team leader and associates have done an outstanding job given the budgetary realities their subprogram has had to deal with. I found the folks managing this subprogram area, in general, and the team leader, in particular, very knowledgeable, friendly, extremely approachable, and easy to work with. I give the team leader "4 out of 4" for managing the subprogram.
- None.
- It was really nice that budget information for FY 2010 was provided to the audience during the presentation.

Hydrogen Delivery Element

1. Was the Subprogram area adequately covered? Were important issues and challenges identified? Was progress clearly presented in comparison to the previous year? (Include information presented in the Plenary presentation of the Subprogram if appropriate.)

- Good job summarizing the different areas.
- The subprogram was very thoroughly covered, with the primary objectives reviewed along with the programs being pursued to meet these objectives.
- The dollars/kg (<1.00 gge) number has not been revised, given today's economics. What is the basis of this threshold? Any thought to revising the number annually?
- Yes, the subprogram was covered adequately. It would have been interesting to include a critical analysis of the subprogram progress (or lack thereof).
- The subprogram was well covered, and progress was identified.
- Not bad. I wish costs were covered more explicitly. I wish customer benefits were covered better. Does a cheaper, high-pressure tank help make hydrogen a good transportation fuel, or is the energy density way too low? I would have like to have a good talk on the zeroing out of the mobile hydrogen program. It is awfully relevant to all those here.
- The subprogram was described with good examples of progress. However, the recent change in focus and funding places large burden on program managers to achieve goals.
- Progress was given, but for some programs it is hard to discern any chronological progress.

- Excellent discussion of the Production and Delivery Subprogram. Critical issues associated with delivery were identified—namely, reducing the cost of compression, increasing capacity of trailers for truck delivery, and lowering liquefaction costs. Good examples were presented of progress being made for truck delivery (i.e., increasing capacity to 600 kg). Issues for pipeline delivery were identified: cost of pipelines, application of polymer composites, and development of advanced pipeline compressor technologies.
- The subprogram was covered. Challenges and their relative importance were not clearly identified; the presentation was more of a status report. Year-to-year progress was not clearly identified.
- The Delivery area was properly covered with challenges identified and major highlights presented.
- The subprogram area was adequately covered and all important issues and challenges were identified and discussed. Progress against the previous year was presented and discussed.
- I could not attend the presentation due to a conflict.
- Yes to all.
- Yes, the subprogram areas were adequately covered with important issues, barriers, and challenges clearly identified. The significant progress was clearly presented and highlighted in comparison to previous years.
- Good discussion of tradeoffs and "big picture" issues that need to be considered in the delivery system. Good overview of near-term vs. long-term challenges and priorities. Good description of how the R&D accomplishments address key barriers and what benefits the R&D will provide.
- I would have liked to have heard discussion on how the decrease in budget from FY 2008 to FY 2009 to the FY 2010 request has/will impact program priorities, plans, and ability to meet targets.
- The subprogram was very well described with excellent background of the DOE Hydrogen Delivery Subprogram. The relationship between delivery storage and use of hydrogen (well-to-wheel) cost and trade-offs were described. The progress was presented as well as the successes to date.
- Good overview of the relevant DOE program elements in hydrogen delivery.
- Challenges and approaches were clearly stated. Complexity of tradeoffs was described. Developments in trucking were described.
- This was an overview. The clarity in progress relative to previous work suffered from the scope of activity being covered. At the same time, it seemed that the presenter was not that well-informed on quantitative information regarding benefits and deficiencies of the various delivery options. In fairness, the presentation time available to each presenter was clearly inadequate for overview presentations. The presenter had to make choices regarding what would be emphasized and what would not. That generates team disconnects and political problems that frequently cause more damage than a less informative presentation.
- The team leader gave a masterful summary of the programs under his wing. Very clear and concise articulation of long-term and near-term objectives. Very systematic presentation of progress achieved and where the current emphasis lies.
- Excellent summary presentation!
- The technology issues and challenges were clearly identified, and progress was presented. Due to reduced funding, changes in priority were not clearly identified.
- Yes, the subprogram was well covered in adequate detail.
- Very good overview of the subprogram.
- "Yes" to all questions.
- The subprogram areas were adequately covered. Important issues and challenges were not identified uniformly and certainly not with respect to the previous year. Please consider including

a bird's eye view matrix that summarizes, for each delivery project, progress made since last year to achieve and/or approach DOE hydrogen delivery program targets (that should also appear on the matrix/table).

- All items were covered succinctly in the time allowed.
- This presentation also should have been 30 minutes long. The subprogram could not be adequately covered in 15 minutes. Hence, important issues were only briefly covered and left more questions than answers. Also, there was no time to ask questions. I realize more details are provided in the individual talks, but a longer overview is still needed. I didn't get a good sense of the progress that has been made in delivery from the previous year.
- Yes, the subprogram area was adequately covered. Important issues, barriers, and challenges were clearly identified. Progress since last year was clearly presented.
- The team leader covered the Hydrogen Delivery Subprogram well, citing key accomplishments and challenges.

2. Are plans identified for addressing issues and challenges? Are there gaps in the project portfolio?

- Plans are good given the very low budget available.
- A very concise review of planned efforts was given.
- One possible gap in delivery is the possibility of distributed generation through local electrolysis. This would eliminate the long distance physical transport of hydrogen and replace it with transport of energy through electric potential. (This may have been considered and down-selected unbeknownst to the reviewer.)
- Compression technology should be looked at in detail, including costs and breakthroughs in technologies.
- Yes. The forecourt challenges are numerous. As the intersection of multiple technologies, delivery is a critical part of the supply chain. What is not clear is the plan for transition.
- Other specialized carriers should be considered. These should include the materials developed from the hydrogen storage materials centers of excellence. It also does not consider liquid fuel transport as a hydrogen carrier. It also should include fuels which can be transported through pipelines and fuels which can be efficiently produced and reformed at low temperatures, such as dimethyl ether (DME) and methanol.
- No obvious gaps beyond the elephants in the room, as mentioned above: cost, value to the customer, and the zeroing out of the subprogram.
- The project portfolio covers a good balance between clever near-term solutions for delivery of hydrogen to longer-term, cost-effective approaches.
- Plans and descriptions of projects to address major challenges were presented, as evidenced by near-term projects to design advanced compression technologies and explore polymer composite pipelines. Long-term progress on demonstration of pipeline compressors is critical and will depend on continued support at an enhanced level. A critical issue appears to be the "chicken-or-egg" issue found with hydrogen: industry will not get serious about hydrogen delivery until they see a market, and the market will not be developed until they see an infrastructure to provide hydrogen.
- Could have been made clearer.
- Plans for addressing issues were properly identified.
- Plans for addressing issues and challenges were presented. There appear to be no gaps in the project portfolio.
- Existing challenges are receiving priority while new opportunities are folded into the work.
- Plans were not explicitly shown in the subprogram presentation. There are no gaps in the portfolio.

- Yes, plans are identified to address issues and challenges relevant to each project according to the DOE MYPP. There are no gaps in the project portfolio.
- Funding trends would seem to indicate that truck/carrier and compression are being deemphasized. It was unclear whether the funding decrease was based on funding limitations or whether the challenges have been resolved.
- Portfolio gaps include: onsite "polishing" step for hydrogen quality, hydrogen quality sensors or controls, and geologic storage purity/feasibility.
- The goals and objectives of the delivery team were clearly explained, along with the trade-off issues and how the subprogram fits within the total DOE hydrogen roadmap. There are gaps in funding due to the decreased budget in FY 2010, and beyond that, there is a need to address codes and standards to ensure the safety and integrity of the different approaches.
- Good job in presenting overview of the DOE approach and in developing hydrogen delivery systems.
- Gaps are due to lack of funding, not due to failure to recognize or plan. Due to lack of funding, only a few projects are funded.
- The intimate relationships between transport, delivery, and fueling options were not clear to this reviewer. That could be related to ignorance on the part of this reviewer or to lack of presentation clarity.
- Most issues were well laid out, but some needed more clarification. (E.g., what are the key decisions regarding the active magnetic regenerative liquefier (AMRL) and the Praxair ortho-para approach? Have they convinced DOE that such approaches confer useful advantages? Is the rail option adequately defended?
- Due to the significantly lower amount of funding in FY 2009, not all the technologies or analysis can be accomplished, but these were not addressed in the presentation in an adequate manner.
- Plans are nicely addressed over short- and long-term time frames. The challenges are certainly there and are focused on the many technical imperatives necessary to create a hydrogen infrastructure.
- Yes.
- It was not clear to me where each activity in terms of achieving its goals. I expected a much better presentation of the analysis findings and where each technology stood with respect to the hydrogen delivery costs.
- Consideration should be given to re-inserting onsite reforming for hydrogen (if program funding permits). While there are a couple of commercial, small-scale reformers, developmental work remains for multi-fuel capabilities, new catalysts development, and continued work on controls systems.
- Again, due to the time limitation, it was unclear if plans are in place to address the major issues and challenges. How is this subprogram coordinated with the Hydrogen Production Subprogram? For example, Production and Storage each have their costs and energy loss goals. However, that may eliminate some production technologies that minimize the cost and energy loss of distribution, as well as have improved safety, minimal greenhouse gas emissions, and easier coordination of supply and demand. For example, onsite electrolysis is relatively expensive and energy intensive, but it eliminates these distribution issues. How are these types of cross-cutting issues addressed?
- Yes, plans are identified to address issues and challenges relevant to each project. There are no gaps in the project portfolio.

3. Does the Subprogram area appear to be focused, well-managed, and effective in addressing the DOE Hydrogen Program R&D needs?

• Good projects and valuable activities. This is a well-managed subprogram.

- The subprogram is very well organized. The technology development manager has a good grasp of the required technologies and the direction for technical development.
- Yes, given the comments above.
- Generally, yes, but because of previous budget re-allocation, the progress has been slow to come.
- The subprogram is appropriately focused and managed. It should be prematurely focused.
- Fine, except for the elephants in the room, as mentioned above: cost, value to the customer, and the zeroing out of the subprogram.
- The subprogram appears well focused. The subprogram manager correctly cautioned his contractors that the absence of metrics will be weighted heavily against them in the excruciatingly difficult selection process.
- While I applaud the manager's approach to turn the dramatic decrease in funding into a mechanism for increased focus in the programs, my concern is that the decrease is cutting into the bone and will result in loss of important programs.
- The subprogram appears to be very well managed with a good balance between fundamental R&D and engineering of advanced systems. The severe cutback in funding is limiting progress.
- Yes.
- The subprogram area is well focused, and I could not identify any major gaps in the portfolio.
- The subprogram area is focused, well managed, and effective.
- Yes, the Hydrogen Delivery Subprogram appears focused on the significant challenges that come with transporting this energy carrier. Continued success of this subprogram will bring commercially available hydrogen-fueled cars towards reality.
- Yes, it does.
- The subprogram area is well focused and well managed. Provided adequate funding, progress of the projects will address the DOE Hydrogen Program R&D needs in the out years.
- The subprogram needs consistent funding, at least at the FY 2009 level, in order to continue important R&D progress on cost-effective delivery of hydrogen. Given the erratic and relatively low-level of funding that the program has experienced, the subprogram has been very well managed, focusing on top priorities and making good progress on addressing the challenges.
- The involvement of industry in defining priorities has been good, and collaboration on pipeline R&D through the Pipeline Working Group has been very beneficial and should be continued.
- The subprogram areas appear to be focused and well managed. However, due to the reduced budget in FY2010 and beyond, the timeline to commercial use will need to be adjusted.
- Accomplishments in the DOE subprogram for Hydrogen Delivery were clearly summarized.
- Yes. Good blend of short- and long-term projects. At this stage, many delivery options are still on the table. With limited funding, the subprogram has not been able to adequately fund critical research.
- It was not clear from the presentation that all the issues relating to interfaces between production, storage, delivery, and fueling are engaged in the subprogram. It could be that some of these problems were addressed elsewhere in the program. Nevertheless, it seems important to have all this rolled up into a single program element.
- Definitely well managed, but final resolutions not spelled out as strongly as I had hoped. (E.g., mechanical versus electrochemical compression: which stands out, or will both continue to be further developed as options?)
- The subprogram is well managed and has identified key challenges to the large scale delivery of hydrogen. However, it is not clear what technology has the greatest potential during a transition strategy as the market advances for hydrogen. If the funding is reduced further, based on the analysis model, which technologies must be stretched out to allow the original equipment manufacturers (OEM) to make the commercialization decision?
- Yes.

- Well focused and well managed.
- Yes.
- The subprogram appears to include a large collection of potentially viable hydrogen delivery techniques. However, only one technology was downselected (e.g., N-ethylcarbazole-"like" liquid carrier). I expected more downselects!
- The DOE team does a great job.
- From the limited information given in the introduction, this subprogram seems focused, well managed, and effective. My main concern is how cross-cutting issues among the various subprograms are treated.
- The subprogram area is focused, well managed, and effective in addressing the DOE Hydrogen Program R&D needs.

4. Other Comments:

- Analysis work needs to consider the car side of the work and include the effect of the car on infrastructure performance and cost.
- This subprogram is a necessity in order to bring together the ancillary technologies for hydrogen to become a commercial reality. Funding should be increased to demonstrate the required technologies.
- Listening to the Delivery team progress, it is natural to question if funding was allocated correctly to all aspect of the program. Would it have been more effective to support some of the more achievable technologies in delivery and forecourts at the expense of storage, for example? Delivery could have been a low-risk, high-reward play in the entire portfolio. Some of the technologies being considered here have far-reaching applications beyond hydrogen.
- This subprogram does not appear to have funding in the administration request. This subprogram is critical to the long-term success for fuel cell technology. It does not make sense how hydrogen will be available without funding for hydrogen delivery. This area needs to be funded.
- I would have liked to hear a good talk on the zeroing out of the mobile hydrogen program. It is extremely relevant to all those here.
- Only regrets are the cuts to an important program.
- The subprogram manager should be commended for this program that involves basic/fundamental research coupled with applied/engineering design studies. A delivery test loop facility should be established at a national lab to address pipeline and compressor issues.
- The presentation was clear and conducted in an excellent manner.
- None.
- Excellent program goals and objectives. Well-thought-out modeling and analysis ensure that delivery infrastructure options are in step with the fuel cell development and commercialization.
- A good presentation. Some additional attention to the role of collaborations and to future work would have been helpful.
- It is interesting to note that both Japan and the European Union spend more on production and delivery R&D than storage. The U.S. R&D budget is dominated by storage.
- Need to address questions of how this subprogram might proceed with minimal funding.
- The missing ingredient in all this is a commercial business plan that assures that different roles and responsibilities are adequately identified and accommodated in a dynamic enterprise that would be responsive to unexpected events. The issue is more important because system obstacles could bring down regional transportation that relies on daily, and possible several daily, distribution events.
- Keep up the comparisons, but clearly spell out the priorities if a decision needs to be made today.
- Solid subprogram and well managed.

- Some of the technologies, such as the higher capacity tube trailers, seem to be viable to replace current high strength steels. Is this technology being accelerated for commercial applications? If not, should that not be a higher priority when the funding is cut by more than 50%?
- Why was there such a large decrease in funding from FY 2008 to FY 2009? This, coupled with reputed further decreases for FY 2010, does not bode well for serious infrastructure R&D required if we are really serious about hydrogen.
- With the impression on the requested DOE FY 2010 budget allocation, it is unclear what the DOE long-term goal/strategy of Hydrogen Production and Delivery Subprogram is.
- The DOE Hydrogen Analysis Model (H2A) cost analysis summary for each technology should be included in one summary slide.
- None.
- It appears that the distribution of hydrogen from large-scale production facilities has many insurmountable challenges such as cost, energy loss, hydrogen loss, materials, safety, public acceptance, etc. If this is not true, a better case could have been made in this introduction. It would be desirable to increase the presentation time to 30 minutes, so that more details can be learned.

Hydrogen Storage Subprogram Comments

- 1. Was the Subprogram area adequately covered? Were important issues and challenges identified? Was progress clearly presented in comparison to the previous year? (Include information presented in the Plenary presentation of the Subprogram if appropriate.)
 - Yes the technology gaps were adequately identified; the targets and explanations of new directions were adequately addressed. Progress was demonstrated via the gap chart and new materials discovery.
 - The subprogram area was adequately covered, important issues and challenges were identified and the technical progress and accomplishments over the past year were summarized.
 - Yes, the subprogram area was covered quite well. The challenges were identified and progress highlighted.
 - The subprogram was covered adequately. However, the challenges were not defined adequately. Considering that we are in the fourth or fifth year of this program, a more detailed analysis was warranted.
 - The presentation was, in general, thorough; it would have been interesting to discuss the status of other storage systems target besides gravimetric (i.e., volumetric targets and filling/kinetics comes to mind). Modeling hypotheses as to the determination of systems hydrogen storage density from materials hydrogen storage density should have been stated more clearly in the presentation. (I didn't have time to ask this question during the session.)
 - Yes to all questions.
 - The subprogram area adequately covered most of the important issues and challenges identified. The most important progress compared to last year is the target update and the new Engineering Center of Excellence (CoE), which is the leading effort in DOE Hydrogen Program.
 - Good overview of the subprogram area and its strategy, technical goals, main achievements, and developments during the reporting period.
 - One of the goals and objectives were stated for off-board storage (stationery, portable); however, these targets were not shown, discussed, or established.
 - The team leader was very knowledgeable about the ongoing activities in hydrogen storage. She presented a comprehensive overview of all the areas of storage including the expanded engineering effort. The highlights of accomplishments made in some selected areas were useful.

- Important issues and roadblocks in hydrogen storage were appropriately identified. A nice summary of progress made in the past year was presented. The subprogram area was more than adequately covered. Overall, the presentation gave a clear and concise picture of the status and challenges in hydrogen storage.
- The subprogram area was adequately covered. The important issues and challenges were identified; however, the reasons for revised targets were not clear.
- The goals of the program were succinctly stated relative to the major issues of cost mass volume fill time. Others were included by reference. New targets were explained. Progress was shown by the CoE giving the highlights like mild alane regen, improved spillover kinetics, improved range and durability from the demo, and allied life estimate in many dimensions. It is clear what progress remains to be accomplished.
- "Yes" to all the questions based on the subprogram presentation. I did not hear the Plenary presentation.
- Yes, the presentation gave a very thorough description of the subprogram including goals and objectives, issues, challenges, and progress.
- The subprogram was clearly described both in terms of the revised targets for system storage and the current state of progress for materials discovery. However, current status for materials and systems was not accurately represented in the presentation. In particular, blanket statements such as "currently no technology is able to meet the revised 2015 targets" are not wholly accurate. Achievement of the DOE targets is a complicated matter that deserves a fair quantitative assessment of which milestones or targets have been met to date and which ones are far from being met. There will be compromises to be made for certain targets but, in aggregate, the storage system may exhibit a surprisingly favorable performance. This can be qualified by noting that the recent system-level modeling carried out by Argonne National Laboratory on cryosorption in metal-organic framework (MOF)-177 yields better performance results than originally thought possible based on gravimetric capacities alone.
- Overall challenges were communicated, and the progress was captured. The progress for the "new concepts/other materials" category was not presented and not visible; information on these would be helpful especially given that the 2009 budget appropriation will increase for this category.
- Very good overview of progress in the subprogram area. Excellent description of overall progression of material capacity/temperature is given in slides 12-15. That information provides a useful snapshot of the current status and emerging trends.
- A greater emphasis on critical issues, obstacles, and challenges faced by each of the specific technology areas (i.e., chemical hydride, metal hydride, sorption) would have been helpful. Without that information, it is difficult to put the progress into proper context.
- Although they remain challenging objectives, the revised performance and cost targets are generally much better aligned with expectations and projections based upon current data and future projections.
- Unable to review due to conflict.
- Yes.
- Excellent presentation.
- The subprogram was covered pretty well.
- The year's progress in areas of hydrides, chemical, adsorbents, testing, gas storage, etc. were covered well.
- The subprogram area has been covered in an adequate manner. Progress in respect to previous years has been clearly presented and discussed. Although no major breakthroughs have been achieved (storage is a really challenging problem), all important aspects have been addressed.
- The subprogram presentation covered all relevant topics including challenges, progress, changes, etc., with the exception of the 2010 budget. The breakdown for progress in each area of storage

(i.e., CoEs, analysis, etc.) was informative and 2008 progress was apparent. The rationale for changes to the targets was clear.

- Two graphs on volumetric and weight density progress were good, but the two added points to the gravimetric/volumetric density plot mixed material properties with system properties and real data with estimated values for systems.
- Good review of recent progress by PIs covered all major areas.
- A comprehensive overview was given of the subprogram. The new targets for this subprogram were presented, and the rationale for the new targets was explained (i.e., based on real world experience of current fuel cell vehicles). The challenges were then presented in relationship to meeting the 2015 targets. Highlights of progress from the different centers were given, providing a flavor of the exciting new work coming out of the subprogram.

2. Are plans identified for addressing issues and challenges? Are there gaps in the project portfolio?

- The Engineering CoE will play a key role in providing feedback to the material research PIs regarding what other material characteristics will be critical for an effective system design. To many of the PIs who previously concentrated on only two high-level targets (i.e., weight, volume), this center should provide valuable feedback regarding the importance of other characteristics such as heat capacity, thermal diffusivity/conductivity, packing geometries, agglomeration effects, etc.
- The presentation identified the issues and challenges and discussed the revised performance and cost targets. Not enough information was presented to pick out gaps in the project portfolio.
- Plans are identified. Storage systems and performance targets for real market applications are being developed, which shows confidence in meeting DOE goals in the near future.
- Partially. It is important to have a "look back" and gap analysis in the near future.
- The overdue Engineering CoE would have addressed most of the outstanding issues in the field. The Storage Subprogram should have addressed the nearer-term application for hydrogen energy technologies, and set application-specific storage targets (e.g., public transportation in buses, materials for hydrogen storage in portable applications, etc.).
- Yes, plans were adequately identified. There are no apparent gaps.
- The plans sufficiently address the issues and challenges.
- Critical areas and challenges were adequately discussed along with the revised performance and cost targets. There are no apparent gaps in the project portfolio. What was missing was a reference to the future work plans (possibly as a result of the current discussions and uncertainty on future funding). This issue was only addressed when asked by the reviewers during the presentation.
- Everyone knows that funding for the Hydrogen Storage Subprogram has been zeroed out in next year's budget proposal, yet DOE does not seem to have any plan to address this challenge. The only plan mentioned was to "bring the Hydrogen Storage Subprogram to an orderly close." I sincerely hope that we can do better than this!
- Storage needs and performance targets need to be defined based on progress in the project portfolio.
- The plans identified issues and challenges. Close collaboration with basic science seems lacking.
- The gaps were made clear in the presentation. In Q&A, the plan was to bring the Center to an orderly close in compliance with the budget request. A database to make all learnings accessible will be developed. If funded by Congress, they will manage that to the degree possible with the funds allowed.
- Plans for addressing issues and challenges were adequately addressed.
- I am sure there are a few gaps, but no major ones come to mind right now.

- Yes, the subprogram is very comprehensive and covers the area of hydrogen storage for vehicular applications very well.
- Few or no details were given on addressing current and future issues or challenges. This gap in the presentation is, however, understandable given the uncertainty of future funding of the vehicle hydrogen and fuel cell program.
- The plans to tackle the existing challenges could have been elaborated upon more (i.e., presentation of a timeline). Also, the plan and next steps for the added early market application could have been included.
- The issues and challenges did not receive sufficient emphasis in the presentation. At this stage of the overall program, there are critical barriers that remain (some may be "showstoppers"). Although the presentation described progress in each of the technology areas, very little information was provided concerning the status of the project with respect to the most serious obstacles. Likewise, virtually no information was provided about plans to address those challenges. One or two additional slides (after slide 20) describing problems and mitigation strategies would have been helpful.
- Looks very good.
- DOE has very recently decided to eliminate the need for vehicular hydrogen storage, so this program element may be reconfigured to support the areas of stationary fuel cells and portable power.
- Explanations of new targets were useful.
- The Engineering CoE seems like a good addition at this stage.
- Stationary storage seems like a worthy technical area for this subprogram, but it was hardly addressed at all.
- Hybrid high pressure gas/hydride tanks seem to be an important part of the Japanese on-board storage effort. Is there a role for this approach (including established, lower-capacity hydrides) within the DOE program?
- Nothing was said about the future (if any) of the materials CoE concept.
- The subprogram has reached a level of maturity that contributes substantially towards timely identification of plans to address the main challenges. The portfolio has grown to a level that seems to cover almost all essential issues without leaving major gaps. The only topic I would like to see more extensively covered relates to hybrid (high pressure, solid) storage systems investigation and development.
- The most pressing issue and challenge is the proposed discontinuation of funding in storage, which would make progress impossible.
- From a technical standpoint, given the addition of the Engineering CoE, it is unclear how the other Systems Analysis projects (e.g., ANL or TIAX) will be effectively integrated. The models and information they have provided are invaluable and should be leveraged going forward. The added goal of looking at early market storage applications was presented here, but has not been disseminated to PIs in a timely way for them to be included in their work plans this year.
- There was no clear discussion on why an increase in analysis work is needed.
- There was no discussion of future plans.
- Alternative applications have been identified (which are likely to be earlier-to-market opportunities) and are being incorporated into the subprogram (e.g., stationary, portable electronics, niche vehicle), but targets are needed for these new applications. This new direction should be commended because the vehicle-only applications were overly restrictive for the subprogram.
- Given the uncertainty of funding for the next 12 months, the orderly wrap-up of the subprogram was indicated as a priority. However, if this subprogram ceases to exist, this will be a major hole in the DOE program. It is inconceivable that DOE will not continue to support work into one of the key technological barriers for hydrogen systems. The United States is currently leading the

hydrogen field, but risks playing catch-up with other major economies (e.g., Japan). This will be a detriment to U.S. industry because early-to-market industries will have a crucial competitive edge over the rest. Hence, the continuation of the work in some shape or form must be a priority for DOE.

3. Does the Subprogram area appear to be focused, well-managed, and effective in addressing the DOE Hydrogen Program R&D needs?

- There is a subprogram manager for each of the four areas, which allows good communication between the different areas. It is clear that the cross-fertilization of ideas is occurring between the different CoEs and that redundancies are being eliminated through the effective project management of the team and the CoE leads.
- The subprogram area appears to be focused, well managed, and effective.
- The subprogram is well managed.
- It may be useful to include some additional basic studies to identify a few additional storage systems/approaches. Hydrogen storage in organic materials may be worth a closer look.
- Generally "yes," but there needs to be further improvement. With some work on "look backs," lessons learned, and gap analysis, some of the bottleneck issues can be addressed. This is a reflection of the technical difficulty of the subject matter.
- New storage targets are much more realistic. Dumping the "old vehicle architecture assumption" is refreshing. The subprogram does appear to be well focused.
- Yes.
- The subprogram areas are all well managed.
- The Storage Subprogram is well managed and has a diverse R&D portfolio with clear ties to technical targets.
- Large efforts within relatively small domains of materials for each project resulted in difficulties in downselecting. It became very time consuming to discover new domains of storage materials.
- The subprogram is well focused and the CoEs are functioning well. The performance and cost targets for hydrogen storage are clear.
- The subprogram area appears to be very well focused and well managed to achieve DOE Hydrogen Program needs.
- The subprogram area is important to addressing the DOE Hydrogen Program. It seems focused and well managed.
- The program has an appropriate broad spectrum of projects for a materials discovery mission. Within that broad approach is a disciplined go/no-go structure to ensure focus on programs with potential to improve hydrogen transportation.
- The short answer here is "yes."
- Yes.
- The subprogram is not focused enough toward addressing the DOE Hydrogen Program R&D needs in a reasonable timeframe. DOE program managers have not engaged themselves enough with the Materials Centers of Excellence to impose no-go decisions on material classes that show little or no chance of ever meeting gravimetric or volumetric targets early on. The statistics presented for downselecting various materials at each of the MCoEs represent, in many cases, materials of very similar class or composition, and any permutation or combination of them is not likely to meet the stated targets. Nevertheless, work has been allowed to persist for these classes of materials year after year, sacrificing valuable resources that could have been used on more promising materials.
- The subprogram appears to be well managed and focused.
- The subprogram area is very well managed and has been shown to effectively address the DOE needs for hydrogen storage. The CoE "model" is working well and is providing opportunities for

interaction and collaboration that would be unlikely if projects were funded independently. There appears to be more inter-Center collaboration as well. As some project areas between CoEs begin to merge, this collaboration is healthy and greatly benefits the overall program.

- Yes.
- Yes.
- Yes.
- Yes, generally.
- I think that the management of the subprogram has been one of its main positive assets over the years, and this seems to continue now too. It has been quite effective in addressing the various R&D needs of the DOE Hydrogen Program, and nowadays it appears to be sufficiently focused on the challenges. The launching and first activities of the Engineering CoE and the synergy with Basic Research projects are very positive aspects that I noticed this year.
- The subprogram is extremely well managed. Coordination and monitoring of projects and resources is done effectively to maximize technical progress. Project scopes appear to be efficiently directed to keep priority on high-impact, high-value research. Coordination with CoE managers also appears to be effective for cascading information and suggested directions.
- The subprogram has been well managed in past years and has shown important progress in the area of hydrogen storage.
- This seems to be a very well managed subprogram. The different types of solid state materials are the focus of the individual CoEs, ensuring the program has breadth but retaining a necessary level of focus.
- Very significant advances have been made for the various material systems, bringing materials closer to the system targets of the DOE Hydrogen Program. This work needs to continue.

4. Other Comments:

- The audience would have preferred a slide on the impact of the President's proposed budget on the subprogram. Even a timeline outlining programmatic decisions would have been appreciated.
- The work on advanced hydrogen storage materials and systems should continue.
- A sudden termination of this project may significantly hamper our quest for alternative energy sources and reduce our chance to resolve energy deficit before it turns into a global energy crisis.
- One of the ways to satisfy growing energy requirements is the conversion of solar energy. This energy can be immediately used in the form of electricity to power a broad variety of tools and devices. It can also be stored in a chemical form in hydrogen-rich chemical substances: hydrides. It is worth noting that conversion of solar energy into materials with high hydrogen content, such as oil and natural gas (carbon hydrides), is the way in which fossil fuels formed in nature. Biomass production and its conversion into hydrogen gas/biofuels is another example of when solar energy is stored in the form of carbon-based hydrides.
- In view of the 2010 budget issues and the challenges still facing the storage, it is warranted to engage in a systemic cradle-to-grave evaluation and look backs.
- Some questions to consider: How could we have done this differently? Were the goals even achievable? What are the lessons for the next material-discovery project? How can we recover the most out of this work?
- There are still many questions about the target setting and relevancy of the targets. The revised targets do not reflect the technical and economic challenges and new realties facing the subprogram. It is imperative to revise the entire set of targets and change the basis on what has been learned and established.
- I am surprised that this subprogram is being cut, despite the spectacular progress that has been achieved over the last five years—the steady progress and all the potential applications that will arise from this work in the fields of storage, gas purification, and even battery materials science.

It is the opinion of this reviewer that this decision is unsound. Restarting this subprogram in a few years, when it is realized that this issue is unavoidable even for the new fuel cell focus of the program (i.e., forklift trucks, portable applications), is likely to result in a permanent loss of leadership in the field. This subprogram could have been saved in line with the new shorter-term priorities by adding application-specific storage density targets for shorter-term applications (e.g., forklift and intensive mobile indoor applications, portable applications, public transportation applications), while keeping longer-term targets.

- More information regarding alternate plans and directions to be taken in regard to recent DOE FY 2010 budget announcements would have been helpful.
- The downselection process has obviously greatly benefited the project, focusing the resources on the most promising material systems.
- The CoEs are proving to be an excellent tool for mobilizing resources and expertise.
- Interactions of Materials CoEs among themselves and with the Engineering CoE should be strongly encouraged. Also, all data generated so far should be properly recorded and stored. This is to ensure conservation of the results and full exploration of the materials data gathered over all these years, even if the funding of the program is finally substantially reduced, pending current discussions.
- It is a great disappointment that work in hydrogen storage will be reduced at a time when so much progress has been made over the past several years.
- There seems a potential for MOF material in the area hydrogen storage, but not much was discussed. Overall, the presentation was good.
- Other aspects were also covered, such as the H Prize. Also, the presentation covered the desire for feedback and noted the process for reviews again.
- Re-evaluating and re-adjusting of the hydrogen storage system targets (for whatever rational reason DOE chooses to offer) was essential to both the real and perceived success of the subprogram. The prior target values were unrealistic from day one and unnecessary. Solving our energy problems cannot be done by technology alone. There needs to be major transformations in cultural habits and in the way people think.
- I believe that the area of metal-particle-decorated materials, as predicted by simulations and other • theoretical calculations, should not be funded anymore. I believe that this work originated largely as an attempt to somehow legitimize the very early and completely erroneous work on hydrogen uptake by carbon nanotubes and fibers [that turned out to be only metal impurity particles that do the absorbing of hydrogen (or just plain wrong)]. The idea that somehow those metal particles or atoms can decorate carbon structures, remain stable, and absorb lots of hydrogen has not ever really been convincingly demonstrated experimentally, and consequently, seems to be wishful thinking and not based in reality. It seems that the "spillover" effect is another manifestation of this mind-set. It is long past time to move on to materials that have a real chance of being real and practical hydrogen storage materials. I also believe that part of the difficulty of moving on to real, valid experimental results is the fact that hydrogen sorption measurements are very complex and quite difficult to do correctly. We have seen many, many times over the past 15 years, results that are first sensational, then unbelievable, and finally dismissed as spurious or due to an experimental issue. We need more focus on good-quality, robust, accurate, and believable experiments. That is where more funding should go.
- There appears to be good two-way communication between DOE program management and CoE managers and project PIs. This is essential for facilitating progress, focusing technical efforts, and resolving conflicts in a program of this scope and depth.
- None.
- It will be interesting to see how the Hydrogen Storage Subprogram element reconfigures itself in light of recent DOE decisions. Hopefully, some aspects of hydrogen storage will remain. Attention should be given to characterizing hydride storage materials if their thermodynamics are

such that the operating temperature is near room temperature. If high temperature is required kinetically for thermal activation, then rehydrogenation will be kinetically inhibited. PIs should keep in mind the question of what synthesis and/or characterization methods would be required to detect a good, reversible hydrogen storage material that operates near room temperature. How can the kinetics be made adequate to allow rehydrogenation at laboratory pressures?

- Comments on longer term funding would have been helpful. Although mentioned only briefly in response to a question, the zeroing of the FY 2010 storage budget seems to be highly problematic. Implications of this event should have been discussed.
- In my opinion, this is a successful subprogram that deserves to be supported to fulfill its aims over the coming years.
- Given the progress made by the CoEs, it would be a calamity for all the work to stop over the next few months. Some contingency plans need to be developed to ensure this essential work continues in some form.

Fuel Cells Subprogram Comments

- 1. Was the Subprogram area adequately covered? Were important issues and challenges identified? Was progress clearly presented in comparison to the previous year? (Include information presented in the Plenary presentation of the Subprogram if appropriate.)
 - The subprogram overview was sufficient. The major players in this program have stayed the same for quite some time now, so in-depth review beforehand is not necessary. The most important/relevant aspects of this presentation, budget/appropriation by year and the 2010 proposed budget, was not discussed at all, which was very disappointing.
 - In both the Fuel Cells Subprogram overview and the Plenary presentation, the Fuel Cells Subprogram was clearly covered in a direct and concise manner. The progress based on a comparison with the previous year was clearly described and the challenges identified.
 - The presenter focused heavily on the fuel cell stack components such as catalysts and membrane work. This is where the focus of the subprogram really should be. In that sense, the concentration on those elements is appreciated. However, since this is supposed to be an overview of all the activities, other elements perhaps should have been presented, such as the balance of plant components (almost as large a percentage of cost as catalysts) or stationary work on solid oxide fuel cells (SOFC). Understandably with time constraints on the presentation, these portions may have had to have been put aside.
 - Yes. The presentation adequately covered the goals for the stationary power and other early markets. The presentation also discussed the goals and challenges and for the transportation applications.
 - "Yes" to all questions.
 - The subprogram was well covered; the challenges and progress were identified.
 - The subprogram seems to be making excellent progress on the cost targets.
 - As of Wednesday at noon, my sense is that the research that is done is adequately covered, but there are at least two glaring holes: (1) The customer—no talk has addressed what he/she would get, who the target customer for each project is, or what it would cost him/her to use the hydrogen/fuel cell technology relative to other options like making the car lighter or going to high-efficiency diesel. (2) With funding zeroed out for mobile fuel cell/hydrogen, one would expect someone from DOE to explain to us what they would like us to do now.
 - Good overview of the subprogram. Main issues of technical targets were identified. Progress was both in the form of cost projections and highlights from specific programs. If there was a highlight in water management, that would have been nice to include. Progress was represented

as a function of being relative to the target from DOE. A similar comparison of the contractor's progress relative to last year would have been informative too.

- The subprogram area was well covered.
- In several cases, progress was not clearly presented compared to the previous year.
- An adequate subprogram overview was presented. Goals were discussed including 2011 distributed generation—fuel cells operating on natural gas or liquefied petroleum gas (LPG), with 40% electrical efficiency, 40,000–hour durability, and a cost of \$750/kW. Other goals for consumer electronics, auxiliary power, and transportation were identified. Transportation was deemphasized this year. Early market entry is a major goal and challenge; also, job creation, increased public awareness, and establishment of a domestic supplier base are goals. Challenges in durability, reliability, and the cost of materials and subsystems were identified. Major accomplishments were presented, including \$73/kW modeled cost for transportation fuel cell systems projected to 500,000 units/year, high-conductivity membrane milestone met, and catalyst loading decrease exceeding the milestone.
- Subprogram areas were adequately discussed as goals have changed little from previous years.
- Discussion on the reduction of the Hydrogen Fuel Cell budget for 2010 was notably absent. How can the program representatives just ignore this "900-pound gorilla" in the room?
- It was inconsiderate that the subprogram representatives took no questions.
- The presenter covered the subprogram area completely and thoroughly identified important issues.
- Clear progress was made towards the DOE targets. Progress on catalyst, membrane, and cost targets were shown. Membrane electrode assembly (MEA) durability progress and improvements in fundamental understanding of electrocatalysts are impressive. Targets are being met on time.
- Yes, the subprogram was adequately covered and important issues were identified; good progress was demonstrated.
- The Fuel Cell Technologies segment of the program was adequately covered with the reiteration of overall goals and timelines. Increased attention to stationary and portable applications was also highlighted.
- Important issues and challenges were identified at the component level (i.e., catalysts, membranes, MEAs), and new progress from FY 2009 was clearly stated (i.e., Brookhaven, Giner, 3M).
- The stationary combined heat and power (CHP) approach needs to provide more details, with more systems consideration. To achieve 40% electrical efficiency with the target cost the system will require better integration of the stack and fuel processor. With DOE's current emphasis on high temperature proton-exchange membranes (HT PEM), achieving this target will be difficult. The stack needs to operate at around 160-200°C for CO sensitivity and ability to use stack waste heat for integration with the fuel processor.
- The subprogram area was adequately covered with good rationales for why particular areas are targeted. Progress was presented, but it was not clear where the stationary applications are and what the progress is here. Fuel processing for stationary is a "mystery."
- The overview of the Fuel Cell Technologies Subprogram provided a good summary of the subprogram's most remarkable achievements.
- Yes, the subprogram was adequately covered.
- Progress on fuel cell cost reduction was well documented.
- The subprogram area was covered in full. Issues and challenges were clearly identified. Progress was adequately identified.
- Excellent summary.
- The team leader adequately covered the subprogram and summarized the important issues and challenges. Progress on proton conducting membranes was not adequately presented. Half of the membrane projects met the DOE go/no-go conductivity target. This should have been emphasized

in the presentation, especially because the target was very challenging. Also, about half of the membrane projects were terminated because they did not meet the go/no-go target. This too should have been mentioned in the talk because it clearly indicates DOE's seriousness when it comes to material performance.

- Cost estimates and breakdown of projected costs by component were useful in providing guidance on research needs. A number of specific challenges were identified with specific approaches that addressed them. In the past, I have seen breakdowns of subprogram funding based on fiscal year (including estimates of out year) that allowed one to see the changing priorities of the subprogram and better understand how research priority changes were being addressed.
- Coverage was adequate; clear focus on remaining technical barriers was maintained, and progress from last year was demonstrated.
- Yes, it was fully covered.
- Yes. The presenter had the difficult task in explaining the future redirection of the subprogram, but did it well. Importantly, the presentation focused on the fact that this meeting was not a conference, but a review of work performed in the last year and project plans for the remainder of the awarded effort.
- The presentation was well done. Accomplishments were featured. Challenges were mentioned.
- I would like to see a breakdown of areas where cost reductions have been achieved, and where they are expected, i.e., percent improvement in membrane, air management, etc. with respect to time. This would show trends in specific areas. It would also be relevant to show what are seen as the largest impediments to meeting goals, in addition to showing the accomplishments. Perhaps a slide showing the relationship between individual tasks and specific, or most important, goals or objectives would illustrate how the balance between activities and relative importance is planned.
- Understandably, the plans for transportation were limited.
- The subprogram area was adequately covered, and important issues were indentified. However, for several of the presentations I attended, progress relative to one year ago was not clearly presented.
- The subprogram was presented with an emphasis on membranes and catalysts, which is somewhat appropriate. It is unfortunate that wide ranges of projects (i.e., plates, water transport, impurities, analytical techniques) were not covered. It should be emphasized that the government's ability to provide fundamental knowledge is also part of helping non-public entities further develop the technology.
- Some of the progress shown for catalysts and membranes was a bit "overhyped" compared to what the results truly are.
- The subprogram was redirected with increased emphasis on stationary fuel cell systems, consumer products, and auxiliary power units (APU). These are important and new challenges. The transportation cost challenge was identified at \$45/kW, which is a difficult target. It was not clear what approach would be used to achieve the \$45/kW target. Is lower platinum content the key, or a reduction in balance of plant? For balance-of-plant (BOP), the compressor/expander module (CEM) still appears to be a major cost challenge when thermal management, fuel management, water management, and air management are included.
- The review appeared complete. Progress was clearly met with many projects.

2. Are plans identified for addressing issues and challenges? Are there gaps in the project portfolio?

• The key challenges are reducing cost and improving durability primarily of fuel cell MEA components. The team is heavily centered on these topics. Balance-of-plant (BOP) components are somewhat weak, however. Much of the cost reduction with balance-of-plant can be attributed

to engineering from industry (i.e., not suitable for high-risk DOE funding). Currently, most of the components of BOP are made from expensive stainless steels and pressure fittings. These materials are not suitable for high volume manufacturing. Work is needed to develop cheaper tubing and fittings. Work should be dropped on enthalpy wheels. (They just don't provide enough benefit for the cost.)

- Cost and durability are key for fuel cell commercialization. DTI cost analysis shows steady progress to achieving the cost targets; however, a road map should be discussed showing how that will be achieved to guide research.
- Initial investment on manufacturing equipment needs to be discussed because no company will make heavy capital investment in this field without a future, particularly based on recent comments made by the Secretary of Energy.
- The plans for addressing the existing challenges were presented. It appears that the portfolio is well structured, without gaps.
- The major milestones and future solicitation were identified. Not enough information was presented to judge the future plans or identify gaps in the project portfolio.
- Yes, plans were identified, and there are no gaps.
- Gaps appear to be present if the DOE program shifts emphasis to near-term applications.
- The missing areas were like an "elephant in the room." We would have asked about them, but the microphones were removed at the relevant sections, and there was no Q&A there either. The collapse of the auto industry also hangs in the air over this. Will anyone build the fuel cell vehicles we are working on? Does anyone want to? Will anyone buy one?
- Plans were presented in a general, high-level roadmap for next several years. Specifics on targets underneath those goals were not noted (i.e., "bipolar plates" is listed, but no cost or technical targets mentioned on slide 7).
- There are significant gaps in DOE's fuel cell portfolio, particularly in the area of durability, which I hoped would be addressed with last year's solicitation. It is an embarrassment that, over a year after the Funding Opportunity Announcement, the awards have not been announced.
- Several go/no-go decision points are planned designed to move fuel cells into the marketplace. A gap would be inadequate funding for the transportation-specific application, which is a more distant goal. This could cause this objective to move even further out.
- A major gap exists in how the low-cost targets are ultimately to be met. How will projects be taken through the "valley of death," from lab experiment to commercial production?
- The presenter completely addressed all pertinent areas expected in an overview.
- More information could have been presented on plans for the Hydrogen Program for 2010 and beyond. The next four to five years are critical.
- Additional work on evaluating catalyst performance at low relative humidity is needed.
- Yes.
- Plans were identified at a level of detail appropriate for an overview presentation. Since the main challenges for fuel cells are in materials development, the fuel cell team is pursuing the proper areas of R&D.
- The biggest gap in my mind was absence of medium-temperature fuel cells (160-200°C). This is the sweet spot (from a performance, durability, and cost point of view) for stack operation and integration with a fuel processor to achieve high electrical efficiency.
- Fuel processing for stationary is not clearly defined. Plans for addressing membranes, catalysts, and MEAs are identified but need better rationales for priorities.
- Component-level projects (e.g., MEA, bipolar plates) need to share more information about cost and manufacturability.
- No known gaps in the portfolio.

- Actions for addressing issues and challenges were adequately identified. I was not aware of any gaps in the project portfolio.
- Issues and challenges are being addressed, especially with the re-direction of the program activities.
- The presenter could have spent more time on identifying future issues and challenges for hydrogen fuel cells and how EERE plans to address future such issues and challenges.
- I feel quite comfortable with the Fuel Cell Subprogram, although from only the presentation, it would be difficult to make this assessment. This is the difficulty of trying to represent such a broad subprogram in such a limited setting, and I do not believe it could be significantly improved.
- Yes.
- Plans for addressing challenges are clear. The extent to which these will be relevant, given the possibility of significant shift in mission/goals associated with new administration and new budget, is not clear. Stationary CHP is probably not represented to the extent that it should be to adhere to administration priorities.
- The fuel cell development for vehicles is sound as it is. Considering a weakened automotive industry in the United States, national laboratories like ANL might be granted a more important role in systems development. The strong focus on the fuel cell stack rendered good results. Systems development becomes increasingly important as stack research materializes.
- This is hard to answer at this point; a program redirection and refocus is not yet defined. Rationale for change was laid out. Targets and progress toward them were discussed.
- Yes, plans are OK. However, it was mentioned that a new "roadmap" is being addressed.
- It would be beneficial to show a correlation between the operating constraints and the limitations in applicable fuel cell operations. For example, what are the limitations if a fuel cell operates at a constant condition versus at large load cyclic conditions?
- Analyses of the gains in each of the most critical areas would be very useful. For example, while the performance of the catalysts at BNL show an improvement over platinum (Pt) only, what are the limitations and barriers that have been identified (if they have been identified)? Besides the positive, which is important, what new or different challenges have the results or analyses presented? Not every improvement or advancement is final. This could serve as a yardstick over time.
- The portfolio is appropriate for the current goals relating to hydrogen-fueled fuel cells for transportation.
- There are gaps in the project portfolio (i.e., BOP), but it is difficult for the DOE to find the right parties who can conduct a project in that area without the project being about producing a commercial device.
- In terms of research dollars, plans were shown for addressing issues and challenges, but it is hard to say if DOE has a technical strategy on fuel cell development, which is good to a greater extent. At the moment, both metal- and carbon-based plates are funded, both perfluorinated sulfonic acid (PFSA) and hydrocarbon membranes are funded, both nanoparticle and thin film catalyst designs are funded, and so forth. The plan has been to not eliminate anything before it needs to be eliminated.
- The plans for addressing the challenges for the stack appear to focus on high temperature membranes, but the examples given suggest that sulfonic acid membrane will be used. This would indicate high pressure operation that was shown in the ANL presentation to increase the cost of the CEM. It is not clear how this will be achieved. The durability of the membrane systems (Giner and Case Western Reserve University) was not addressed. Have extended stack evaluations been done with the new membranes? If alternative membranes with phosphoric acid are used, they will demand higher platinum contents on the cathode to compensate for anion adsorption; this topic was not discussed.

• The new program portfolio will need much pruning unless funding is restored. Many current projects (e.g., APUs) clearly fit into the technology-neutral program described by the plenary speaker (Acting Program Manager) on May 18, 2009.

3. Does the Subprogram area appear to be focused, well-managed, and effective in addressing the DOE Hydrogen Program R&D needs?

- The team is generally well focused. However, as a FreedomCAR program, the team is conducting research on too many stationary or heavy-duty applications. I understand that this team is likely the only "home" for these applications; however, DOE can extract more value from funding light vehicle duty research. Much of what is learned in this field will likely spill over into all the other markets since vehicle-level fuel cells are the most challenging in terms of cost, power density requirements, cycling, etc. Knowledge learned from stationary applications (e.g., SOFCs) will likely find little use in light duty vehicle applications (i.e. FreedomCAR).
- The subprogram is effectively run. A go/no-go decision was made recently on the membranes under the high-temperature program, but the results have not been made public at this time.
- The managing of this portfolio is exemplary. It is a key component of the Hydrogen Program. The subprogram area is pretty focused, well managed, and effective.
- Yes. This subprogram is well managed and covers the required development areas, with the possible exception of changing priorities.
- The subprogram is in complete disarray after telling the researchers they were being zeroed out for the main application they were building towards. Current researchers are trying to redirect. Fuel cell manufacturers no longer have obvious customers. Several previously defunded researchers presented. They were doing what they think is best, but seem to lack direction.
- Yes, addresses all the critical subcomponents.
- The DOE Hydrogen Program R&D needs are not well defined at this time. It is impossible to answer this question without clear understanding of DOE's priority on automotive fuel cell system development.
- The program addresses current needs and is focused on most recent changes in direction in the program (i.e., early market penetration and transportation de-emphasized). The program manager is new, but has many years experience and program appears to be well managed. New direction in program office will require adjustments. Next year, review will be more telling in regard to effectiveness.
- The presentation appeared completely effective.
- Yes. Much progress is being made due to the focused effort.
- No, the current administration is backing off hydrogen. This is a mistake considering how close DOE is to solving many of the critical issues. The program should refocus on hydrogen fuel cells.
- The subprogram was focused, well managed, and effective for FY 2009. Notable materials breakthroughs occurred under their management.
- It appeared very well managed.
- The program is switching targets, so this area seems a little confused at the moment. This area should work with analysis group to sharply define goals and stick with them.
- The subprogram appears to be well managed.
- When there are parallel efforts across several projects, it would be helpful to have some means of side-by-side comparison and/or exchange of information so that each project's relative success can be evaluated on the same metric.
- The Fuel Cell Subprogram is well focused on addressing the key barriers, particularly the durability and cost issues. The subprogram is very well managed.
- The subprogram appears to be adequately managed and effective in addressing the identified needs of DOE Hydrogen Program R&D.

- Yes. The program is very well focused and managed. It is effectively addressing DOE needs. Clear evidence of this can be found in the membrane projects which met DOE's extraordinarily high proton conductivity target of 0.1 S/cm at 120°C and 50% relative humidity. The DOE managers are to be commended for selecting the correct projects and pushing the researchers to achieve a high conductivity.
- Yes, but again this has more to do with this reviewer's knowledge of the Fuel Cell Subprogram and the impact that it has had rather than from information passed along during the plenary session or subprogram overview talk.
- Yes. A number of the projects I reviewed did not appear to fit into the Fuel Cell Subprogram goals well, or it simply was not explained. Also, a number of projects are quite immature given the dates associated with the Subprogram goals.
- Yes. The DOE subprogram is very well managed, focused, and addresses the R&D needs as defined in the program. A major factor is the technologically very knowledgeable staff DOE assigns to this research area.
- Yes, the subprogram continues its history of defining, supporting, and managing relevant work and making demonstrable progress toward challenging goals.
- This R&D plan has been on the roadmap "road" for some years. There have been a few detours, and missed turns, if the "truth were told." However, there has also been considerable success, and the challenge now is to build on that strong result. The DOE team is working on this, and that task will be far easier because things have gone well up to now.
- The coverage seems to address all areas. However, the benefits of the modeling of catalysts and fluid dynamics in water transport and the correlation between advances made in the experiments and preparations and modeling projections is absent. This is an area that needs to be expanded in order to take advantage of the analyses of problems and how we can justify taking risks in areas that may have larger payoff within the current work.
- I think this area is appropriately focused and managed. Effectiveness is varied; several projects in the membrane area seem to be very poor, and those efforts did not improve over the past year. Despite the focus on conductivity-based milestones, it appears that a lot of effort went into characterizing and making fuel cells with polymers that were not sufficiently conductive to be of further interest. Projects in the catalysis area were more effective, I think, in making advances and avoiding wasted effort.
- The subprogram may not appear focused from the perspective of people who believe the DOE research should be delivering a product, but it is focused from the perspective that DOE research should merely be supporting the development of new materials, the acquisition of fundamental knowledge, and the adaptation of new analytical tools.
- At a minimum, DOE is funding topics that are highly relevant. DOE could better manage the approach of each individual project, but the relevance is extremely high.
- It is up to private consumers of DOE research data to develop fuel cell products, not DOE. DOE should not be held accountable for the development of fuel cell products or for the validation of those products and systems.
- The subprogram needs to have a clearer focus on the cost reductions associated with BOP. The catalyst efforts are making progress, but it is still unclear if high temperatures will result in catalyst recrystallization.
- The subprogram area is well managed and addresses DOE R&D needs.

4. Other Comments:

- It is difficult for the industry to plan future activities based on a very unclear 2010 DOE budget/scenario for hydrogen/fuel cells.
- This subprogram has a chance to catalyze the ultimate success of the DOE Hydrogen Program.

- The audience wanted clarity and elaboration of the impact of President's budget on the fuel cell portfolio. Perhaps, this was not possible because of the timing.
- If DOE intends to concentrate on near-term applications, additional technologies require funding (e.g., reformate anode tolerant catalysts, portable power systems, methanol oxidation catalysts). Operating conditions likely shift for stationary applications, making durability measurements difficult due to the length of time.
- If someone in DOE wants continuation of this work, it would be nice to know who, or what for.
- The rapid shift away from hydrogen for transportation applications was well presented.
- I hope we can have more fuel cell sessions at future meetings. The current situation is a "huge mess."
- None—the overview was everything one could expect.
- As indicated by the mention of multiple focus areas in the slides (i.e., stationary, portable, and transportation), FY 2010 will be challenging for everyone. The fuel cell team should communicate effectively with researchers to clarify the current focus for each project and be realistic in what any single project can do simultaneously towards different applications. Trying to do everything at once will likely create poorly focused and useless results. For example, durability projects will need to select one set of Accelerated Stress Tests tailored to either transportation, stationary, or portable demands.
- Thanks for all the hard work. Congratulations.
- The program is in flux at the moment. The best plan is to identify the need, define technical goals, and set programs to attain the goals regardless of changing priorities.
- Availability of funding appears to be the main barrier to accelerating the R&D efforts. The good momentum in the Fuel Cell Subprogram needs to be sustained to achieve targets.
- Skillfully done!
- The projects that are earmarks should continue to be reviewed. Being reviewed helps the PI focus and improves the likelihood of getting something useful out of the project. And, the reviewers' comments can also help steer the projects to get the most "bang for the buck."
- It will be interesting to see how the Fuel Cell Subprogram reconfigures itself, given the redirection from DOE.
- More funding and extended time of funding should be provided to those DOE-EERE fuel cell projects that have been highly successful in meeting/exceeding the DOE performance targets.
- Presentation did what it needed to do, in that it provided a clear introduction to the session and a general overview of the subprogram. More information on the future plans/budget based on component/approach would have been useful to the extent that it is understood.
- Given the tremendous progress made toward viable, light-duty transportation under this subprogram, and the long-term promise of sustainable transportation for which we have precious few alternatives, I would hope that the transportation focus is not entirely lost as the program is redirected and refocused.
- Of course, it is hard to project what is in store with the new administration.
- The DOE program on fuel cells is a long-term effort that has produced a lot of progress towards creating systems that avoid the use of foreign oil, that do not emit greenhouse gases, and that use energy more efficiently than thermally-limited conversion processes. A lot of great work has been done over the past 20 to 25 years in PEM fuel cells, and future generations will profit from it greatly. Not all the benefits (in fact, hardly any) of this program have yet been realized in commercial products, but given commercial delivery timelines, that is to be expected. The benefits, however, will be realized in the fullness of time.
- Overall, the recognition of the early, pre-automotive applications should be beneficial. The key issue appears to be the increase in temperature and its effect on the BOP.

Systems Analysis Subprogram Comments

- 1. Was the Subprogram area adequately covered? Were important issues and challenges identified? Was progress clearly presented in comparison to the previous year? (Include information presented in the Plenary presentation of the Subprogram if appropriate.)
 - Year-to-year progress and direction, issues, and challenges were all very clearly explained. The subprogram was well covered and issues identified. The presentation was well laid out to convey the needed information.
 - Good discussion of program objectives with highlights of 2013, 2014, and 2015 programmatic goals and objectives. Early emphasis on stationary electrical generation in using the Macro-System Model was followed by environmental studies and resource requirements. The manager provided a breakdown of subprogram tasks on studies and analysis, development of models, support functions, and systems integration. A good balance of support was found within these areas with a major emphasis on evaluating synergies of integrating transportation and stationary fuel cell systems and barriers to implementing these strategies. Primary issues and challenges identified included inconsistency of existing data, market complexities, and assumptions. A good presentation was given on past analysis priorities and transition to current focus on incorporating stationary fuel cell systems with transportation needs and the potential to implement distributed hydrogen generation at stationery fuel cell sites.
 - A clear flowchart was presented showing various domains of work and the interplay between them. Crisp targets and milestones.
 - Various issues related to the transition to a hydrogen economy were identified and approaches were evaluated; useful new insights were gained.
 - The subprogram was very well represented, as were important issues and challenges. Progress was clearly shown in comparison to the previous year.
 - The area was covered, but perhaps needed to be prioritized better. Lots of different factors were discussed for both stationary and vehicle uses, but each application has different technical requirements. This made identification of the important issues and challenges difficult. Simplify the message to get everyone on board. Progress was shown, but it was not clear from where and to where.
 - The Analysis Subprogram covers a very broad range of activities, and these were adequately covered in the review. Significant progress was presented in developing new models and methods and providing a consistent set of analysis tools. Significant new results were adequately presented.
 - Model/tool development needs were addressed, as well as progress in developing tools to analyze various impacts (environmental, economic, cost, etc.).
 - The coverage was excellent. There was a lot of material, but it was covered in a timely and clear manner. The speaker did an excellent job.

2. Are plans identified for addressing issues and challenges? Are there gaps in the project portfolio?

- The Systems Analysis Subprogram seems to assume a pervasive hydrogen infrastructure based on dominance of the hydrogen car. While the subprogram and the associated projects address this scenario very well, they do not seem to consider the case of a more limited deployment of hydrogen cars sharing the road with electric vehicles.
- The project portfolio should include assessments of distribution and use profiles consistent with what this reviewer believes to be the most likely future: a large numbers of electric cars, a grid

that supports them, and hydrogen competing with fossil fuels in certain markets less suited to electric cars.

- Setting cars aside, there is a huge existing market for hydrogen in industrial processes. Central hydrogen generation scenarios should focus on refinery and agricultural uses of hydrogen.
- It is not clear how the overall analysis can be validated and verified to be accurate. This was briefly mentioned (e.g., data inconsistency), but how it was to be overcome was not clearly addressed.
- Good presentation of future plans to address issues associated with co-production of hydrogen at stationary fuel cell sites. New tasks were brought on board to address the impact that a transition to a hydrogen economy would have on job creation. Also, an analysis was conducted to show the impact future government funding would have to accelerate the deployment of fuel cells. A shortfall still appears to exist on bringing the cost of stationary fuel systems down in spite of accelerated government expenditures—\$40-55B in government expenditures to introduce two million FCVs. This is a rather expensive subsidy of FCVs; at \$20,000 per vehicle, this is a large gap. (DOE note: Reviewers assumptions were incorrect. Government expenditures of \$55B were for ~5.5M vehicles by 2023.)
- The project portfolio is quite diverse and covers most of the related aspects of hydrogen infrastructure development and its implications. There are a lot of useful tools for use by industry and academia to assess intended and unintended impacts.
- Plans where identified for future improvements, although some projects seemed to be anticipating little or no funding in FY 2010.
- Plans are given but, again, it is difficult to see where the priorities lie. The Analysis Subprogram should provide the information with which to formulate policy, but this is all over the map. I am not aware of any significant gaps in the portfolio of projects.
- It is not clear that overall energy models such as the National Energy Modeling System (NEMS) and the MARKet ALlocation) Model (MARKAL) adequately include the potential impact of hydrogen technologies. Efforts to (more appropriately) incorporate hydrogen technologies into these models should be considered.
- The plans were well identified with no obvious gaps.

3. Does the Subprogram area appear to be focused, well-managed, and effective in addressing the DOE Hydrogen Program R&D needs?

- It is well focused and managed with respect to the DOE Hydrogen Program R&D needs; I suggest in my answer to Question #2 that the program might consider the possibility of hydrogen not being the dominant transportation fuel.
- Yes. Connecting all the analytical tools will be important to make them all useful.
- The subprogram appears to be well managed although, from a perspective of a novice in hydrogen analysis, it is difficult to understand the relationship between the 17 different models under development.
- The program is instrumental in assessing the overall progress in the DOE Hydrogen Program. It is very well managed with focus on delivery and cross-interaction with various technology areas. The subprogram seems to be well focused.
- No. It seems to be addressing everything and needs to be divided into clearer subsections so that the analysis presents clear options for policy decisions.
- The Analysis Subprogram is very well managed, considering the broad spectrum of tools being developed and analyses being conducted.
- The development of a suite of tools has progressed logically, and current focus on the potential impact of various government policies is appropriate.
- It appears to be focused and effective. There is no basis for a judgment of management.

4. Other Comments:

- There may be duplication of effort between AN-13 and AN-14.
- Keeping the information up-to-date might be a challenge.
- The Systems Analysis Subprogram, in general, plays a critical role of putting hydrogen and fuel cell R&D programs into perspective and shows a path to how it can be deployed successfully in the marketplace. DOE should continue funding this program.
- This is a critical activity for DOE. Whether or not there should be a hydrogen economy is still being debated and is not a settled issue. Many projects would benefit by directly asking the questions, "Is hydrogen the fastest way to bring renewable energy into the market?" and "Is hydrogen the ultimate solution for a renewable energy future?"
- The switch to stationary and early market applications is clearly causing problems. The stationary aspects need to be assessed against competing technologies such as redox flow batteries, which are much more efficient.
- The results of the environmental modeling of a transition to a hydrogen economy suggest that there are no major problems with even the most successful hydrogen penetration scenarios. If so, future work on the fine details may be of lesser importance and could be wrapped up, if necessary, under tight budget constraints.
- It would have seemed appropriate to have at least mentioned the possible effects of the budget request.

Manufacturing R&D Subprogram Comments

- 1. Was the Subprogram area adequately covered? Were important issues and challenges identified? Was progress clearly presented in comparison to the previous year? (Include information presented in the Plenary presentation of the Subprogram if appropriate.)
 - This subprogram area was adequately covered. Important issues and challenges have been identified, and good progress is evident.
 - Yes to all of the above questions.
 - Great to see the challenge of growing a domestic supplier base addressed.
 - The subprogram was adequately covered, and issues and challenges were identified. A more thorough comparison with the previous year could have been presented.
 - Good overview of the subprogram.
 - This presentation failed to highlight two key requirements of managing a manufacturing portfolio:
 - What are the key gaps that must be closed to make fuel cell manufacturing viable? Where are the bottlenecks that drive cost, quality, and/ or flexibility of a process? What benchmarks are you aiming for?
 - What is the long-term viability of a process?
 - Once the gaps have been identified, what processes are specific to a particular material or technology? Can that translate to future or similar processes? Fuel cell technology is fast moving and changing. The subprogram must exercise judgment to identify processes that will carry through all the iterations of a technology.
 - The overview presentation was poorly prepared and delivered. Only a very brief description of the program was given. Little attention was paid to the critical technologies required and challenges needing to be addressed and overcome.

2. Are plans identified for addressing issues and challenges? Are there gaps in the project portfolio?

- Plans for addressing issues and challenges were appropriately covered, and there were no significant gaps in the project portfolio.
- Most focus seems to be on fuel cell components. Some additional focus on manufacturing of infrastructure manufacturing might be helpful including high pressure components for gas compression, dispensing systems, and metering.
- See above (question 1).
- Critical challenges were not clearly elucidated, and no plans for addressing challenges were offered.
- There appears to be no element related to the stack assembly process. Are there other projects looking at robotics, assembly line design, or other critical cost elements for stack (and system) assembly that would lead up to the 2013 goal?

3. Does the Subprogram area appear to be focused, well-managed, and effective in addressing the DOE Hydrogen Program R&D needs?

- The subprogram is well focused, well managed, and effective in supporting the R&D challenges and goals.
- The subprogram has elements that address the stated goals for reducing the barriers to commercialization in cost reduction, quality control, and production improvements.
- The subprogram area appears to be focused, well managed, and effective in addressing the DOE Hydrogen Program R&D needs, with one exception—in general, the assessment of potential cost reductions needs to occur earlier in many of the individual projects.
- The DOE team appears to be doing a great job.
- The subprogram does not appear to be focused. (See reasons above.) They seem to be working on projects that were submitted to them without first having taken a holistic view of the entire value chain.
- This is a relatively small subprogram with a tremendous array of challenges that need to be addressed. Yet, it can only address a small number of the challenges in reducing manufacturing cost and increasing quality. These results, in a segmented program with little focus, are not the fault of subprogram management.

4. Other Comments:

- Development of the technologies required to reduce manufacturing costs will minimally impact the commercial application of these technologies in an environment where competing energy technologies are cost competitive.
- Assessment of manufacturing readiness levels for low rate initial production is an important tool in aiding industry stakeholders in marketing strategies.

APPENDIX C: GENERAL PROJECT EVALUATION FORM

Reviewer:	Panel (circle one): AN / ED / FC	Panel (circle one): AN / ED / FC / MF / PD / SCS / ST	
Presentation ID	Title	Principal Investigator	

<u>**1. Relevance**</u> to overall DOE objectives – the degree to which the project supports the Hydrogen Program and the goals and objectives in the Multi-Year RD&D plan. (Weight = 20%)

- □ 4 Outstanding. Project is critical to Hydrogen Program and fully supports DOE RD&D objectives.
- **3** Good. Most project aspects align with the Hydrogen Program and DOE RD&D objectives.
- **2** Fair. Project partially supports the Hydrogen Program and DOE RD&D objectives.
- □ 1 Poor. Project provides little support to the Hydrogen Program and the DOE RD&D objectives.

Comments:

<u>2. Approach</u> to performing the work – the degree to which technical barriers are addressed, the project is well designed, feasible, and integrated with other efforts. (Weight = 20%)

- □ 4 Outstanding. Sharply focused on technical barriers; difficult to improve approach significantly.
- **3** Good. Generally effective but could be improved; contributes to overcoming some barriers.
- **2** Fair. Has significant weaknesses; may have some impact on overcoming barriers.
- **1 Poor.** Not responsive to project objectives; unlikely to contribute to overcoming the barriers.

Comments:

<u>3. Technical Accomplishments and Progress</u> toward overall project and DOE goals – the degree to which progress has been made, measured against performance indicators and demonstrated progress towards DOE goals. (Weight = 40%)

- **4 Outstanding.** Excellent progress toward objectives; suggests that barrier(s) will be overcome.
- **3** Good. Significant progress toward objectives and overcoming one or more barriers.
- **2** Fair. Modest progress in overcoming barriers; rate of progress has been slow.
- **1 Poor.** Little or no demonstrated progress towards objectives or any barriers.

Comments:

APPENDIX C: EVALUATION FORM

<u>4. Collaboration and Coordination with other institutions</u> – the degree to which the project interacts with other entities and projects. (Weight = 10%)

- □ 4 Outstanding. Close, appropriate collaboration with other institutions; partners are full participants and well coordinated.
- **3** Good. Some collaboration exists; partners are fairly well coordinated.
- **2** Fair. A little collaboration exists; coordination between partners could be improved.
- □ 1 Poor. Most work is done at the sponsoring organization with little outside collaboration; little or no apparent coordination with between partners.

Comments:

<u>5. Proposed Future Work</u> – the degree to which the project has effectively planned its future in a logical manner by incorporating appropriate decision points, considering barriers to the realization of the proposed technology and, when sensible, mitigating risk by providing alternate development pathways. (Weight = 10%)

- **4 Outstanding.** Plans clearly build on past progress and are sharply focused on barriers.
- **3** Good. Plans build on past progress and generally address overcoming barriers.
- **2** Fair. Plans may lead to improvements, but need better focus on overcoming barriers.

1 - **Poor.** Plans have little relevance toward eliminating barriers or advancing the program.

Comments:

Project Strengths:

Project Weaknesses:

Recommendations for Additions/Deletions to Project Scope:

Go to https://peernet.orau.gov to record your comments in PeerNet.

HYDROGEN STORAGE CENTER OF EXCELLENCE EVALUATION FORM

Reviewer:	Pan	el (circle one): ST COE
Presentation ID	Title	Principal Investigator

1. Approach to performing the R&D including Center Management – the degree to which the DOE EERE Multi-year Program Plan (RD&D Plan) technical barriers are addressed; the overall CoE effort is well-designed and technically feasible. The technical approach clearly leverages partners' unique skills to complement activities and avoid duplication. The CoE management approach includes, and has demonstrated, effective down-select/decision points and criteria. CoE progress and technical direction are periodically internally "audited" for effectiveness, efficiency, and benefits. (Weight = 25%)

- □ 4 Outstanding. The Center is well managed. The overall center is sharply focused on one or more key technical barriers to development of on-board hydrogen storage technology (focused on 2010 targets). It would be difficult to improve the approach significantly.
- □ 3 Good. The Center is reasonably well managed. The approach is generally well thought out and effective but could be improved in a few areas. Most aspects of the center projects will contribute to progress in overcoming several of the barriers.
- □ 2 Fair. The Center is somewhat well managed. Some aspects of the center projects may lead to progress in overcoming some barriers, but the approach has significant weaknesses.
- □ 1 Poor. The Center is not well managed. The approach is not responsive to project objectives and unlikely to make significant contributions to overcoming the barriers.

Comments:

<u>2. Technical accomplishments and progress toward DOE goals</u> – the degree to which the CoE research has achieved progress across the center. CoE's actual progress and technical accomplishments are measured against performance indicators and quantitative milestones as related to DOE's RD&D plan.</u> (Weight = 25%)

- □ 4 Outstanding. The overall CoE has made excellent progress toward objectives and overcoming one or more key technical barriers. Progress to date suggests that several of the barriers may be overcome.
- □ 3 Good. The overall CoE has shown significant progress toward its objectives and to overcoming one or more technical barriers.
- □ 2 Fair. The overall CoE has shown modest progress in overcoming any barriers, and the rate of progress has been slow.
- □ 1 Poor. The overall CoE has demonstrated little or no progress towards its objectives or any barriers.

Comments:

<u>**3.** Proposed future research approach and relevance</u> – the degree to which the CoE has effectively planned its future, considered contingencies, built in optional paths or off ramps, etc. (Weight = 20%)

- □ 4 Outstanding. The future work plan clearly builds on past progress addressing identified issues and is sharply focused on one or more key technical barriers in a timely manner. Future work includes well developed optional path(s) and/or off ramps.
- □ 3 Good. Future work plans build on past progress addressing identified issues and generally address removing or diminishing barriers in a reasonable period. Future work considers optional path(s) and/or off ramps.
- 2 Fair. The future work plan may lead to improvements, but should be better focused on removing/diminishing key barriers in a reasonable timeframe. Future work does not consider optional path(s) and/or off ramps.
- □ 1 Poor. Future work plans have little relevance or benefit toward eliminating barriers or advancing the program. Future work does not consider optional path(s) and/or off ramps.

Comments:

<u>4. Coordination, collaborations and effectiveness of communications within the CoE</u> – the degree to which the partners interact, interface, or coordinate with other partners within the CoE. The center director/coordinator provides a mechanism to foster partner interaction, interfaces, or coordination within the CoE. The center coordinator has helped to leverage resources to achieve progress and obtained maximum benefit from the center's overall funding. (Weight = 20%)

- □ 4 Outstanding. Close coordination is evident among the majority of partners with continuing cross center communications and collaborations.
- □ 3 Good. Some coordination exists; full and needed coordination could be accomplished fairly easily.
- 2 Fair. A little coordination exists; full and needed coordination would take significant time and effort to initiate. Some partners appear to be insufficiently aware of other work occurring in the CoE.
- □ 1 Poor. Communications among and between partners appears to be insufficient. It appears as if unnecessary duplication of work may be occurring.

Comments:

<u>5. Collaborations the CoE</u> – the degree to which the CoE interacts, interfaces, or coordinates with the other DOE CoEs and with other institutions and projects and the degree to which technology developed within the CoE is communicated and disseminated to outside the CoE. (Weight = 10%)

□ 4 - Outstanding. Collaboration with other DOE CoEs and other institutions is in place and appropriate; Good coordination is allowing the CoE to clearly leverage other work occurring in the subject area; very effective dissemination of the CoE's activities through publications, presentations, patents, collaborations and etc.

- 3 Good. Outside collaboration exists but could be expanded; coordination is allowing the CoE to partially leverage other work occurring in the subject area; Good dissemination of the CoE's activities through publications, presentations, patents, collaborations and etc.
- 2 Fair. A little collaboration exists; coordination could be improved to allow the CoE to leverage other work occurring in the subject area; the CoE does not appear to be fully aware of other major R&D efforts occurring in a particular subject area; the CoE's activities are not widely disseminated to outside entities.
- □ 1 Poor. Most of the work done within the CoE; There appears to be little outside collaboration; There is little or no apparent coordination to leverage other work occurring in the subject area; there is little apparent dissemination of the CoE's activities to the outside world.

Comments:

Overall Center Strengths:

Overall Center Weaknesses:

Recommendations for Additions/Deletions to Project Scope:

Go to https://peernet.orau.gov to record your comments in PeerNet.

SUBPROGRAM EVALUATION FORM

Reviewer:

Subprogram (circle one): AN / ED / FC / MF / PD / SCS / ST

Using the following criteria, rate the work presented in the context of the Program objectives and provide specific, concise comments to support your evaluation.

*** Write/print clearly please. ***

1. Was the Sub-program area adequately covered? Were important issues and challenges identified? Was progress clearly presented in comparison to the previous year? (Include information presented in the Plenary presentation of the Sub-program if appropriate.)

2. Are plans identified for addressing issues and challenges? Are there gaps in the project portfolio?

3. Does the Sub-program area appear to be focused, well managed, and effective in addressing the DOE Hydrogen Program R&D needs?

4. Other Comments:

Go to https://peernet.orau.gov to record your comments in PeerNet.

Project ID	Project Title	PI Name	Organization
PD-01	Low-Cost Hydrogen Distributed Production System Development	Frank Lomax	H ₂ Gen Innovations, Inc.
PD-27	Indirectly Heated Biomass Gasification	Richard Bain	NREL
PD-33	Geologic Storage of Hydrogen	Anna Snider Lord	SNL
PDP-08	Photoelectrochemical Hydrogen Production	Malay Mazumder	University of Arkansas, Little Rock
PDP-09	Photoelectrochemical Generation of Hydrogen from Water Using Visible Light Sensitive Semiconductor Nanotube Arrays	Mano Misra	University of Nevada, Reno
PDP-11	Design of Advanced Manufacturing Technologies for Low Cost Hydrogen Storage Vessels	Ken Johnson	PNNL
PDP-23	Innovative Hydrogen Liquefaction Cycle	Martin Shimko	Gas Equipment Engineering Corporation
ANP-02	DOE Hydrogen Program Risk Analysis in Support of EERE's Portfolio Analysis	Mike Duffy	NREL
ANP-04	A Business Case for Stationary Fuel Cells and Hydrogen Co-Production	Daryl Brown	PNNL
ANP-05	Stranded Biogas Decision Tool for Fuel Cell Co-Production	Michael Ulsh	NREL
ST-14	Hydrogen Storage Engineering Center of Excellence	Don Anton	SRNL
ST-31	Multiply Surface-Functionalized Nanoporous Carbon for Vehicular Hydrogen Storage	Peter Pfeifer	University of Missouri, Columbus
STP-05	Hydrogen Storage Materials with Binding Intermediate between Physisorption and Chemisorption	Juergen Ekert	University of California, Santa Barbara
STP-06	SRNL Technical Work Scope for the Hydrogen Storage Engineering Center of Excellence: Design and Testing of Metal Hydride and Adsorbent Systems	Ted Motyka	SRNL
STP-07	Systems Engineering of Chemical Hydride, Pressure Vessel, and Balance of Plant for On-Board Hydrogen Storage	Darrell Herling	PNNL

APPENDIX D: LIST OF PROJECTS NOT REVIEWED

APPENDIX D: PROJECTS NOT REVIEWED

STP-08	Advancement of Systems Designs and Key Engineering Technologies for Materials Based Hydrogen Storage	Dan Mosher	United Technologies
STP-09	Chemical Hydride Rate Modeling, Validation, and System Demonstration	Troy Semelsberger	LANL
STP-10	Key Technologies, Thermal Management, and Prototype Testing for Advanced Solid-State Hydrogen Storage Systems	Joseph Reiter	NASA JPL
STP-11	System Design, Analysis, Modeling, and Media Engineering Properties for Hydrogen Energy Storage	Matthew Thornton	NREL
STP-12	System Design and Media Structuring for On-board Hydrogen Storage Technologies	Darsh Kumar	General Motors
STP-13	Ford/BASF Activities in Support of the Hydrogen Storage Engineering Center of Excellence	Don Siegel	Ford Motor Company
STP-14	Microscale Enhancement of Heat and Mass Transfer for Hydrogen Energy Storage	Kevin Drost	Oregon State University
STP-15	Development of Improved Composite Pressure Vessels for Hydrogen Storage	Norman Newhouse	Lincoln Composites
STP-16	Hydrogen Storage by Novel CBN Heterocycle Materials	Shih-Yuan Liu	University of Oregon
STP-24	NaSi and NaSG Powder Hydrogen Fuel Cells	Michael Lefenfeld	SiGNa
STP-31	A Joint Theory and Experimental Project in the High-Throughput Synthesis and Testing of Porous COF and ZIF Materials for On-Board Vehicular Hydrogen Storage	David Britt	UCLA
STP-32	Capacitive Hydrogen Storage Systems: Molecular Design of Structured Dielectrics	Robert Currier	LANL
STP-33	New Carbon-Based Porous Materials with Increased Heats of Adsorption for Hydrogen Storage	Joseph Hupp	Northwestern University
STP-34	Hydrogen Trapping through Designer Hydrogen Spillover Molecules with Reversible Temperature and Pressure- Induced Switching	Angela Lueking	Penn State University
STP-35	Neutron Characterization in Support of the Hydrogen Sorption Center of Excellence	Dan Neumann	NIST
STP-47	Design of Novel Multi-Component Metal Hydride-Based Mixtures for Hydrogen Storage	Christopher Wolverton	Northwestern University

APPENDIX D: PROJECTS NOT REVIEWED

STP-48	Tunable Thermodynamics and Kinetics for Hydrogen Storage: Nanoparticle Synthesis Using Ordered Polymer Templates	Mark Allendorf	Sandia-Livermore
STP-49	Fundamental Reactivity Testing and Analysis of Hydrogen Storage Materials	Don Anton	SRNL
STP-50	Quantifying & Addressing the DOE Material Reactivity Requirements with Analysis & Testing of Hydrogen Storage Materials & Systems	John Khalil	UTRC
STP-51	The Reactivity Properties of Hydrogen Storage Materials in the Context of Systems	Daniel Dedrick	Sandia-Livermore
STP-52	Carbide-Derived Carbons with Tunable Porosity Optimized for Hydrogen Storage	Yury Gogotsi	University of Pennsylvania/ Drexel University
FCP-01	Fuel Cell Testing at the Argonne Fuel Cell Test Facility	Ira Bloom	ANL
FCP-05	International Stationary Fuel Cell Demonstration	John Vogel	Plug Power

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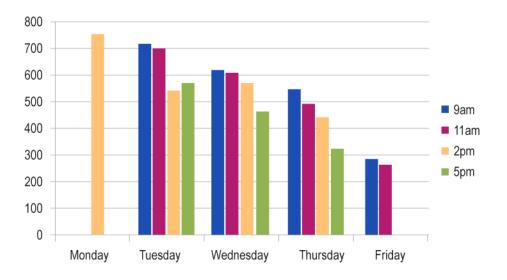
APPENDIX E: 2009 ANNUAL MERIT REVIEW SURVEY QUESTIONNAIRE RESULTS

This report documents two separate activities: 1) feedback from a meeting held May 22, 2009—just after the conclusion of the 2009 DOE Hydrogen and Vehicle Technologies Programs' Annual Merit Review and Peer Evaluation Meeting and 2) results from a survey questionnaire given to all participants. At the feedback meeting, results were presented from the 55 questionnaires completed by the end of the meeting. Following the meeting, the questionnaire was posted online and all 1,568 attendees were solicited via email to complete the questionnaire. As a result, an additional 181 questionnaires were completed, bringing the total to 236 (15% of the total attendees).

Meeting Overview

The 2009 DOE Hydrogen and Vehicle Technologies Programs' Merit Review and Peer Evaluation Meeting was held May 18-22, 2009 in Crystal City, Virginia. A plenary session was held on Monday afternoon. Oral presentations were held in eight parallel sessions all day Tuesday, Wednesday, and Thursday, and a half day on Friday. There were 232 oral Vehicle Technologies presentations and 174 oral Hydrogen Program presentations for a total of 406. Poster sessions were held Monday through Thursday evenings. There were 95 Vehicle Technologies posters and 124 Hydrogen Program posters for a total of 219. In total, 625 presentations were given during the meeting.

A total of 1,568 people attended the meeting. Attendance of the sessions was counted daily and is shown in the following graph.



2009 AMR Session Attendance by Day

Notes from the AMR Feedback Meeting on May 22, 2009

Numerous Vehicle Technologies and Hydrogen Program staff, Alliance Technical Services personnel who managed the review, and Oak Ridge Institute for Science and Education staff who managed the reviewers of the review, attended the feedback meeting. The following are specific comments and recommendations made during this meeting.

- Presentations should include a Gantt chart to plot project progress.
- Session assignments for reviewers were not always clear.
- Need to see clocks from the podium and moderator locations.
- Use pop-up responses for answering simple questions on reviewer form.
- Hard to tell what is new from year to year in the presentations.
- Add more time for sub-program overview presentations.
- Presentation template was a plus.
- 20 minutes were not enough to assess progress.
- Some reviewers didn't know their schedule until Monday, which was problematic.
- Putting the same reviewers on same projects would be preferred.
- Identifying slides as "new" would be good; helps reviewers sort through previous results.
- Templates were sort of boilerplate—suggested pop-up options in questions for reviewer ease.
- Past presentations being available was good.
- Maybe have DVDs optional and distribute separately from registration packet—also consider thumb drives.
- Reviewer feedback sessions must be added to overall schedule as reminder to the TDMs.
- Solicit areas of expertise going forward for future reviewers.
- May need one more large session room next year.
- Consider having the same reviewers each year for continuity and the ability to assess progress.
- Should consider reducing the number of posters to be reviewed.
- Consider doing the meeting questionnaire online only.
- It was suggested that reviewers indicate their area of expertise on the registration form.
- It was proposed that when the Save the Date goes out next year, we should ask if reviewers want to sign up at that time. (Editorial note: This recommendation was implemented as part of the email soliciting completion of the Web-based questionnaire.)

2009 AMR Survey Questionnaire Results

The following pages present the results of the 2009 survey questionnaire with comparison to 2007 and 2008. Note that no editing of the survey response was done. Following are selected comments and recommendations pertinent to the 2010 meeting.

- Networking and information gathering/exchange were frequently mentioned as the most important aspects of this meeting.
- There were several comments that the hotel was too costly.
- Reviewers would like their assignments earlier to head off conflicts.
- Presenters should use larger fonts.

- There should be water in the session rooms.
- The agenda needs to be clearer with times listed when food is served.
- Presentations were too long and many were allowed to exceed their time limit, reducing time for questions.
- A "not applicable" category should be included in the questionnaire.
- There were too many projects for the time available.
- Sub-program overview presentations and materials did not have sufficient depth for review.
- The criteria used for evaluation do not fit all projects. There should be at least one question to the effect of "Do you think this project should continue to be supported?"
- The review is too large—most projects do not need to be reviewed every year.
- It would be good for the DOE program manager to introduce the speaker and explain how the project fits with his/her portfolio.

The following table presents the results of the questionnaire. Note that other than where totals are given, the answers to the questionnaire questions are averages based on the following scale:

Strongly Agree = 5 Agree = 4 Neutral = 3 Disagree = 2 Strongly Disagree = 1

2007	2008	2009	
61	78	236	Total Number of Respondents
			DEMOGRAPHIC QUESTIONS
			1. Attendee Role and Affiliation:
			a. What was your role in the review?
14	19	45	Peer Reviewer
11	23	90	Presenter of a Project – Oral or Poster
1	1	6	Presenter of Program Overview
34	36	90	Attendee, neither Reviewer nor Presenter
			b. What is your affiliation?
0	2	14	Government agency directly sponsoring the program under review
16	31	81	National/government lab, private-sector or university researcher whose project is under review
16	16	70	In an industry directly involved in the program under review
6	4	21	In an industry with interest in the work under review
3	3	28	Government agency with interest in the work
11	4	17	National/government lab, private-sector or university researcher not being reviewed, but who has an interest in the work
5	13	13	Other (descriptions below - not all provided descriptions) German delegation, Public non-U.S. government agency, consultant Retired university faculty Italian Governmental Agency Consultant (3) Consultant, Under contract to ORNL DOE consultant (2) Educational nonprofit organization/DOE EERE grant award recipient

			QUESTIONS FOR ALL ATTENDEES
4.6	4.6	4.5	2. Purpose and scope of the Hydrogen Program Review were well defined.
4.3	4.4	3.9	3. The plenary presentations were helpful to understanding the direction of the Hydrogen Program.
4.3	4.3	4.2	4. Sub-program overviews were helpful to understanding the research objectives.
			5. The quality, breadth, and depth of the following were sufficient to contribute to a comprehensive review:
4.1	4.2	4.1	a. Presentations
3.9	4.2	4.1	b. Question & Answer periods
3.8	3.9	3.9	c. Answers provided concerning programmatic questions
3.9	4.1	4.1	d. Answers provided concerning technical questions
4.2	4.4	4.2	6. Enough time was allocated for presentations.
4.0	4.2	4.0	7. Time allowed for the Question & Answer period following the presentations was adequate for a rigorous exchange.
3.8	3.7	3.7	8. The questions asked by reviewers were sufficiently rigorous and detailed.
0.0	0	•	9. There were no problems with:
4.5	4.4	4.3	a. Groupings of projects by technical area
4.3	4.4	4.2	b. Proprietary data (should not be any at this Review)
3.9	3.9	4.0	c. Quantity/level of the information presented
4.5	4.7	4.6	10. The review was conducted in an organized fashion.
			11. The frequency (once per year) of this formal review process for this Program is:
98%	96%	90%	About Right
0%	4%	8%	Too Frequent
2%	0%	1%	Not Frequent Enough
0%	0%	0%	Don't Know the Frequency of Reviews
4.6	4.5	4.4	12. Logistics and amenities were satisfactory
4.0	4.3	4.3	13. The visual quality of the presentations was adequate. I was able to see all of the presentations I attended.
4.3	4.5	4.4	14. The audio quality of the presentations was adequate. I was able to hear all the presentations I attended.
4.3	4.7	4.3	15. The hotel accommodations were satisfactory.
4.5	4.4	4.5	16. The information about the Review and the hotel accommodations sent to me prior to the Review was
			adequate.
			17. What was the most useful part of the review process?
			 Consistent presentation format made them easy to follow. Common grouping of presentations. Knowledgeable reviewers with good questions.
			 Provides considerable interaction of researchers in the hydrogen field, which does not occur at other gatherings.
			 Board outside room.
			 Opportunity to have an overview of all projects funded by the DOE under the H2 and vehicle programs.
			 Opportunity to talk with participants - especially at posters.
			Networking.
			Meeting with fellow colleagues to discuss research ideas.
			 Easy to see and hear presentations. Program eventions and technical advances/future direction of projects
			 Program overviews and technical advances/future direction of projects. Meeting others of similar business interests and goals.
			 Seeing high-quality technical content in the context of practical goals.
			 Networking.
			 Exchange of information and suggestions between organizations and labs.
			Program details.
			Networking.
			 Progress update and program direction. Good improvement. The reviewers were much more constructive and respectful in their comments than last year.
			 Good improvement. The reviewers were much more constructive and respectful in their comments than last year. Discussion with colleagues and collaborators.
			 Opportunity for exchange with other researchers.
			 Meeting program organizers far-flung collaborators.
			Keeping Schedule.
			Learning about other projects.
			Presentations, contacts, and informal discussions.
			 Seeing what the national labs are working on versus industry.
			 Presentations. Getting reasonably complete updates on all the projects in this program.
			 Getting reasonably complete updates on all the projects in this program. Comparison of funded programs and projects.
			 Review of fund allocation.
			Review of progress and tasks to be completed.
			 In Energy Storage, the battery projects' reviews were very useful!
			Having the presentations available on CD.

- Talking to people at breaks. Some of the presentations were useful. Presentations To keep me informed on the process in the relevant area and to lean new developments. · Learning about progress in the technology. Hallway discussions. CD with the briefs – there were too many parallel sessions to sit in on them all, but can review later. · Presentations. · Meeting peers working on similar projects. • Exchange of technical details and opportunity for further collaborations. • I learned a lot about the actual status of projects and the many results obtained. Cross industry/government/academic interactions. • Compared to the NETL peer review, this EERE review is significantly more helpful. • Meeting collaborators and peers. • Overview of total range of programs. Ability to compare presentations from similar projects. • Ability to guide research and program into most useful channels. Ability to see the entire DOE research portfolio in one meeting. · Amount and quality of information, ability to speak directly to others in industry. • As a general attendee (not presenter or reviewer), this annual review was very good chance to understand how the whole DOE program is going, and I've learned a lot about the state of the art of lithium ion battery research in the U.S. Both the talks and the poster session were extremely helpful to me in getting a perspective on the current directions of battery research in the U.S. The talks had the right level of detail and the presenters were generally clear and concise. Comments by the reviewers. · Discussions with reviewers and peers. · Efficiently meeting everyone involved in this area. · Everything is good! • Exchange of ideas among peer groups. • Exchange of technical information and networking. · Feedback on program and results. Getting an overview of the new direction for the DOE program and getting information on new advances. In many cases the technical progress is perhaps not as great as at the last review, but I think this mainly reflects that the program was redirected to look at some much tougher areas (such as higher energy density anodes); also the last review was really an 18-month review. The PeerNet system worked much better than the last time. although I did lose one review early on and had to recreate it when PeerNet wouldn't save it. · Facilities were very good; food was great! · Getting the latest state of the art technology information. Going to talks in subjects other than my own. · Good detail on projects of interest. • Good organization. Enough time for the speaker. · Great opportunity to meet up with program administrators, as well as experts in the field. Wonderful information gathering. Great snapshot of the breadth of research projects being funded by DOE. Liked the fact that H2/FC and Vehicle Technologies were co-located this year in nearby hotels. Having access to presentations prior to talks. Having the opportunity for asking questions. Having all the presentations and presenters together in one place at one time. • Having the same consistent first page of each presentation layout the same critical information. • I appreciated learning about the other areas in our program and what they are doing, within a short period of time. · I find the Review an information meeting and where I can connect with government personnel and other companies. • I liked the poster sessions where a direct dialog is possible with authors/PIs. . In addition to having the opportunity to attend the presentations I was most interested in (and to ask questions of presenters), it was very valuable to have the opportunity to interact with some of our colleagues who work in Washington and with some of our subcontractors who had flown in to attend the Peer Review at breaks and when they came to our poster presentation. Face to face meetings are not frequent over the course of the year due to budget constraints; however, these annual meetings give us a valuable opportunity to interact in this way. In several cases, the upcoming review seemed to be a primary motivation for researchers to complete certain parts of their work and to organize it. I think the review process actually helps keep many projects on track. Information - technology status & updates. Overall program direction. Commercial status of technologies. Interacting with colleagues and discussions with poster presenters. It gave a good overview of the goals of the programs and the results obtained to date.
 - It is useful to hear about the progress made in the Hydrogen Program.
 - Learn the progress made up to date.
 - Learning and understanding what and why others are doing particular R&D.
 - Learning from others.

 Learning on a technical level what DOE is funding and the direction of the research. Learning what has been tried; even when the no-go conclusion was obtained. Synthetic methods used for other
 purposes. Listening to the other oral presentations - plenary and technical.
 Meeting others in the hydrogen community and networking.
 Meeting various representatives from industry, universities, and national labs.
Most interesting and helpful.
My own education was valuable.
Networking.
 Networking. Networking with other scientists and industry.
 Networking with others for my research.
Networking.
 Opportunity for networking and the chance to see progress in technical areas other than my own.
Opportunity to learn more.
 Opportunity to meet with the PIs and network.
Oral and poster sessions.
 Organized well. I was able to attend and learn from presentations in the same category/field.
 Overview of what is going on in several areas of the hydrogen and fuel cell car programs. Overviews of subprogram group
 Overviews of subprogram areas. Plenary session from DOE.
 Poster sessions and adequate number of oral presentations, keeping strict timing for people to attend the parallel
sessions and enough breaks.
 Poster sessions and presentations.
Posters and discussions.
 Presentation of all aspects of hydrogen energy at a single meeting. Opportunity to meet various researchers
working on different areas of hydrogen storage.
Presentations.
 Presentations – keeping research relevant to the current problems and not reflecting on "pie in the sky" research. Presentations – both and negtor: interactions; and networking.
 Presentations, both oral and poster; interactions; and networking. Project status.
Question and answer period.
 Question and answer session for each presentation.
Questions from the audience, suggestions from peers during breaks, poster sessions, the enthusiasm of
attendees, and the willingness to help each other with guidance.
The review was well organized and provided an excellent opportunity to assess progress. For the most part, the
new online review process worked well.
Seating and tables for reviewers.
 Seeing the wealth of projects. Communication and partnerships. Providing lunches and dinners kept people on site.
 Seeing an industry-wide review of PHEV & EREV research.
 Talking directly with the program folks from DOE.
 Technical presentations of on-going projects/programs.
 Technical presentations on projects being reviewed.
 Technical progress in the important energy storage area.
The AMR is both an excellent opportunity to see the progress of current research and to facilitate discussions
among researchers.
 The breadth of the presentations allowed insight into the overall state of technical progress.
 The chance to see other projects related to the Hydrogen Program along with the great opportunity to network and discuss with the breadth of knowledge in one area on this topic.
 The flexibility to be able to choose which presentations one wanted to sit in on was nice. Providing none conflicted
with each other due to time, but overall I was able to sit in on any and all that I found of relevance and interest.
The informal networking ability outside of the schedule.
The materials.
 The morning intro sessions and schedule of presentations outline.
 The most important part of the meeting for me was to learn about the development status of the fuel cell
technologies supported by DOE.
 I got incredibly condensed and useful information regarding what was going on across the different fields of fuel cell industry, and how far or close.
 How close we were to full-scale commercialization in certain areas, and what needs to be done in order to achieve
 How close we were to full-scale commercialization in certain areas, and what needs to be done in order to achieve the industry goals.
 The most useful information presented is the new, updated, and breakthrough information from the projects and
the programs.
 The opportunity to interact with fellow participants, particularly at the poster series.
The opportunity to interact with the researchers and the excellent question and answer sessions after each
presentation.
 The opportunity to meet key researchers and talk about their research activities was extremely valuable, and

• The opportunity to meet key researchers and talk about their research activities was extremely valuable, and

758

 much appreciated. By the way, thank you for the lunches and refreshments between sessions! The prepared handouts with registration were also quite useful to understand who's who and who's working with whom. The presentations and the exchange during the poster sessions. The presentations from the FCV and refueling industry representatives. If anything, these were FAR too short. When you have programs that eat up \$40 million of DOE's program budget at a crack, these programs absolutely require more explanation, more detailed results, and status discussions. Instead, the program organizers allocated equal presentation and discussion time. This is not acceptable. Moreover, DOE MUST require the industry "partners" to be true partners. Cost-shared funding should mandate info sharing. DOE (and NREL) has become very lax in this regard. Far too many important R&D findings (and costs) are hidden from public and academic view. The presentations themselves. The presentations were kept on a reasonable schedule. The presentations were systematic and well prepared. The presentations.
The Q and A.
 The question and answer sections of the presentations were very informative and pretty rigorous.
 The review process allowed me to gain a more thorough insight into the scope of the DOE program.
 The review provides an opportunity to summarize data collected in the past year. Meeting other researchers doing similar work and in related areas is probably the best part of conducting a review in this manner.
 The talks were excellent and provided an up-to-the-minute snapshot of current research.
The technical presentations.
This was a great opportunity to become exposed to a cross section of the work being done on hybrids and
alternative powertrains.
 Sessions were generally very informative. To see the activities currently on going with the vehicle technology program.
 Web-based review platform.
Well-organized review process. Apart from some minor glitches, the new online review process worked well.
18. What could have been done better?
• The review is too large - most projects do not need to be reviewed every year. Combining the two large programs
only exacerbated this issue. There is very little overlap. Please do not repeat.There was not enough communication on when and where food was provided. Too many required slides on
 There was not enough communication on when and where rood was provided. Too many required sides on background and context for time allotted. Font was too small on many presentations.
Cheaper hotel for the meeting.
The Fuel Cell section needed a larger session room.
Too BIG - combining Hydrogen and VT is a BAD idea.
 Individual subprogram reviews were much better, i.e. systems/materials/engines. The amount of time devoted to formal presentations should be shortened and more casual meetings should be
 The amount of time devoted to formal presentations should be shortened and more casual meetings should be encouraged where researchers can freely discuss.
 Their ideas – find new collaborations.
 Presentations should finish by 5:00pm and not start before 8:00am.
Presenters need to use bigger font so that the audience in the back of the room can see/read it.
 Distribute data on a to memory stick instead of CD. A more there use a way is a sound be presented on subpreserves.
 A more thorough overview should be presented on subprograms. Hotel rooms are too expensive.
 Poster displays were not uniform in display format, size of text, and figures. Some were difficult to read,
particularly for "older" eyes.
 If the formats of slides (such as the minimum font size) were defined, it would help the audiences follow the presentation.
 More time for reviewer/researcher interaction. This meeting is not useful as a review. Consider a half-day of brief overview presentations followed by a half-day
 This meeting is not useful as a review. Consider a nan-day of biter overview presentations followed by a nan-day of posters – where only reviewers are permitted in poster session presentations during that "on" day. Then the public goes to posters on another "off" day.
Battery developers provided too little data.
 A less formal review with lots of group discussion may be more productive and far less expensive.
Temperature control - many sessions were too cold.
 The venue was OK, much better than last year. Organization is fine and I looked at the poster/talk breakdown. Some presentation rooms needed to be bigger.
 Some presentation rooms needed to be bigger. Nothing.
 Questions/criteria/presentations preliminary better controlled for uniformity.
 Making sure that OEM's recurring money has to show data with real units on. Two GM presentations were unacceptable with little or no data or missing axis. They should not get funding if they are going to do this.
Water at breakfast. The field of the statement to state and the statement to state and the statement to state and the statement to statement to state and the statement to statement
 The fuel cell section got moved to a room that was way too small. It would have been helpful if DOE staff could have been more forthcoming regarding the implications of the
 It would have been helpful if DOE staff could have been more forthcoming regarding the implications of the Secretary's proposed budget changes. Questions during the plenary session.
 Questions during the plenary session. Water should be available for reviewers.

- DOE should work with presenters to come up with press releases and other promotions to identify value of work. Project work may be supported by public and Congress with more PR. Some valuable work progress should be released.
- In Energy Storage the ABRT presentations said much too little about the technology specifics and science specifics involved. I know there were 25 posters covering this, but I live in Gaithersburg: 90 minutes on Metro, briefings from 8:15 to 7:45, 90 more minutes on Metro. How was I supposed to have time to review 25 posters on subjects I care about? Energy storage could have used Friday to give some of these posters as presentations.
- Room numbers should have been provided ahead of time along with the agenda.
- DOE is spending too much money unnecessarily instead of hiring two people who are sitting around most of the time to monitor questions and take microphones around the floor, why doesn't DOE just have a standing floor microphone and have people line up behind the microphone to ask questions?
- Poster sessions are stigmatized both presenters and attendees feel the poster sessions are consolation for those who can't make "the cut" (not good enough to be assigned for oral presentation) and assigned "after hours" when most attendees are gone.
- The format of the presentations is not conducive to understanding a project you didn't already know about.
- Clearly state that breakfast and lunch are included.
- · Allow presenters to take part remotely by Web-based meeting software.
- Seating logistics.
- Thermal sessions in APE and AC were scheduled at same time (Friday morning). The same problem occurred last year.
- Need to ask what sessions will be attended during registration process. The initial room for the energy storage session was far too small for what is definitely a key area. The room was changed, but seemed to take a lot of complaints to make that change happen. Also, this didn't make up for missed talks because the room was full and people were standing in the hall.
- I think it would be good for the DOE program manager to introduce the speaker and explain how the project fits with his/her portfolio.
- Allow more time for Q&A to allow the collective knowledge to progress.
- · More snacks in the morning!
- Several things were improved compared to last year especially with respect to Internet access and PCs available to reviewers.
- This is not really a review; it is a Kangaroo Court. The DOE program managers should engage in asking hard program and feasibility questions.
- The meeting is expensive, with not much choice for hotel accommodations.
- The meeting should be held in ONE venue! Two sites caused me to miss talks.
- The larger programs (> \$1M) get too little time; small ones (~\$100K) could be shorter.
- A few of the presentations used too small type. Most, by far, were OK.
- A lot. It is really surprising to see the focus on hydrogen and fuel cells when there are no clear technological
 solutions or solicitations for short- to near-term technologies to meet and exceed the current government targets
 for fuel efficiency. For technology start-ups in attendance, this year's review may have missed a key focus in
 today's auto market.
- The presentations were outdated. Numerous speakers spoke to the fact that the data was old compared to what they had. Apparently DOE required them to submit final presentations three months before. It's better if they were asked to submit two weeks in advance and upload to a website. Attendees can download them on their memory disk, from the Web, or even come to the conference and take a disk if needed.
- All presentations should be in one hotel; could not go back/forth because of the location distance.
- Arrange appropriate conference rooms for the hot topic so that attendees can have a seat and be actively involved.
- As often the case with such meetings, one is occasionally confronted with two talks of specific interest that are scheduled at the same time in different sessions. Another problem was the difficulty of moving between the two meeting hotels to catch talks of interest.
- Assignments of rooms. Those of us interested in both Fuel Cells and Batteries were in a tough spot. Once the switch was made, the Fuel Cell room was a bit small. If an audience member did not use the microphone, the speaker should be requested to repeat the question for everyone's benefit before answering.
- Assignments for reviewers. I told the AMR team that I was arriving Wednesday afternoon, but I was assigned hydrogen production projects reviews for Tuesday. After this was corrected, I was then at the last minute assigned fuels technology projects again on Tuesday.
- Assignment of reviews according to personal expertise.
- Attendance by Secretary Chu, in general and especially due to recent announcement.
- Better explanation of why the Hydrogen Program was decimated. The DOE staff was either "muzzled" or did not know. Of course the story is still unfolding.
- Better overview to first-time presenters for oral review regarding what to expect, format, size of audience, and etc.
- Can't think of any thing; job well done.
- Crowd control.
- Do not know.
- DOE plenary presentation should be longer in time allocation and more detailed.
- DOE representatives could/should have better clarified the new administration's intention and direction on fuel cells R&D.
- · Don't know; everything seemed well organized to me.

760

- Earlier and more consistent notification and confirmation of potential reviewers. Everything was fine. · Fewer parallel sessions - there were several times during which I wanted to attend sessions that were happening simultaneously. Please also try to have posters available on the CD given to attendees. Focus more on fuel cells of all types, not just hydrogen. • Free wireless Internet. Given the extensive nature of the program, I believe the review was well organized. In many cases, the rooms were way too small for the audience. I had to stand in the back (or leave) for more than half of the presentations I wanted to addend. Insufficient food at dinner poster sessions. It may be difficult or impossible, but more accurate planning of room size for potential audience size for each session would have been beneficial. · It seems it would make sense for DOE program managers to assess in advance what level of progress was made on a particular project throughout that year, and then decide if an oral or poster presentation is more appropriate to present findings. It wasn't clear how format was selected but some progress especially that which is primarily pictorial lends itself better to poster than to oral, whereas hard data needs the oral format. · It was hard to see some of the slides because of the light level in the room. Some slides contained too much information in too small of a font. I realize that I can get the slides online and read them, but what's the point of projecting a slide that has minimal value to the oral presentation. • It went very well. I can't think of a way to improve. • It will be helpful to have all the sessions in one place. It would be great to have additional rooms available to everyone to organize meetings with co-workers from other labs. It would have been helpful to allow more time for questions and discussion after oral presentations. It would have been nice to not split the meeting between two hotels - but I assume this is the reason for the new venue next year. Also, one of the meeting rooms was a bit cramped. • I've felt that over the past three years that I have attended, the Peer Review has become more organized and focused, and this past meeting was the best of the three. I can't think of anything that I would suggest changing. · Larger facility. Having the meeting in two different hotels is not a good idea. Never schedule the meeting the week before Memorial Day. • Larger font size for the timetable of events. Larger room for the fuel cell session. Less time for presentations; more oral presentations. · Logistics and costs. • Make it a bit smaller. · Many of the presentations moved so fast that they were hard to follow. This is likely because the presenters wanted to include everything to show that they used their funding to the fullest, so I'm not sure what can be done about it. But combining the pace of the talks with the lack of proprietary information sometimes requires leaving out a lot of detail that could be helpful. Many reviewers are currently DOE-funded project PIs. If their expertise areas are the same, it could cause conflict of interests; if not, they are not the most qualified. Such a practice definitely limits DOE's view on the quality of the projects and the future directions. · More information about hotel service. More information could have been provided earlier to the reviewers about the scheduling and agenda. More seating needed for FC presentations. N/A • No particular ideas at this time. No particular suggestions. • Not much. With a group this size, it was all handled very well. Nothing. Nothing – no complaints. Perhaps separating the Hydrogen and Vehicle Technologies programs back out would ease confusion and overcrowding of plenary session review room. · Please arrange for all sessions in one location. Having two hotels was inconvenient. Please give more time for the reviewers to ask more questions. • Please list the reviewers and their affiliations for each session. Please provide water in the conf or presentation room. Presentations were outdated material because of the limitations of no proprietary information and the several months that lapsed between the time when the presentations were due and when they were given. Presenters could have considered their audience better. Provide refreshments at all times, not just at the breaks. Raise the display screens for the video projectors to make the bottom of the presentations visible to the entire room Really, this is very good. Better Internet connectivity for the HTML-based review process would have prevented frustrating disconnection in the middle of a review.
 - Revert to the former system for inputting reviews. The Web-based system is poorly adapted to this process; it is better suited for reviewing confidential proposals. The FedEx packages containing nothing more than a password

were a ridiculous waste of money. Better to hand each reviewer a flash drive with all information on it to be returned at the end of the review so that Internet connection is not required. Rooms were sometimes overfilled. Panel discussion was avoiding topics of very high interest, i.e. development of budget for H₂ program. Seating capacity for some sessions was inadequate. This created a situation where people had to stand in the aisles or outside the meeting room. It was somewhat disruptive. There were audio/visual equipment problems in one of the sessions that contributed to a delay. Set dates for the meeting early, advertise the dates, and try not to change the dates. Some confusion between Battery and Fuel Cell related presentations. Hydrogen/fuel cell and vehicles presentations could have been organized in the same hotel/space for ease of intermingling between the two areas. Some initial problems in the online review with reviewer assignments - i.e., assignments were added and deleted at the last minute without notification. Hopefully this is simply a "break-in" problem that won't occur in the future. Many of the presenters failed to address remaining obstacles/barriers to progress. As a reviewer, it was often difficult to "read between the lines" and determine the actual status of the project with respect to technical barriers. Some of the presentations were light on detail; I would prefer if more detail were available. Outside of that -- I learned a lot and am looking forward to next year. Some of the rooms were crowded (most were good). Some rooms were too small and could not accommodate people who came to attend the presentation. Some, but not all, of the talks from the commercial companies were basically marketing fluff and too vague for a merit review. While I recognize that this is an open forum, they should be able to sanitize the data sufficiently to at least say something. From a reviewer's point of view, one or two talks were devoid of any useful information whatsoever; it appeared to me that they didn't care what we thought because they were going to get funding anyway. The real problem of course is that this can be used as a ploy to hide really shoddy work. Several topics really need the ability to show movies as part of their presentations, but generally this was not allowed (or if it was it didn't work). Try and permit this in future. Sometimes, the schedule was too tight. For example, the review started 8:00am and ended 9:00pm. I believe that, especially, the reviewers (and of course also the presenters) would be very exhausted at that time. For the good review, I think it is necessary to schedule the review process not too tight. The meeting is too big, and the speakers can only be well selected. • The presentation rooms were too cold; the lobby area was too crowded. The question and answer sessions could have been longer in order to provide a more thorough understanding of the results obtained and possible problems not considered or addressed by the presenter. The reviewers could have been notified earlier as to exactly how many and which reviews they had to do. I got my information late and was assigned 23 reviews 4 of which overlapped (were at the same time with other reviews I had). I did manage to work this out and get down to a reasonable number of 12 reviews. The Reviewers did not seem to be technically good enough to ask good tough questions. In fact often they did not ask any questions at all. It seems they are trying hard to be nice as they may have some stake in the outcome. Experts from fields should be carefully chosen and changed every year or every two years. Not good to have the same reviewers every year. The talks given by the European representatives were inconsistent. One or two of their talks were poorly executed and not informative. The talks given by the DOE representatives were very useful. The time reminder for the presenter could have done better. The timing conflict between BATT and Fuel Cell sessions made it difficult, if not impossible, to attend all sessions of interest. There needs to be time for Q&A at the plenary session. • There was a slight problem with the room size being too small initially, but this was quickly rectified. The food was excellent. Very large review. This hindered discussion for my specific program. There were not enough chairs in some rooms, and it was hot. The room ventilation was poor. It's hard to focus on the discussions when sweat is running down your forehead. There were problems with reviewer assignments in the online review. Review assignments were added/removed without notification. This created some confusion; hopefully it was simply a problem associated with first-time use of the review method. · There's not sufficient time to present all data accumulated during the year. So the presentations end up being marketing talks, instead of being technical talks. This is critical—in order to accurately assess technical work, the details must be presented. This is impossible without an NDA, and is the reason for my negative ratings. • This is too large. Too many presentations. Too many people. • To limit presenters to complete their presentations within the assigned time. Some presenters left very little or no time for questions that is a very important part of the reviewing process. Too many programs were reviewed all at once by a review panel whose members are also being reviewed! Given that a vast number of programs are being reviewed it must be exhausting for the review panel to keep their focus during the whole week. It will be better to split the meeting so that a smaller number of programs get reviewed much better. We had a lot of problems with reviewers. The reviewers did not know what projects they were reviewing. The reviewers did not show up. The status of reviewers was not provided to the program leads. A better communication process for reviewers and informing the program leads needs to improve.

• When you switch rooms for a series of presentations, you might want to make things a bit clearer ... something as

4.0		4.0	simple as a yellow post-it note with directions.
4.3	4.4	4.2	19. Overall, how satisfied are you with the review process?
000/	0.001		20. Would you recommend this review process to others and should it be applied to other DOE programs?
00%	96%	93%	Yes
0%	4%	7%	No
			21. Please provide comments and recommendations on the overall review process.
			The online process used this year is easy to use and convenient.
			 Need clearer agenda with times and locations for food. Time for each presentation was OK, but the required "context and background" slides should not be presented. Focus on what was achieved and conclusions. Use
			larger font.
			 The annual review meeting is becoming too large. It may serve the needs of the sponsors, but the review has
			become too unwieldy and rigid to be of much use for the researchers.
			 Reviews should be based on research topic (fuel cells, hydrogen/batteries/engines/components/etc.) and not all-
			encompassing DOE offices.
			The process is very well organized. Rich Bechtold and the colleagues should be commended for an outstanding
			job. Coffee breaks, continental breakfasts, and lunches were very good. Plenty of time provided for meetings ar
			networking between sessions. Good job keeping everything on schedule so people can move around between
			sessions.
			Improve readability of posters.
			The review was very well planned.
			 I do not understand why this review is open to the public. I baliave reviewers were averablemed by the paster session. I'm not sure if projects were not "projudged "
			 I believe reviewers were overwhelmed by the poster session. I'm not sure if projects were not "prejudged." I liked the overall organization of the meeting.
			 Fliked the overall organization of the meeting. Feedback from reviewers needs to be within two months; otherwise, don't bother providing the comments.
			 The hotel cost at \$250 is getting a bit too high to afford for many of us.
			 Require presenters to start with the status of last year's review and focus mostly on work done over the past year
			Too many talks had more than half of their talks the same as last year.
			I don't like mega-reviews with many parallel sessions! Since I am primarily a battery person, I was forced to miss
			all of the Hydrogen work and only caught the SOFC sessions for fuel cells. Also, none of the Basic Energy
			Science sessions!
			• Vehicle Technologies program presentations were extremely short changed. Too few sessions, and the papers
			were so condensed that most lacked any appreciable depth!
			 A representative from U.S. DOT (e.g. Federal Motor Carrier Safety Administration), which participates in the 21st Century Truck Partnership, should have been invited as a reviewer!
			 Too big, too noisy, and too shallow. Review smaller program chunks in more depth.
			 Seating in salons was unsatisfactory. On Tuesday, Energy Storage was crammed – Standing Room Only. The
			rest of the week Fuel Cells was jammed. Someone came to count people in the FC session but she missed the
			times when all seats were taken and people were still jammed at the doorway and on the floor.
			 I think this is a very time and resource expensive process.
			Facilities and organization were superb.
			• Technical details and discussion should be extended to all research groups year round as it becomes available.
			• The review should be held someplace other than DC. If you want it to be a review, then the DOE program
			managers need to be more involved.
			 A great job, with great planning and wonderful accommodations. A real pleasure to be there and a great source of informal connections and information exchange. I will highly recommend that we keep attending in the future.
			 Again, the review was quite large. This may make for simpler and cheaper coordination, but I do not feel that it
			 Again, the review was quite large. This may make for simpler and cheaper coordination, but i do not reer that it lead to improved discussions between folks in battery, fuel cell, hydrogen storage, etc.
			 Biggest criticism: For a peer review to be meaningful, it needs to be closed, with the peer reviewers signing Non
			Disclosure Agreements. The success or failure of these technologies often hinges on specific technical issues
			and the details/data, etc. are, unfortunately, almost always proprietary. Consequently, the value of the peer
			review suffers because the peer reviewers only see high-level information.
			Feed back! The presenters would like to know the outcome of the review and a summary of constructive
			criticisms that reviewers may have had after presentation, preferably confidential (within a few days upon
			 compilation of the results). First of all, congratulations to the organizers of this meeting! Everything went so smoothly and as planned. Keep
			doing a great job!
			 For a DOE review it would be a better display to the press and public if the energy generated (as well as local
			transportation) was coming from the technology being reviewed.
			• From a reviewer's point of view, I found this to be better than last year. By having us rate every other talk or so,
			we could keep up with our tasks and in my view give a more thoughtful response with the detailed commentary
			that I (and I think the DOE) find more useful than the scoring system. The downside was that I could not always
			follow the talks I was not covering, but you can't have everything. There is still not enough time for the presenter
			to really explain what they have done, still trying to cram too much into the week. However, by using posters
			instead of talks for some people, it was better than before. Although I understand that those giving posters may
			 not have been happy, I actually find them a good way to get a true Q&A dialog going. Funds received did not always reflect quantity/quality of work being reported. Often two similar programs with
			 Funds received and not always reflect quantity/quality of work being reported. Other two similar programs with similar goals would present back to back but one program would receive twice the funding. Presenters should

763

explain where a majority of the cash was spent (i.e. total man hours, major capital investments).Good.
Good.
Good job Rich and team.
Great job.
Great job!
 Having a merit review gives researchers an external view of their projects, and DOE has an external view of the projects they fund
projects they fund.Helpful and feel confident on what we are doing after the review process.
 Hotel room rates, even though discounted were too high (~\$285/night). Some presentations could have been
grouped better to minimize the number of days a reviewer would need to stay.
• I am satisfied with the overall process.
• I can see how this review must take a considerable effort to prepare and present in such an organized manner.
Those involved at DOE should be commended for a job that always seems to be so well organized.
 I didn't know which projects to review till Monday, May 18th.
• I felt that the whole story was not being told. The auto makers presented that this was still a viable project, which it
isn't as reflected by DOE's lack of funding. This was the only thing the car company's can agree upon between them. I think the costs are not being presented accurately and not frequently enough.
 I found the review very informative. I got a sense of the scope and strategy of the programs and enough detail to
identify potential collaborators.
 I was satisfied and found it a good experience for my first year involved with the DOE AMR.
 In addition to us benefiting from the meeting more each year, we have recommended to some of our
subcontractors that they attend in order to get an idea of what others in the industry are doing and perhaps get
ideas from others at these meetings which might speed up their contributions on our timeline. This has
consistently been a motivator for the progress of our project.
 In my view, a large panel reviews a vast number of programs. Given the length of the AMR meeting the review process may get compromised. This also will be overwhelming for the program managers.
 It is important that the reviewers truly understand the project. Sometimes the scientific/academic types are out of
touch with the industry approaches and understandings.
• It seems that we continue to push the deadline for getting the review material into the hands of the reviewers.
Earlier is better.
 It was the first time I attended. I was impressed with the entire event. Good job!
It went very well. Thank you.
Last year I did not receive my review until the actual review summary was published on the DOE website. I would have that I would receive my review before publishing this year.
hope that I would receive my review before publishing this year.More (or less restrictive) categories for input in the review process would desirable.
 More (or less restrictive) categories for input in the review process would desirable. Most of the presentations were too long. The number of slides should be restricted to a maximum of 30, and time
allotted should be controlled properly by the session lead. Reviewers should be changed every year or 2 years
and experts in the field should be chosen.
• N/A.
No comments.
Of the presentations I saw, I feel that the peer reviewers and many presenters see the merit review as a
presentation of a technical paper and not a program review. There was too much data, which initiated too many
questions regarding data. With regard to Office of Vehicle Technology programs, it is becoming more of a DEER type conference where the presentation is just a version of an SAE paper. Based on the outline and guidance I
was given for the review, I would reduce presentation time to 15 minutes and 5 minutes for questions – and cut
presenters off at exactly 15 minutes.
On condition that it answers is short and near term technologies. We cannot leap into hydrogen and fuel cell
powertrains just yet so the full scope of mainstream hybrid powertrain solutions, for example, is critical at this
point.
 Overall satisfactory. It was nice but personally I wanted to more news and comment for next future funding for hydrogen vehicle side from DOE officials. It was not clear for future activity for vehicle demonstration.
 Overall, the review was very well organized and provided a good opportunity to evaluate progress in the Hydrogen
Program. The schedule was well thought out, and parallel sessions worked well.
 Presentations should be updated material and allowed to be updated until they are presented.
Procedure is all right for such a large program. Smaller programs should have a more informal setting for
discussion between reviewers and presenters.
• The process ran smoothly; the presentation schedule was well thought out. Parallel sessions worked well.
The review was good. In addition to the various categories, it would be nice if each presenter was asked to
address a goal (cost, efficiency etc) and bottom-line numbers so that technologies can be compared. Comments about the outdated presentations are in question 21.
 The review was well conducted.
 Rich Bechtold was great to work with very responsive and most helpful. I thank him for all his guidance. Specific
to this survey design, I would ask that you allow for a "not applicable" response, as many of these questions did
not apply to me, as I had no basis to evaluate.
• See 18.
• See item 17. Especially the last three sentences. Too much industry R&D is veiled. There should be a common
FCV R&D project with shared results, not five different, isolated, secret, industry R&D projects. There also needs

764

			to be more strategic thinking. The Nuclear Hydrogen program is facing project down selecting. Why? It's because
			of the nuclear moniker and not because of the technology being researched. High- temp electrolysis research is important for "green" solar and geothermal applications and not just "nuclear" applications. Linking this important R&D on chemically assisted electrolysis and heat-assisted electrolysis to ADVANCED NUCLEAR POWER PLANT DESIGNS was a mistake. Now, good programs will be cancelled because the reactor concept was
			unworkable. That is not right. Finally, there was a HUGE gap in coverage regarding the safety of creating genetic mutations (e.g., algar) in order to produce hydrogen. A SAFETY analysis should be a necessary requirement of EVERY genetic mutation contract that DOE requires and a discussion of the safety measures proposed should b an essential part of every review and contract award. Existing projects do not meet this or become sloppy.
			 DOE could save a lot of money by not making the meeting so extravagant. I enjoyed it, but a lot of the expensive parts of the meeting were unnecessary.
			 The hotel was well appointed and comfortable but relatively very expensive even at the discounted rate. Perhaps there are other more reasonable (under \$200 per night) choices that could be considered next year. The organization part of the review was excellent – nothing to complain about. The devil is in the details. It is obvious that many of the reviewers are not at an arm's length from the PIs and they were very reluctant to ask
			 critical questions. In many occasions, the presenter would tease the reviewers about enough questions. The planning, accommodations, and quality of technical presentations were outstanding. The process is pretty reasonable given the large number of presentations. Congratulations to the DOE team for
			 efficiently reviewing such a large number of projects! The program leads should not be placed at the side of the projection screen because we could not determine the status of the presenter in their presentation. The presenters were shining the laser pointer in the eyes of the
			 program leads at the head desk. The reviewers presented adequate information on the background and resources used on the projects This is too large. Too many presentations. Too many people.
			Very nice job.Very well planned and executed.
			• While rare, there were a few presenters who seemed to be very ill prepared. If possible, such people should not take part, or at least not present, in subsequent reviews.
			 Reviewers should sign NDAs and have access to important technical details that more often than not are keys to assessing the viability of the work. Would like to get reviewers comments back sooner and a have chance to discuss their comments with them
			immediately. In the past, at least the reviewer's comments were made with the reviewer being unaware of specif DOE program manager instructions to a project team as to the direction and emphasis of a project's approach.
3.6	3.5	3.8	QUESTIONS FOR PEER REVIEWERS ONLY 22. Information about the program/project(s) under review was provided sufficiently prior to the review session
4.0	4.2	4.1	23. Review instructions were provided in a timely manner.
3.4	3.8	3.8	24. The information provided in the presentations was adequate for a meaningful review of the projects.
			25. The evaluation criteria upon which the review was organized were clearly defined and used appropriately.
4.2	4.2	4.0	1 – Relevance
4.2	4.3	4.2	2 – Approach
4.2	4.4	4.3	3 – Technical Accomplishments and Progress
3.5	4.2	3.9	4 – Technology Transfer/Collaboration
3.5	4.3	4.1	5 – Proposed Future Research
			26. Explanation of the questions within the criteria was clear and sufficient.
4.0	4.5	4.1	1 – Relevance
4.2	4.5	4.1	2 – Approach
4.2	4.5	4.2	3 – Technical Accomplishments and Progress
3.8	4.5 4.4	4.1 4.2	4 – Technology Transfer/Collaboration
4.0	4.4	4.2	 5 – Proposed Future Research 27. The right criteria and weightings were used to evaluate the project(s)/program.
3.9	4.2	3.9	1 – Relevance
0.0	4.3	4.1	2 – Approach
43	+.0		
4.3 4 1		41	3 – Technical Accomplishments and Progress
4.1	4.4	4.1 3.9	3 – Technical Accomplishments and Progress 4 – Technology Transfer/Collaboration
4.1 4.2	4.4 4.3	3.9	4 – Technology Transfer/Collaboration
4.1 4.2 3.9	4.4 4.3 4.2	3.9 4.0	4 – Technology Transfer/Collaboration 5 – Proposed Future Research
4.1 4.2 3.9 3.9	4.4 4.3 4.2 4.4	3.9 4.0 4.2	 4 – Technology Transfer/Collaboration 5 – Proposed Future Research 28. During the review, reviewers had adequate access to the Principal Investigators.
4.1 4.2 3.9 3.9 4.4	4.4 4.3 4.2 4.4 4.7	3.9 4.0 4.2 4.3	 4 - Technology Transfer/Collaboration 5 - Proposed Future Research 28. During the review, reviewers had adequate access to the Principal Investigators. 29. Information on the location and timing of the projects was adequate and easy to find. 30. The number of projects I was expected to review was:
4.1 4.2 3.9 3.9 4.4 1.9	4.4 4.3 4.2 4.4 4.7 2.7	3.9 4.0 4.2 4.3 3.0	 4 - Technology Transfer/Collaboration 5 - Proposed Future Research 28. During the review, reviewers had adequate access to the Principal Investigators. 29. Information on the location and timing of the projects was adequate and easy to find. 30. The number of projects I was expected to review was: Too Many
4.1 4.2 3.9 3.9 4.4 1.9 2.3	4.4 4.3 4.2 4.4 4.7 2.7 2.8	3.9 4.0 4.2 4.3 3.0 2.7	 4 - Technology Transfer/Collaboration 5 - Proposed Future Research 28. During the review, reviewers had adequate access to the Principal Investigators. 29. Information on the location and timing of the projects was adequate and easy to find. 30. The number of projects I was expected to review was: Too Many Too Few
4.1 4.2 3.9 3.9 4.4 1.9 2.3 4.0	4.4 4.3 4.2 4.4 4.7 2.7 2.8 4.7	3.9 4.0 4.2 4.3 3.0 2.7 3.9	 4 - Technology Transfer/Collaboration 5 - Proposed Future Research 28. During the review, reviewers had adequate access to the Principal Investigators. 29. Information on the location and timing of the projects was adequate and easy to find. 30. The number of projects I was expected to review was: Too Many Too Few About Right
4.1 4.2 3.9 3.9 4.4 1.9 2.3 4.0 3.8	4.4 4.3 4.2 4.4 4.7 2.7 2.8 4.7 4.3	3.9 4.0 4.2 4.3 3.0 2.7 3.9 3.6	 4 - Technology Transfer/Collaboration 5 - Proposed Future Research 28. During the review, reviewers had adequate access to the Principal Investigators. 29. Information on the location and timing of the projects was adequate and easy to find. 30. The number of projects I was expected to review was: Too Many Too Few About Right 31. The reviewers in your session had the proper mix and depth of credentials for the purpose of the review.
4.1 4.2 3.9 3.9 4.4 1.9 2.3 4.0	4.4 4.3 4.2 4.4 4.7 2.7 2.8 4.7	3.9 4.0 4.2 4.3 3.0 2.7 3.9	 4 - Technology Transfer/Collaboration 5 - Proposed Future Research 28. During the review, reviewers had adequate access to the Principal Investigators. 29. Information on the location and timing of the projects was adequate and easy to find. 30. The number of projects I was expected to review was: Too Many Too Few About Right

			meaningful review. (Additional comments are provided below.)
			 Subprogram overview presentations and materials did not have sufficient depth for review. The projects assigned to me were mostly well outside my areas of expertise. I can't recall if I gave info when registering as a reviewer regarding my background, but this could be helpful. Bring back the water!
			 The presentations were too short to put work in context. Maybe some reviewers should follow for years. Explanation of the questions within the criteria was often not appropriate for the work.
			 Also - time for our side meeting Monday morning was a half hour so all DOE folks attending the meeting were late.
			 Did not receive materials in advance. Should send user ID and password electronically, or send it much earlier. Inadequate time to access website prior to review because didn't get info in FEDEX package early enough due to travel. Especially important if feedback is needed on conflict of interest or overlapping review assignments. Good.
			 Having last year's presentation available to evaluate true progress was very helpful. Except for personal emergencies of a medical nature, PIs should present, not their grad students! I would tie future funding to that requirement.
			 I attended remotely- I can't comment on questions that can only be answered via physical attendance. I can't uncheck and leave anything blank. Since I was not a reviewer this should have been blank. I really hope that the DOE ceases the current problems in the auto industry to challenge experts especially outside private companies to get involved with innovative solutions.
			 I was not a reviewer. In many cases I agree with the above, although please see the comments I made before about the commercial presentations, some of which were frankly pathetic. The program is still too rushed for an in-depth review, but is much better than last year. N/A.
			 Review materials should have been available in advance via email / website. See earlier comments.
			• See previous comments about lack of focus by the presenters on remaining technical obstacles/barriersa candid assessment by the presenters concerning the status with respect to those barriers would help to provide a context for reviewing progress.
			 See previous section for comment. The criteria used for evaluation do not fit all projects (although I am aware that you must have standardized criteria). There should be at least on question to the effect "Do you think this project should continue to be supported?" You would get quite a few enthusiastic yes responses and a few enthusiastic no responses. The presentation scheme does not fit completely with the reviewing criteria.
			 The questions in this survey are poorly written as they assume I was a reviewer, even though the first question listed possible affiliations. The Relevance, Approach, and Technical Accomplishments should be more heavily weighted than the Collaborations and Future Work sections. Also, what's the point of scoring the Future Work category for projects
			 There should not be a "Not Applicable" option for these survey questions. I was not a reviewer, so many of these
			questions do not apply to me QUESTIONS FOR PRESENTERS ONLY
4.7	4.7	4.2	33. The request to provide a presentation for the review was provided sufficiently prior to the deadline for
			submission.
4.8	4.7	4.4	34. Instructions for preparing the presentation were sufficient.
4.8	4.3	4.1	35. The template for the presentation was helpful.
4.8	4.3	4.1	36. The PDF format provided adequate functionality for my presentation.
4.9	4.0	4.1	37. The time limit for my presentation was adequate to present the information needed by reviewers.
4.8	4.4	4.3	38. The audio and visual equipment worked properly and were adequate.
AE	4.6	2.0	39. The evaluation criteria upon which the review was organized were clearly defined and used appropriately.
4.5	4.6	3.8	1 – Relevance
4.5 4.6	4.7 4.6	4.0 4.0	2 – Approach 3 – Technical Accomplishments and Progress
4.0	4.0	3.8	4 – Technology Transfer/Collaboration
4.5	4.4	4.0	5 – Proposed Future Research
4.U	- .0	- - .0	40. Explanation of the questions within the criteria was clear and sufficient.
4.5	4.5	3.8	1 – Relevance
4.5	4.5	4.0	2 – Approach
4.7	4.5	4.1	3 – Technical Accomplishments and Progress
4.5	4.5	3.9	4 – Technology Transfer/Collaboration
4.6	4.5	4.0	5 – Proposed Future Research
			41. The right criteria and weightings were used to evaluate the project(s)/program.
4.6	4.5	3.8	1 – Relevance

4.6 4.	3.9	2 – Approach
4.6 4.6	3.9	3 – Technical Accomplishments and Progress
4.7 4.6	3.8	4 – Technology Transfer/Collaboration
4.5 4.5	3.9	5 – Proposed Future Research
4.2 4.2	3.7	42. During the review, presenters had adequate interaction with the reviewers.
4.4 4.0	3.9	43. Altogether, the preparatory materials, presentations, and the Question & Answer period provided sufficient depth of review. (Additional comments are provided below.)

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