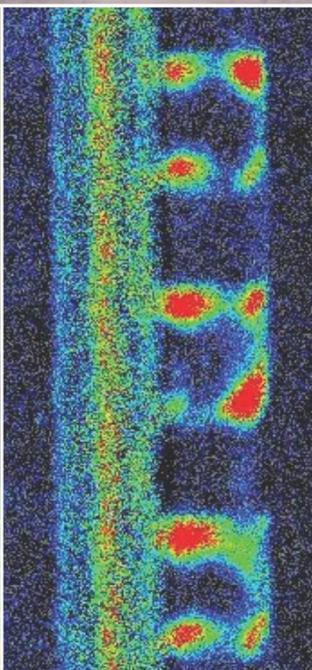
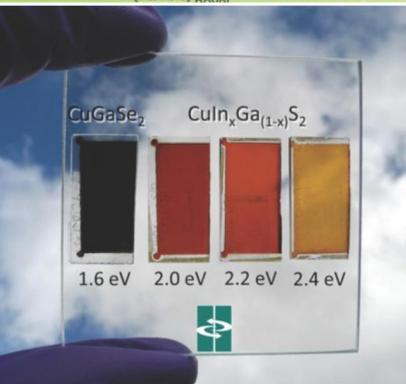
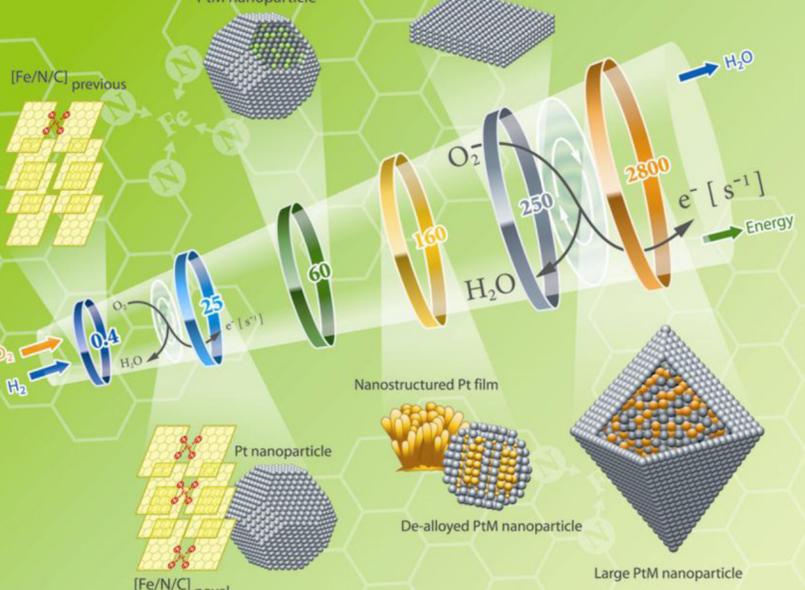


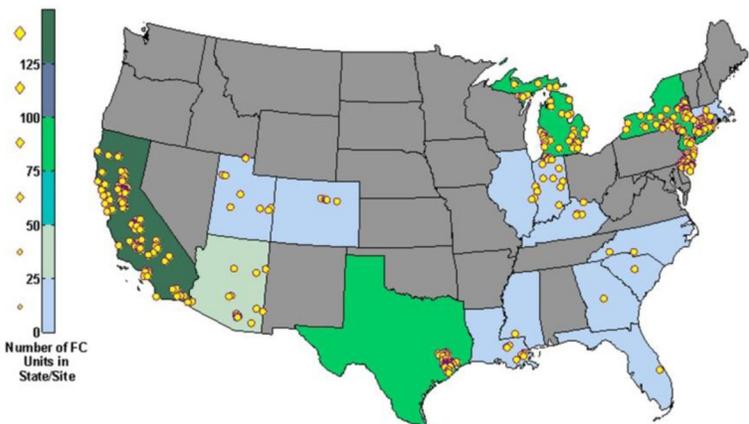
# U.S. DEPARTMENT OF ENERGY

## Hydrogen and Fuel Cells Program



## 2013 Annual Merit Review and Peer Evaluation Report

May 13–17, 2013  
Arlington, Virginia



## About the Cover

Photo collage (from top to bottom, left to right):

*Development of nanosegregated cathode catalysts with ultra-low platinum loading at Argonne National Laboratory (ANL). Image courtesy of ANL. (NREL 27573)*

*Bandgap tuning in copper chalcopyrite thin films for photoelectrochemical hydrogen production. Photo courtesy of the Hawai'i Natural Energy Institute. (NREL 27570)*

*A diaphragm compressor by PDC Machines. Photo courtesy of PDC Machines. (NREL 27575)*

*A Los Alamos National Laboratory (LANL)/Lawrence Livermore National Laboratory (LLNL)-developed hydrogen safety sensor operating in a convenient, easy-to-handle package. Photo courtesy of LLNL, LANL, and the National Renewable Energy Laboratory (NREL). (NREL 27571)*

*Neutron imaging at the National Institute of Standards and Technology (NIST) provided this high-resolution (~10 micron) image of membrane electrode assembly (MEA) water content to study fuel cell flooding and water-related degradation in catalyst layers. Photo courtesy of NIST. (NREL 27572)*

*Fuel cell backup power units deployed (Q1, 2009–Q4, 2012). Image courtesy of NREL.*

Photo on right:

*U.S. Capitol Building. Photo courtesy of [www.istockphoto.com](http://www.istockphoto.com).*

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**DOE/GO-102013-4177**

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## Prologue

Dear Colleague:

This document summarizes the comments provided by peer reviewers on hydrogen and fuel cell projects presented at the fiscal year (FY) 2013 U.S. Department of Energy (DOE) Hydrogen and Fuel Cells Program Annual Merit Review and Peer Evaluation Meeting (AMR), held in conjunction with the DOE's Vehicle Technologies Office AMR on May 13–16, 2013, in Arlington, Virginia. In response to direction from various stakeholders, including the National Academies, this review process provides evaluations of the Hydrogen and Fuel Cells Program's projects in applied research, development, demonstration, and analysis of hydrogen and fuel cells. A joint plenary session opened the meeting with a keynote address from Dr. David Danielson, Assistant Secretary for Energy Efficiency and Renewable Energy, followed by overview presentations from the Vehicle Technologies Office, the Fuel Cell Technologies Office (representing the Hydrogen and Fuel Cells Program), and the Basic Energy Sciences Program. A plenary for Hydrogen and Fuel Cells Program participants included overviews on each of eight program areas: Hydrogen Production and Delivery; Hydrogen Storage; Fuel Cells; Manufacturing R&D; Market Transformation; Technology Validation; Safety, Codes and Standards; and Systems Analysis.

DOE values the transparent, public process of soliciting technical input on projects from relevant experts. The recommendations of the reviewers are taken into consideration by DOE technology managers in generating future work plans. The table that follows lists the projects presented at the review, evaluation scores, and the major actions to be taken during the upcoming fiscal year (October 1, 2013–September 30, 2014). The projects have been grouped according to program area and reviewed according to appropriate evaluation criteria. The weighted scores for all of the projects are based on a four-point scale. To furnish principal investigators (PIs) with direct feedback, all of the evaluations and comments are provided to each presenter; however, the authors of the individual comments remain anonymous. The PIs are instructed by DOE to fully consider these summary evaluation comments, along with any other comments by DOE managers, in their FY 2014 plans. In addition, DOE managers contact each PI individually and discuss the comments and recommendations as future plans are developed.

In addition to thanking all participants of the AMR, I would like to express my sincere appreciation to the reviewers for your strong commitment, expertise, and interest in advancing hydrogen and fuel cell technologies. You make this report possible, and we rely on your comments, along with other management processes, to help make project decisions for the new fiscal year. We look forward to your participation in the FY 2014 AMR, which is presently scheduled for June 16–20, 2014, in Washington, D.C. Thank you for participating in the FY 2013 AMR.

Sincerely,



Sunita Satyapal  
Director  
Hydrogen and Fuel Cells Program  
U.S. Department of Energy

## Hydrogen Production and Delivery

Project Number	Project Title <i>Principal Investigator Name &amp; Organization</i>	Final Score	Continue	Discontinue/ Further Review	Completed or CDP*	Summary Comments
PD-014	Hydrogen Delivery Infrastructure Analysis <i>Marianne Mintz; Argonne National Laboratory</i>	3.6	X			Reviewers applauded the efforts of this analysis and noted the effective collaboration between national laboratory partners and industry. Recommendations included revising the modeling as updates are made to the H2A Delivery Scenario Analysis Model (HDSAM) and Hydrogen Analysis (H2A) models and to SAE J2601, expanding the analysis to include terminal costs for high-pressure tube trailer delivery, and increasing stakeholder input.
PD-022	Fiber Reinforced Composite Pipelines <i>Thad Adams; Savannah River National Laboratory</i>	3.4	X			Reviewers commended the progress in fatigue testing of pipeline materials and the collaboration with ASME. Reviewers recommended that testing be expanded to include higher temperatures and pressures and environmental stressors, and that results be documented in a peer-reviewed journal.
PD-025	Hydrogen Embrittlement of Structural Steels <i>Brian Somerday; Sandia National Laboratories</i>	3.4	X			Reviewers were impressed with the project's progress. More research into alternative welding methods and the impact of on-site welding was suggested. Reviewers also recommended accelerating the rate of progress and including cost analysis in the project.
PD-028	Solarthermal Redox-Based Water Splitting Cycles <i>Al Weimer; University of Colorado</i>	3.3	X			Reviewers praised the innovative approach to redox kinetics and materials selection for the isothermal hercynite cycle. They suggested that water vapor partial pressure effects, simultaneous O <sub>2</sub> and H <sub>2</sub> production, and prolonged high-temperature operation continue to be addressed. Reviewers also recommended that the packed bed reactor design and scale-up, as well as H2A analysis of cost and performance, receive more attention.
PD-035	Semiconductor Materials for Photoelectrolysis <i>Todd Deutsch; National Renewable Energy Laboratory</i>	3.1	X			Reviewers were impressed with this group's advancements in the durability of high-efficiency III-V photoelectrochemical (PEC) materials and devices through nitrogen ion surface treatments. They also commended the group for its strong collaboration with other researchers, especially in their leadership role with the PEC working group. There is some concern over the need to establish better reproducibility in the patent-pending surface treatment, and to test the efficiency and durability of the PEC devices under realistic on-sun conditions.

Project Number	Project Title <i>Principal Investigator Name &amp; Organization</i>	Final Score	Continue	Discontinue/ Further Review	Completed or CDP*	Summary Comments
PD-036	Maximizing Light Utilization Efficiency and Hydrogen Production in Microalgal Cultures <i>Tasios Melis; University of California, Berkeley</i>	3.3			X	Reviewers praised this project for being applicable to both algae and cyanobacteria and noted its applicability to areas outside of H <sub>2</sub> production. Reviewers recommend that the project provide more quantitative information, study stability and fitness of the strains under relevant conditions, reevaluate progress, and establish a target timeline in order to better determine future work. This project is fully funded and anticipated to end in January 2014.
PD-037	Biological Systems for Hydrogen Photoproduction <i>Maria Ghirardi; National Renewable Energy Laboratory</i>	3.3	X			Reviewers commended this project for successfully removing the native hydrogenase from green algae and adding an O <sub>2</sub> -tolerant clostridial hydrogenase, which allowed small amounts of H <sub>2</sub> to be produced in the presence of O <sub>2</sub> . The importance of this effort in meeting long-term goals for photobiological H <sub>2</sub> production was noted. Reviewers recommended increased collaboration as well as investigations of ways to increase H <sub>2</sub> production in the system and of the long-term performance of the mutant strain.
PD-038	Fermentation and Electrohydrogenic Approaches to Hydrogen Production <i>Pin-Ching Maness; National Renewable Energy Laboratory</i>	3.1	X			Reviewers commended the project's progress, including meeting milestones ahead of schedule. Most reviewers considered the collaborations productive and beneficial to technical progress in the project. Recommendations included consideration of alternative feedstocks and examination of practical and economic issues of the system design.
PD-039	Hydrogen from Water in a Novel Recombinant Oxygen-Tolerant Cyanobacterial System <i>Phil Weyman; J. Craig Venter Institute</i>	3.2			X	Reviewers remarked on the project's effective integration of multiple methods for improving H <sub>2</sub> evolution. Suggested areas for future consideration included system scaling and strain fitness under H <sub>2</sub> production conditions, and tests to examine protein folding and metabolic pathways, gene expression, and <i>in vitro</i> hydrogen evolution. The reviewers look forward to future work examining the H <sub>2</sub> production by intact cells. This project is fully funded and anticipated to end in January 2014.
PD-058	Characterization and Optimization of Photoelectrode Surfaces for Solar-to-Chemical Fuel Conversion <i>Tadashi Ogitsu; Lawrence Livermore National Laboratory/National Renewable Energy Laboratory</i>	3.5	X			Reviewers praised this project for providing critical theoretical modeling of III-V semiconductor interfaces under PEC operating conditions and for collaborating effectively with the DOE Office of Energy Efficiency and Renewable Energy PEC H <sub>2</sub> Production Working Group. Reviewers suggested that future research emphasize experimental efforts to validate the modeling, especially for the high-efficiency GaInP <sub>2</sub> PEC systems. Continued refinement of research and development priorities based on needs of the PEC research community is needed.

Project Number	Project Title <i>Principal Investigator Name &amp; Organization</i>	Final Score	Continue	Discontinue/ Further Review	Completed or CDP*	Summary Comments
PD-081	Solar Hydrogen Production with a Metal Oxide Based Thermochemical Cycle <i>Tony McDaniel; Sandia National Laboratories</i>	3.3	X			Reviewers commended the excellent work in materials design, evaluation of kinetics, analysis of performance requirements, and reactor design for a two-step reaction cycle. Reviewers felt that, in addition to the dish array configuration presented, a solar tower configuration should be modeled and analyzed. Reviewers also recommended that high-temperature reactor operation be tested, including the impact on particle attrition.
PD-088	Vessel Design and Fabrication Technology for Stationary High-Pressure Hydrogen Storage <i>Zhili Feng; Oak Ridge National Laboratory</i>	3.6	X			Reviewers noted this project's accomplishments and high potential to reach DOE targets for forecourt storage. Recommendations included more realistic capacity analysis for underground storage and a more robust cost analysis, including scaling of the storage vessel size. A suggested next step was planning for demonstration of the technology, including finding a project partner and location, and providing a clear design of the mock-up vessel.
PD-092	Rapid High Pressure LH2 Refueling for Maximum Range and Dormancy <i>Salvador Aceves; Lawrence Livermore National Laboratory</i>	3.1	X			Reviewers were interested in the accomplishments of this project and the potential benefits of pumping liquid hydrogen (LH2) into fuel cell vehicles. Future work should include a cost model and energy efficiency analysis of the process in order to determine the potential of the system for reaching DOE target goals. It was suggested that collaborations be extended to additional industry partners.
PD-094	Economical Production of Hydrogen through Development of Novel, High Efficiency Electrocatalysts for Alkaline Membrane Electrolysis <i>Katherine Ayers; Proton OnSite</i>	3.0	X			Reviewers praised the efforts of this early research, development, and demonstration Small Business Innovation Research (SBIR) project to reduce the capital cost of alkaline membrane electrolysis by using inexpensive catalyst materials. Reviewers suggested that H2A cost analysis of this technology should be performed and that more focus should be placed on membrane performance and durability issues.
PD-095	Probing Oxygen-Tolerant CBS Hydrogenase for Hydrogen Production <i>Pin-Ching Maness; National Renewable Energy Laboratory</i>	3.4	X			Reviewers commented positively on the project's approach, with multiple paths to address the O <sub>2</sub> -tolerance issue. They also noted the successful application of different methodologies and useful collaborations, as well as the need to integrate the results of the promoter-based gene expression work with the maturation gene identification. Suggestions for future work included testing of <i>in vivo</i> H <sub>2</sub> production by an organism with all of the improvements incorporated, and examination of potential issues such as protein folding.

\*Congressionally directed project (CDP)

## Hydrogen Storage

Project Number	Project Title <i>Principal Investigator Name &amp; Organization</i>	Final Score	Continue	Discontinue/ Further Review	Completed or CDP*	Summary Comments
ST-001	System Level Analysis of Hydrogen Storage Options <i>Rajesh Ahluwalia; Argonne National Laboratory</i>	3.3	X			The project is commended for good coordination with stakeholders and providing realistic system performance projections and data. The reviewers commented that the project can improve by highlighting areas of uncertainty in the models including input assumptions, as well as continue to compare modeling results with available physical testing data for model validation. Input assumptions for balance of plant of the compressed hydrogen storage system should be examined and updated. The reviewers also recommended that the project examine modeling results with regard to sensitivities to fiber winding model assumptions.
ST-004	Hydrogen Storage Engineering Center of Excellence <i>Don Anton; Savannah River National Laboratory</i>	3.6	X			This project is part of the Hydrogen Storage Engineering Center of Excellence (HSECoE, Center). Overall, reviewer sentiment was very positive acknowledging all aspects of the project including management, engineering development, and effective collaboration. The reviewers noted that the Center approach has proven much more successful than if the tasks were attempted by individual partners and specifically that communication among Center participants were very well coordinated. The reviewers acknowledged that the Center has done a great job in addressing material behavior and component design, and in developing models to project system performance that will add value to the research community. Interest was expressed about knowing the results of the recent go/no-go decisions for the transition to Phase III and a more detailed Phase III technical plan.
ST-005	Systems Engineering of Chemical Hydrogen, Pressure Vessel, and Balance of Plant for Onboard Hydrogen Storage <i>Jamie Holladay; Pacific Northwest National Laboratory</i>	3.3	X			This project is part of the HSECoE. Overall, the reviewers praised the various contributions of the project toward the success of the Center. The reviewers commented that while quality work had been accomplished on slurry development and modeling of reactor designs, those materials will likely be nonstarters for automotive applications and emphasis should be placed on non-slurried liquid fuel forms or pressure vessel designs for cryogenic applications. The reviewers indicated that the work on friction stir welding and dynamic cost modeling could have significant impacts outside of the HSECoE as well.

Project Number	Project Title <i>Principal Investigator Name &amp; Organization</i>	Final Score	Continue	Discontinue/ Further Review	Completed or CDP*	Summary Comments
ST-006	Advancement of Systems Designs and Key Engineering Technologies for Materials Based Hydrogen Storage <i>Bart van Hassel; United Technologies Research Center</i>	3.3	X			This project is part of the HSECoE. The reviewers found the approach of the project to be well formulated and addresses several important issues including gas-liquid separations, impurity mitigation and risk abatement, that are key to the successful implementation of hydrogen storage systems. While the reviewers appreciated the relevance of the work and found the collaborations to be managed effectively, some commented that more specific details on future technical tasks were needed for complete evaluation. Additionally, the reviewers noted that the plan forward should consider a contingency to translate the work to alternative materials or systems during Phase III.
ST-007	Chemical Hydrogen Rate Modeling, Validation, and System Demonstration <i>Troy Semelsberger; Los Alamos National Laboratory</i>	3.2	X			This project is part of the HSECoE. The reviewers found the general approach to be effective in evaluating the practical performance of the various system designs considered. The reviewers agreed that the project showed significant progress, especially toward reactor designs and fuel purification, that will be valuable for the research community; however, they also commented that more focus should have been maintained on materials with a simpler regeneration route or that remained a liquid through desorption. Overall, the reviewers found that the project demonstrated good collaborations within the Center and most noted that a more detailed plan for the future would have been useful to completely evaluate the project.
ST-008	System Design, Analysis, Modeling, and Media Engineering Properties for Hydrogen Energy Storage <i>Matthew Thornton; National Renewable Energy Laboratory</i>	3.3	X			This project is part of the HSECoE. The reviewers commended the principal investigator (PI) for the thorough discussion of the approach and noted that vehicle level modeling is a critical piece for validating hydrogen storage systems. It was suggested that a sensitivity analysis be performed between vehicle powertrains to observe any changes in storage system requirements. The reviewers also commented that the project seems to show good coordination within the Center and other U.S. Department of Energy (DOE)/original equipment manufacturer efforts and deliver timely results for the level of funding.

Project Number	Project Title <i>Principal Investigator Name &amp; Organization</i>	Final Score	Continue	Discontinue/ Further Review	Completed or CDP*	Summary Comments
ST-009	Thermal Management of Onboard Cryogenic Hydrogen Storage Systems <i>Mei Cai; General Motors</i>	3.0	X			This project is part of the HSECoE. Overall, the reviewers thought the approach of modeling coupled with experimental validation of thermal management was adequate, but they also thought that more emphasis should have been placed on expediting results. The reviewers maintained that the project is of high value to developing a prototype system and a clear plan for transferring this effort is critical to further success. The reviewers found the results on the influence of particle size and shape on charge/discharge to be valuable, especially for future material efforts. There was concern among the reviewers about the communication of the knowledge base from this project to the Center and public and the transfer of technology developed within this project because it was not clearly discussed.
ST-010	Ford/BASF-SE/UM Activities in Support of the Hydrogen Storage Engineering Center of Excellence <i>Mike Veenstra; Ford Motor Company</i>	3.4	X			This project is part of the HSECoE. Overall, reviewers were impressed with the project's accomplishments, which included fuel cell modeling, supporting cost studies, leading the failure modes and effects analysis, materials evaluation, and serving as system architect; all of these were noted as important to the overall success of the HSECoE. Reviewers also noted the importance of the involvement of a major automobile manufacturer in providing a "real-world" perspective of these efforts. The only potential concern noted was related to the HSECoE's decision to focus on metal organic framework-5 (MOF-5), which cannot meet DOE's targets. It was therefore unclear to the reviewers how representative this material may be for a full range of sorbent materials.
ST-019	Multiply Surface-Functionalized Nanoporous Carbon for Vehicular Hydrogen Storage <i>Peter Pfeifer; University of Missouri</i>	2.2		X		The reviewers noted that boron doping resulted in an increase in binding energy. However, they also pointed out the limitations of this approach as increasing amounts of boron may also result in reduced surface area and the formation of boron oxide, all of which can negatively impact hydrogen uptake. As a result, reviewers questioned the ability of boron-doped materials to meet the DOE targets. The reviewers were pleased that Missouri was working with the National Renewable Energy Laboratory to validate its capacity results, but they also noted that a single validation on a less-than-optimal sample does not necessarily validate past results. Finally, the reviewers were disappointed in the progress of this project over the last year and, as a result, questioned if the project should be moving ahead with monolith development.

Project Number	Project Title <i>Principal Investigator Name &amp; Organization</i>	Final Score	Continue	Discontinue/ Further Review	Completed or CDP*	Summary Comments
ST-021	Weak Chemisorption Validation <i>Thomas Gennett; National Renewable Energy Laboratory</i>	3.3			X	The reviewers acknowledged the thorough work of the international team to provide definitive studies on “spillover” in carbon adsorbents. While they noted discernible spectroscopic signatures from a unique C-H interaction, no technologically significant uptake at room temperature was observed. The reviewers noted the important value of this validation effort that has provided definitive evidence of spillover, while also indicating it may not lead to any significant enhancement of room-temperature adsorption.
ST-024	Hydrogen Trapping through Designer Hydrogen Spillover Molecules with Reversible Temperature and Pressure-Induced Switching <i>Angela Lueking; Pennsylvania State University</i>	2.2		X		Overall, the reviewers did give credit to the researcher for trying to characterize and demonstrate room-temperature hydrogen storage in MOFs via spillover, but they noted that not only has the project fallen well short of its goal of achieving 3 wt.% hydrogen storage, there is a high likelihood that hydrogen storage via the spillover mechanism will meet the DOE targets. This project is currently operating on a no-cost time extension and additional funding is pending a go/no-go review.
ST-028	Design of Novel Multi-Component Metal Hydride-Based Mixtures for Hydrogen Storage <i>Christopher Wolverton; Northwestern University</i>	2.5		X		In general the reviewers acknowledged the project’s strengths in computational expertise, but they found the experimental contributions to be lacking. Reviewers were happy to see that the project team implemented the reviewers’ recommendation from last year’s DOE Hydrogen and Fuel Cells Program (the Program) Annual Merit Review to add nuclear magnetic resonance characterization efforts to the project. However, the reviewers do not see promise in the hydride systems under investigation in terms of practical use for hydrogen storage applications.
ST-044	SRNL Technical Work Scope for the Hydrogen Storage Engineering Center of Excellence: Design and Testing of Adsorbent Storage Systems <i>David Tamburello; Savannah River National Laboratory</i>	3.2	X			This project is part of the HSECoE. The reviewers commented that the approach was well designed and the comprehensive parametric modeling would add significant value to the research community. The reviewers noted that excellent progress had been made on developing an acceptability envelope that integrated material and engineering properties; however, they also noted that several key barriers remained such as loss of usable hydrogen, and volumetric and gravimetric capacities. They acknowledged that this project demonstrated good collaborations across the Center. Finally, the reviewers suggested that a more detailed listing of risks and challenges, as well as forecourt implications, should be provided to determine critical focus areas going forward.

Project Number	Project Title <i>Principal Investigator Name &amp; Organization</i>	Final Score	Continue	Discontinue/ Further Review	Completed or CDP*	Summary Comments
ST-046	Microscale Enhancement of Heat and Mass Transfer for Hydrogen Energy Storage <i>Kevin Drost; Oregon State University</i>	3.0	X			This project is part of the HSECoE. The reviewers acknowledged that the approach of combined simulation and experimental investigations to optimize the design of the Modular Adsorbant Tank Insert (MATI) and the Microchannel Recuperator Heat Exchanger is well conceived. Also, the use of MATI to increase media conductivity is very relevant to the goals of the HSECoE. The reviewers noted that it was not apparent that the system could be scaled to deliver 0.02 g/s/kW to an automotive-scale fuel cell and suggested that scaled testing is needed. The reviewers also suggested a focus on understanding the benefits or trade-offs to/with other cryo-adsorption media because the surrogate material (MOF-5) is unlikely to meet DOE targets.
ST-047	Development of Improved Composite Pressure Vessels for Hydrogen Storage <i>Norman Newhouse; Hexagon Lincoln</i>	3.3	X			This project is part of the HSECoE. Generally, the reviewers considered this project to be a critical aspect of the engineering effort and found Hexagon Lincoln to have the prescribed expertise. They noted that the approach was well thought out; however, they also noted that more data on cryogenic testing of liner and composite materials was needed to support continued efforts on Type 4 tanks. The reviewers acknowledged the switch from Type 4 to Type 1 tanks and thought that this would overcome several of the challenges associated with material's loading and cryogenic operation. The reviewers did note that material loading, sealing, and cryogenic operation of the tank are crucial pieces for the success of the sorbent system.
ST-052	Best Practices for Characterizing Engineering Properties of Hydrogen Storage Materials <i>Karl Gross; H2 Technology Consulting LLC</i>	3.6			X	The reviewers uniformly complimented the continuing effort in documenting methods used to characterize the hydrogen capacity, reaction kinetics, thermal properties, and other engineering parameters necessary to develop materials with the potential of meeting the corresponding DOE performance parameters. They acknowledged the magnitude of the effort and the excellent progress in this work that has incorporated input from experts in the field. The reviewers are interested in having this document finalized with perhaps an update to earlier chapter references.

Project Number	Project Title <i>Principal Investigator Name &amp; Organization</i>	Final Score	Continue	Discontinue/ Further Review	Completed or CDP*	Summary Comments
ST-053	Life Cycle Verification of Polymer Liners in Storage Tanks <i>Barton Smith; Oak Ridge National Laboratory</i>	2.7		X		The reviewers considered the testing methodology to be effective; however, they noted the lack of progress in reporting permeation results due to many experimental equipment challenges. The reviewers suggested collaborations with tank manufacturers and high-pressure equipment manufacturers to overcome the experimental challenges with sample sealing and temperature control. It was also noted that the project should address liner/composite interactions (delamination) as well as other failure mechanisms such as liner buckling in addition to permeation.
ST-063	Electrochemical Reversible Formation of Alane <i>Ragaiy Zidan; Savannah River National Laboratory</i>	3.4	X			The reviewers commended the progress the project has made over the past year in closed cycle generation from MAIH <sub>4</sub> , increases in reaction efficiency, and separation of AlH <sub>3</sub> product. The development of the Cooperative Research and Development Agreement (CRADA) with a commercialization partner and involvement of key collaborators was viewed as very positive. The reviewers suggested that feedback from system analysis to focus priorities might be helpful, considering the limited resources available.
ST-093	Melt Processable PAN Precursor for High-Strength, Low-Cost Carbon Fibers <i>Felix Paulauskas; Oak Ridge National Laboratory</i>	3.4	X			Reviewers commended the project for demonstrating the feasibility of the melt-spun precursor fiber production process. Reviewers commented that the project should shift to further demonstrate the technology using polyacrylonitrile-methyl acrylate (PAN-MA) rather than polyacrylonitrile-vinyl-acetate (PAN-VA) that does not have the properties to produce the necessary high-grade carbon fiber. The reviewers also commented that the project needs to develop a cost model to assess potential cost savings.
ST-098	Development of a Practical Hydrogen Storage System based on Liquid Organic Hydrogen Carriers and a Homogeneous Catalyst <i>Craig Jensen; Hawaii Hydrogen Carriers, LLC</i>	2.8			X	Overall the reviewers commented favorably in terms of the approach and collaboration between the team members. Specific project strengths cited included using the cost of the material as a primary filter for material investigation, and the low catalyst loading of the system (100 ppm). The reviewers felt there was a lack of progress in the past year and emphasized that the DOE targets could not be met with this system. However it was noted that this approach to hydrogen storage could benefit the near-term market strategies of the DOE Office of Energy Efficiency and Renewable Energy (EERE).

Project Number	Project Title <i>Principal Investigator Name &amp; Organization</i>	Final Score	Continue	Discontinue/ Further Review	Completed or CDP*	Summary Comments
ST-099	Development of Low-Cost, High-Strength Commercial Textile Precursor (PAN-MA) <i>Dave Warren; Oak Ridge National Laboratory</i>	3.1	X			Reviewers commented that this is an important project with a good approach to reducing precursor fiber cost. The reviewers commended the project for making good progress, but they recommended identifying specific quantifiable causes and effects to facilitate the progress in optimizing the precursor formulations and conversion process. Reviewers expressed concern that the textile precursor developer was recently purchased by a foreign carbon fiber producer and over the need to identify other available low-cost precursor fiber sources. Reviewers noted that an updated cost analysis to identify potential cost savings is needed.
ST-100	Hydrogen Storage Cost Analysis <i>Brian James; Strategic Analysis, Inc.</i>	3.4	X			Reviewer commended the PI for improving the overall compressed H <sub>2</sub> storage system layout to be more reflective of real-world systems. Reviewers commented that the compressed H <sub>2</sub> storage system cost analysis can be improved by including further cost details on balance of plant (BOP) components and conducting sensitivity analysis to highlight key cost drivers within the tank and BOP. These could include the effects of design assumptions such as pressure and burst factors. It was recommended that the project examine sensitivity to economy of scale, such as learning rate, and carbon fiber pricing.
ST-101	Enhanced Materials and Design Parameters for Reducing the Cost of Hydrogen Storage Tanks <i>Kevin Simmons; Pacific Northwest National Laboratory</i>	3.2	X			Reviewers commended the approach of establishing the validated performance and cost estimator model. Reviewers also commended the broad collaboration that includes key tank manufacturers. Reviewers commented that the project should next focus on determining the optimum compressed H <sub>2</sub> storage operating temperature and pressure for optimized performance to bridge the large gap toward the cost-saving goal of the project.
ST-102	Room Temperature Hydrogen Storage in Nano-Confined Liquids <i>John Vajo; HRL Laboratories, LLC</i>	3.3		X		Even though the experimental results have been negative and have not shown enhanced hydrogen storage using nano-confined liquids, the reviewers commended the excellent experimental methods and high quality of research exhibited by the project. The reviewers felt the computational effort could be strengthened and would recommend the project be discontinued if no evidence of solubility enhancement can be demonstrated by the end of Phase 1.

Project Number	Project Title <i>Principal Investigator Name &amp; Organization</i>	Final Score	Continue	Discontinue/ Further Review	Completed or CDP*	Summary Comments
ST-103	Hydrogen Storage in Metal-Organic Frameworks <i>Jeffrey Long; Lawrence Berkeley National Laboratory</i>	2.8	X			The reviewers acknowledged the highly qualified team with members that bring synthesis, modeling, structural characterization, and hydrogen uptake measurement efforts to this work. They point out that Co and Ni analogues have shown high binding energy at low coverage but drop to typical values at higher coverage. The reviewers were divided in their assessment of the need for high-pressure (350 bar) measurements, because the goal of the Program's adsorbent research has been to find a material suitable for low-pressure (100 bar) storage. Future work should address both mass and volume metrics.
ST-104	Novel Carbon(C)-Boron(B)-Nitrogen(N)-Containing Hydrogen Storage Materials <i>Shih-Yuan Liu; University of Oregon</i>	3.1	X			The reviewers commended the project for the integration of computational and experimental efforts while incorporating fuel cell testing to identify potential issues. The reviewers recommended that the project identify material with higher capacity, as well as identify material impurities under fuel cell operating conditions. The reviewers also recommended further investigation of material intrinsic degradation and thermal stability as well as consideration of spent fuel regeneration complexity of fuel blends before expending extensive material development effort.
ST-107	The Quantum Effects of Pore Structure on Hydrogen Adsorption <i>Raina Olsen; Oak Ridge National Laboratory</i>	3.2			X	The reviewers note the generally sound approach directed toward addressing DOE barriers in storage capacity. An improvement in strengthening the link between experiment and theory was suggested, especially given the hypothesis of hydrogen as a Bose Einstein Condensate in a specially configured pore. The inelastic neutron results show some features that are consistent with the proposed structures, but reviewers felt that the data are not fully convincing. An isotope mix was suggested by the reviewers to confirm the effect.
ST-108	Metallation of Metal-Organic Frameworks: En Route to Ambient Temperature Storage of Molecular Hydrogen <i>Joseph Mondloch; Northwestern University</i>	2.3			X	The reviewers noted that this presentation was a post-doctoral research grant effort to examine two approaches to metallization of coordination polymers (via atomic layer and solution deposition). As an exploratory effort, it was recognized that little progress was made in addressing EERE barriers, given the challenge of post-synthesis metallization, but that "negative results" are of value to the community. A clearer articulation of proposed future work would have been of value.

\*Congressionally directed project (CDP)

## Fuel Cells

Project Number	Project Title <i>Principal Investigator Name &amp; Organization</i>	Final Score	Continue	Discontinue/ Further Review	Completed or CDP*	Summary Comments
FC-006	Durable Catalysts for Fuel Cell Protection During Transient Conditions <i>Radoslav Atanasoski; 3M</i>	3.3	X			Reviewers commented that significant accomplishments and progress have been made toward objectives and overcoming the durability barriers. 3M demonstrated that relatively low catalyst loading (0.029 mg/cm <sup>2</sup> ) can inhibit oxygen reduction reaction (ORR) activity on the anode, and the ORR inhibition has been verified in stack testing. 3M showed that improved cathode protection of 40%–50% during start-up/shutdown over the baseline oxygen evolution reaction (OER) catalyst was attained, and the OER catalyst did not impact the overall fuel cell performance.
FC-007	Extended, Continuous Platinum Nanostructures in Thick, Dispersed Electrodes <i>Bryan Pivovar; National Renewable Energy Laboratory</i>	3.1	X			Reviewers noted that the project has generated some novel catalytic materials with good specific and mass activities. These results show that higher specific activities can be achieved with Pt nanoparticles than had been anticipated. Reviewers also noted the excellent progress in developing new methods to fabricate extended thin-film electrocatalyst structures. However, reviewers noted that progress in membrane electrode assembly (MEA) performance has been disappointing, and that it is doubtful that the MEA performance targets can be met unless this project is extended.
FC-008	Nanosegregated Cathode Catalysts with Ultra-Low Platinum Loading <i>Nenad Markovic; Argonne National Laboratory</i>	3.5	X			Reviewers noted that Argonne National Laboratory (ANL) has met all 2015 U.S. Department of Energy (DOE) targets with respect to catalyst activities and durability, though only in rotating disk electrode (RDE) testing and not in an MEA. Reviewers felt that the technical work has been very thorough. With respect to the mesostructured thin films, reviewers wondered what the stability of the single crystal alloy surface would be after cycling. They felt that the next hurdle is scale-up and determining whether the impressive performance transfers into a fuel cell.
FC-009	Contiguous Platinum Monolayer Oxygen Reduction Electrocatalysts on High-Stability, Low-Cost Supports <i>Radoslav Adzic; Brookhaven National Laboratory</i>	3.5	X			Reviewers noted that Brookhaven National Laboratory is working on very promising catalyst materials, as evidenced by the licensing and scale-up of the core-shell catalysts to N.E. CHEMCAT. They also noted that the Pt nanospheres and the Pt on PdAu nanowires are promising concepts to get to high mass activity, though the true test will be in a fuel cell under realistic load cycling. Several reviewers questioned the use of electrodeposition for catalysts because this technique is quite challenging. Reviewers recommended more work on H <sub>2</sub> /air as well as new work on the possible impacts of contaminants and water management, transport, and ionomer aspects with these new catalysts.

Project Number	Project Title <i>Principal Investigator Name &amp; Organization</i>	Final Score	Continue	Discontinue/ Further Review	Completed or CDP*	Summary Comments
FC-010	The Science and Engineering of Durable Ultra-Low PGM Catalysts <i>Mahlon Wilson; Los Alamos National Laboratory</i>	2.7		X		Reviewers noted that the Pt-PPy nanowire catalyst work was interesting, but that the performance was below the C-based baseline catalyst. They thought that the project included too many different approaches and more materials should be down-selected. They felt that the ceria work is more focused on membrane stability and has little to do with other parts of the project.
FC-013	Durability Improvements through Degradation Mechanism Studies <i>Rod Borup; Los Alamos National Laboratory</i>	3.1	X			Reviewers stated that the approach covers all fuel cell components and the most degrading modes of operation. Reviewers felt that good progress was made in understanding the electrode and membrane degradation, but much less understanding was achieved regarding superimposing factors, specifically how the degradation of one component accelerates the degradation of other components. Reviewers felt that there was too much emphasis on carbon corrosion and they wanted more mitigation recommendations.
FC-014	Durability of Low-Platinum Fuel Cells Operating at High Power Density <i>Scott Blanchet; Nuvera Fuel Cells</i>	3.0			X	Reviewers stated that this project has strong interaction between collaborators, but one reviewer noted it does not include an automotive system integrator. The project was commended for its combined model/experimental approach such that real data and theoretical understanding are both contributing to the outcome and achievements of the project. The use of different cycles—from voltage, load, and drive cycles—is very valuable in establishing the linkage between accelerated stress tests (ASTs) and the real-world linkage to stacks in the field. The accomplishment of the model verification using an electrochemical impedance spectroscopy-based parameter determination approach in order to simulate the AST/performance of the various cell configurations was also commended. Results from the completed project should be used to guide future work.
FC-016	Accelerated Testing Validation <i>Rangachary Mukundan; Los Alamos National Laboratory</i>	3.3	X			Reviewers felt that the approach to achieving the durability technical target is sound and well designed. Reviewers noted the excellent progress toward objectives, specifically identifying how many cycles of accelerated testing correlate to hours of operation of various applications. Several reviewers suggested testing the ASTs on state-of-the-art MEAs, with the caveat that those state-of-the-art MEAs will not have 5,000+ hours of service.

Project Number	Project Title <i>Principal Investigator Name &amp; Organization</i>	Final Score	Continue	Discontinue/ Further Review	Completed or CDP*	Summary Comments
FC-017	Fuel Cells Systems Analysis <i>Rajesh Ahluwalia; Argonne National Laboratory</i>	3.5	X			Reviewers felt that the approach taken was sound. The collaborative work with Ford, 3M, W.L. Gore, and dPoint was commended by the reviewers. Reviewers suggested extending the modeling from high pressure to lower pressure, examining other catalysts besides nanostructured thin film (NSTF), and verifying stack-related performance with actual stack data.
FC-018	Fuel Cell Transportation Cost Analysis <i>Brian James; Strategic Analysis, Inc.</i>	3.6	X			The reviewers agreed with the well-defined assumptions used and the cost estimate methodology, which is widely accepted by industry. FY 2013 data confirm earlier results but with consideration of new components, including quality control. Reviewers were concerned that representative performance characteristics derived from one MEA did not match the newer MEA manufacturing method that was analyzed for cost. Strong collaboration with the ANL fuel cell system model team and industry could enable the necessary performance characterization.
FC-020	Characterization of Fuel Cell Materials <i>Karren More; Oak Ridge National Laboratory</i>	3.6	X			The project's strengths are clearly attributed to the Oak Ridge National Laboratory team's continuous efforts to improve its tools and analysis capabilities; engaging with strong and numerous partners from industry, universities, and national laboratories; outstanding experimental proficiency in imaging; and openness to sharply focus on the requirements of fuel cell development. Reviewers gave this project a perfect score of 4.0 for "Collaborations" and for "Relevance/Impact." This work provides significant contributions to understanding degradation mechanisms. The targeted components such as catalyst nanoparticles, polymers, catalyst support materials, MEAs, etc. are the most important ones for longevity and cost reduction. The research contributes to the most important targets: durability and performance. Reviewers recommend including research for understanding the compression effect of the electrodes during operation, interfacial aspects between the electrode and the membrane, and more comparisons of results to realistic operational conditions.

Project Number	Project Title <i>Principal Investigator Name &amp; Organization</i>	Final Score	Continue	Discontinue/ Further Review	Completed or CDP*	Summary Comments
FC-021	Neutron Imaging Study of Water Transport in Operating Fuel Cells <i>Muhammad Arif; National Institute of Standards and Technology</i>	3.4	X			Reviewers felt that the ability to visualize total water content under operation is a highly valuable tool in correlating observed performance and durability effects to cell design. Reviewers noted that the collaboration of the National Institute of Standards and Technology with many other partners was highlighted and appreciated by other principal investigators (PIs) during the DOE Hydrogen and Fuel Cells Program Annual Merit Review. They noted that significant progress had been made in improving resolution and that the analysis of error and accuracy is important in interpreting results. Several reviewers were interested in whether neutron imaging could be used for stack diagnosis.
FC-026	Fuel Cell Fundamentals at Low and Subzero Temperatures <i>Adam Weber; Lawrence Berkeley National Laboratory</i>	2.7		X		Reviewers stated that the approach is systematic and involves substantial experimentation and modeling efforts to elucidate an understanding of transport phenomena and water/thermal management at low and subzero temperatures. They felt the relevance, future work, and collaborations were quite strong; however, they felt the approach and accomplishments were lacking. Suggestion for improvements included eliminating the membrane morphology portion, including an automotive system integrator perspective, considering non-NSTF materials, and integrating the individual component models into an MEA performance model.
FC-036	Dimensionally Stable High Performance Membranes <i>Cortney Mittelsteadt; Giner, Inc./Giner Electrochemical Systems, LLC</i>	3.1	X			Three viable pathways were investigated for developing dimensionally stable membranes (DSMs): inversion casting, ultraviolet microreplication, and mechanical methods. Reviewers stated that the project has a good plan, strong partnering, a logical approach, and promising test results. However, they felt the project needs a more detailed cost analysis to demonstrate the viability of the proposed manufacturing methods, deeper stress and swelling analysis, and focus on demonstrating DSM performance and durability before further support and fabrication optimization. This former Small Business Innovation Research project began its third and final phase in July 2013 to continue scale-up of its most promising fabrication process.

Project Number	Project Title <i>Principal Investigator Name &amp; Organization</i>	Final Score	Continue	Discontinue/ Further Review	Completed or CDP*	Summary Comments
FC-044	Engineered Nano-Scale Ceramic Supports for PEM Fuel Cells <i>Eric Brosha; Los Alamos National Laboratory</i>	2.7		X		Reviewers noted that Los Alamos National Laboratory has identified promising ceramic material based on molybdenum; however, the performance of this material needs further improvement. Reviewers suggest that cyclic voltammograms (CVs) of these materials should be presented, test conditions for cycling should be given, CO stripping should be used to investigate electrochemical surface area, and mass activities should be presented before and after cycling.
FC-048	Effect of System Contaminants on PEMFC Performance and Durability <i>Huyen Dinh; National Renewable Energy Laboratory</i>	2.9	X			Reviewers commended the project for the amount of data generated and mechanism identified. The study of contaminant mixtures and inclusion of the effect of catalyst loading on the results were also commended. Reviewers gave positive comments regarding the new website. It was recommended that some of the results be reproduced on a large cell or stack scale. One reviewer recommended that rather than developing a universal model to explain voltage loss, the team should focus on how to recover the performance of fuel cells by looking at “classes” of contaminants, and categorizing their introduction to the fuel cell as reversible or non-reversible. It was also suggested to identify additives that are strong contaminants.
FC-052	Technical Assistance to Developers <i>Tommy Rockward; Los Alamos National Laboratory</i>	3.0	X			Reviewers stated that the work appears to be serving a useful and accessible function of sharing technical assistance to developers through fuel cell and material characterization and technical assistance. They also stated that the PI exhibited a wide range of characterization results, from FTIR and relative humidity degradation characterization of membranes to fuel cell performance of gas diffusion layers (GDLs) to water imaging across the membrane. They noted that the list of “clients” is comprehensive, including automotive original equipment manufacturers (OEMs), laboratories, universities, materials and equipment suppliers, and technical institutes. The reviewers would like to see more in the way of proposed future work such as surveying the stakeholders for their inputs on what is most useful in existing technical support and what could be most useful but is currently lacking.

Project Number	Project Title <i>Principal Investigator Name &amp; Organization</i>	Final Score	Continue	Discontinue/ Further Review	Completed or CDP*	Summary Comments
FC-054	Transport in PEMFCs <i>Cortney Mittelsteadt; Giner, Inc./Giner Electrochemical Systems, LLC</i>	2.7			X	By widely varying the transport and structural properties of fuel cell components (mainly membranes), this project seeks to come up with guiding design principles and transport models for fuel cell component development. Reviewers stated that the approach and collaborations (Virginia Tech and the University of South Carolina) were very good. However, the impact and proposed future work were lacking, in that it was unclear how the model and data would be disseminated and used by industrial developers. Also, the relevance is difficult to assess because it may only indirectly assist in improving fuel cell performance, cost, and durability. This project ends in October 2013.
FC-063	Novel Materials for High Efficiency Direct Methanol Fuel Cells <i>David Mountz; Arkema</i>	2.4			X	Reviewers felt the objective, approach, and expertise of the prime contractor were good, but that the execution and final product were not delivered. The new membrane material did not perform significantly better than the perfluorosulfonic acid (PFSA) membrane, and the Pd-based cathode catalysis portion of the project was not successful in reducing costs and improving performance. This project ends in September 2013.
FC-065	The Effect of Airborne Contaminants on Fuel Cell Performance and Durability <i>Jean St-Pierre; Hawai'i Natural Energy Institute</i>	3.2	X			Reviewers stated that the approach is good, straightforward, and based on down-selecting from various contaminants. They noted that the use of low-loaded catalysts (0.1 mg Pt/cm <sup>2</sup> ) is a major improvement and that the addition of cleaning agents and coolants to the contaminants list is appropriate. Reviewers would like to see data showing mitigation/restoration to 90% of cell performance for the seven contaminants for which this has been completed, and information on the mitigation/restoration strategies used for the contaminants.
FC-077	Large Scale Testing, Demonstration, and Commercialization of Fuel Cell Coolant (SBIR Phase III) <i>Satish Mohapatra; Dynalene</i>	2.8			X	Reviewers commented on the innovative use of nanoparticles for improved coolant. Reviewers recommended understanding the effect of the coolants on structural plastics and other materials that may be used in automotive fuel cell systems, as well as full-scale field testing at high voltage in a relevant system. This project ends in October 2013.

Project Number	Project Title <i>Principal Investigator Name &amp; Organization</i>	Final Score	Continue	Discontinue/ Further Review	Completed or CDP*	Summary Comments
FC-081	Fuel Cell Technology Status - Voltage Degradation <i>Jennifer Kurtz; National Renewable Energy Laboratory</i>	2.7		X		Many reviewers commended the project for its collaboration and stated that the information gathered was treated with considerable analytical prowess. They also remarked that the project has been a public source for fuel cell durability information. Reviewers expressed concern over the inconsistent conditions under which hours were accumulated and wondered if data sets with similar conditions could be reported separately. The FY 2014 project will focus on cost/price status versus durability status. Each year the project will rotate between durability status and cost/price status.
FC-083	Enlarging Potential National Penetration for Stationary Fuel Cells through System Design Optimization <i>Chris Ainscough; National Renewable Energy Laboratory</i>	3.4	X			Reviewers noted that their comments from last year's review were addressed and gave the project favorable reviews. The reviewers commended the inclusion of the Commercial Buildings Energy Consumption Survey (CBECS) and user groups for industry feedback. The reviewers indicated that the National Renewable Energy Laboratory (NREL) is developing a valuable tool to model the applicability of fuel cell combined heat and power systems for various building types around the country. It was recommended that proper model validation be performed.
FC-084	WO <sub>3</sub> and HPA Based Systems for Durable Platinum Catalysts in PEMFC Cathodes <i>John Turner; National Renewable Energy Laboratory</i>	2.7		X		Reviewers noted the good, productive collaborations with industry, national laboratories, and universities, and that experts were utilized on the materials investigated. Reviewers also commented on the relevance of this project. However, reviewers were disappointed with the results. Due to the low electronic conductivity of WO <sub>x</sub> and consequent low activity of Pt/WO <sub>x</sub> catalysts, no further work will be conducted in this area. Future work will use alternative nitride and carbide supports as well as the heteropoly-acid (HPA)-modified graphitized carbons in an attempt to meet the DOE targets. This project will be completed in early 2014.
FC-085	Synthesis and Characterization of Mixed-Conducting Corrosion Resistant Oxide Supports <i>Vijay Ramani; Illinois Institute of Technology</i>	3.2	X			Reviewers commended the project for its durability results and for its partnership with an automotive OEM. Reviewers also commented that future plans to reduce particle size were good. Down-selection of supports was recommended.

Project Number	Project Title <i>Principal Investigator Name &amp; Organization</i>	Final Score	Continue	Discontinue/ Further Review	Completed or CDP*	Summary Comments
FC-086	Development of Novel Non-Platinum Group Metal Electrocatalysts for PEMFC Applications <i>Sanjeev Mukerjee; Northeastern University</i>	3.2	X			Reviewers noted substantial progress made over the last fiscal year and that the PI was able to address challenging, critical barriers. Collaboration of an automotive OEM, universities, national laboratories, and materials suppliers was commended. More operation and testing on air were recommended.
FC-087	High-Activity Dealloyed Catalysts <i>Anusorn Kongkanand; General Motors</i>	3.4	X			Reviewers commended the approach, organization, and level of collaboration for this project. They noted the substantial increases in mass activity and durability achieved over the past year, with the project's developed dealloyed catalysts meeting DOE targets. Some reviewers recommended expanding the effort to investigate support durability and optimize catalyst layer properties. It was also suggested that ternary system work needs to concentrate on low-cost component metals.
FC-088	Development of Ultra-Low Platinum Alloy Cathode Catalyst for PEMFCs <i>Branko Popov; University of South Carolina</i>	2.7		X		Reviewers noted the project strengths include good team work to meet milestones, plenty of performance data on novel catalysts, a PI that is highly experienced in synthesizing materials, and some progress in increasing support stability and catalyst activity/durability. Weaknesses included a lack of comparison to commercial materials, questionable test protocols, and too much data with too little interpretation and evidence to support hypotheses. The kinetic activity targets were only marginally met and the MEA performance at high current density is below expectations. There is a go/no-go decision point at the end of September 2013.
FC-090	Corrugated Membrane Fuel Cell Structures <i>Stephen Grot; Ion Power</i>	2.4		X		Reviewers rated the relevance and collaborations as moderate and the accomplishments and potential impact as low. Although the concept is creative and innovative, the challenges in terms of ultimate prospects for increasing power density and lowering manufacturing and materials costs compared to state-of-the-art fuel cell configurations seems too great to overcome. The reviewers also noted that there may be performance issues related to heat and mass transfer, electrical resistance, and durability. They also noted that the full stack issues such as reactant/coolant manifolding have not been considered. The go/no-go decision point, which has a metric of producing power density of at least 70 mW/cm <sup>2</sup> at 0.8 V from a corrugated cell, is at the end of August 2013 and there has been only limited success in fabricating the corrugated cell to test. The major subcontractor, an automotive OEM, is no longer supporting the project.

Project Number	Project Title <i>Principal Investigator Name &amp; Organization</i>	Final Score	Continue	Discontinue/ Further Review	Completed or CDP*	Summary Comments
FC-091	Advanced Materials and Concepts for Portable Power Fuel Cells <i>Piotr Zelenay; Los Alamos National Laboratory</i>	3.2	X			Reviewers noted that the multidirectional approaches are reasoned and sensible. They commented that the PI holds the team together and despite some apparent isolation of the individual efforts, they are all of high quality and are focused on DOE milestones and barriers. Reviewers said that work on “ultrathrified” Pt/Ru/C catalysts is outstanding and other projects are all very good to excellent. They felt that in some cases (e.g., catalysts supported on Cu and on Au), there could be more work done to address durability.
FC-092	Investigation of Micro- and Macro-Scale Transport Processes for Improved Fuel Cell Performance <i>Jon Owejan; General Motors</i>	3.3			X	All nine reviewers seemed to agree on the excellent approach, accomplishments, collaboration, and relevance of this project. A reviewer noted that the project is well balanced between practical in situ characterization/diagnostic experiments and direct insightful modeling. The project addresses the key barriers to understanding and improving the transport issues for lower platinum group metal (PGM) MEAs. The publishing of all project data and models (via website, conferences, and journals) is of tremendous benefit to the PEM fuel cell community at large. An effective transport model will help developers decrease transport losses and achieve high power density with smaller systems, decreasing the cost. This project will be completed in November 2013.
FC-096	Power Generation from an Integrated Biomass Reformer and Solid Oxide Fuel Cell (SBIR Phase III Xlerator Program) <i>Quentin Ming; InnovaTek</i>	3.0	X			Reviewers commented that the project has hit its milestones, met the go/no-go criteria, and addressed the performance barriers. Reviewers commended the achievement of 40% efficiency using bio-kerosene. Recommendations were made to focus on durability. This project will be completed in May 2014.
FC-097	Stationary and Emerging Market Fuel Cell System Cost Analysis – Material Handling Equipment <i>Kathya Mahadevan; Battelle</i>	3.2	X			Reviewers commented that the project strengths include the strong methodology, detailed analysis, and identification of cost drivers (areas where R&D efforts need to be applied). Suggested areas for improvement were better use of collaborators and consideration of the two parallel efforts at Strategic Analysis, Inc. (SA) and Lawrence Berkeley National Laboratory. This project passed a go/no-go decision point in March 2013 after completing its material handling equipment report.

Project Number	Project Title <i>Principal Investigator Name &amp; Organization</i>	Final Score	Continue	Discontinue/ Further Review	Completed or CDP*	Summary Comments
FC-098	A Total Cost of Ownership Model for Design and Manufacturing Optimization of Fuel Cells in Stationary and Emerging Market Applications <i>Max Wei; Lawrence Berkeley National Laboratory</i>	3.1	X			Reviewers noted that this project has a systematic methodology, appears to be making progress toward the objectives, and includes health and environmental benefits analysis. However, it appears to lack accurate cost inputs because companies are reluctant to share that data. It has a high degree of overlap with Battelle and SA, so this should be reconciled to eliminate redundancy. Reviewers questioned why there was a lack of volume effect on balance of plant component costs. This project will have a go/no-go decision in October 2013.
FC-100	High Aspect Ratio Fuel Cell Catalysts <i>Brian Larsen; National Renewable Energy Laboratory</i>	2.8		X		Combining catalyst preparative variations with electrochemical performance evaluation was commended. Reviewers expressed concern, however, about the lack of a systematic approach to design improved materials, lack of collaborations, and lack of durability testing. The project has been discontinued after further review.
FC-103	Roots Air Management System with Integrated Expander <i>Dale Stretch; Eaton Corporation</i>	3.5	X			Reviewers agreed with the approach Eaton has taken to reduce cost and improve performance. They commended the collaboration with Kettering University to provide computational fluid dynamics modeling, ANL to provide system modeling, SA to provide cost modeling, and finally Ballard to provide the integration and demonstration of the system with a stack. There is some concern that results will not be available to support the final design decision on schedule.
FC-104	High Performance, Durable, Low-Cost Membrane Electrode Assemblies for Transportation Applications <i>Andrew Steinbach; 3M</i>	3.0	X			A number of the reviewers stated that this new project is highly relevant, has a good approach, and has good teaming. Some reviewers expressed concern regarding the NSTF technology, including the water management issues to be addressed in this integration activity.

\*Congressionally directed project (CDP)

## Manufacturing R&D

Project Number	Project Title <i>Principal Investigator Name &amp; Organization</i>	Final Score	Continue	Discontinue/ Further Review	Completed or CDP*	Summary Comments
MN-001	Fuel Cell MEA Manufacturing R&D <i>Michael Ulsh; National Renewable Energy Laboratory</i>	3.4	X			Reviewers applauded the new approach planned—focusing more on exploratory studies. They also commended the National Renewable Energy Laboratory (NREL) for coordinating with industry to develop and improve diagnostics critical to fuel cell membrane electrode assembly (MEA) and gas diffusion layer (GDL) manufacturing. One reviewer questioned the new diagnostic to measure the ionomer/carbon ratio as the presentation did not indicate a strong industry need for this diagnostic. Reviewers suggested that NREL indicate how these techniques will be used in a feedback process loop control.
MN-004	Manufacturing of Low-Cost, Durable Membrane Electrode Assemblies Engineered for Rapid Conditioning <i>Colin Busby; W.L. Gore</i>	3.2	X			Reviewers noted that the approach of the project to develop methods to produce fuel cell MEAs in volume is good. Reviewers stated that it was unclear what progress has been made since last year other than selecting a low-cost backer. No results from the University of Tennessee-Knoxville are evident. Reviewers thought that the addition of cost analysis by Strategic Analysis, Inc. was good. Reviewers were concerned about the loss of UTC Power/United Technologies Research Center as stack testers.
MN-006	Metrology for Fuel Cell Manufacturing <i>Michael Stocker; National Institute of Standards and Technology</i>	3.0			X	This project is complete. Reviewers felt that the general approach to the effort was appropriate but that additional input from other researchers at laboratories or in academia may have been useful. They felt that the Large Aperture Projection Scatterometer (LAPS) device has some potential but that there still seem to be some process control issues to resolve. Reviewers felt that the benefits of this technique compared to X-ray fluorescence (XRF) are not clear. They also felt that the ability of LAPS to measure two-sided coatings simultaneously may not be needed. The researchers are urged to get better input from industry.
MN-007	High-Speed, Low-Cost Fabrication of Gas Diffusion Electrodes for Membrane Electrode Assemblies <i>Emory De Castro; BASF</i>	3.6			X	This project is complete. Reviewers felt that BASF laid out and accomplished a methodical approach to addressing the problems in the statement of work. They noted that the throughput (line speed) was significantly increased, the paper gas diffusion electrode (GDE) cost goal was met, and variability now meets acceptable level. In addition, they commended the ink cost savings and the performance gain of the GDE.

\*Congressionally directed project (CDP)

## Technology Validation

Project Number	Project Title <i>Principal Investigator Name &amp; Organization</i>	Final Score	Continue	Discontinue/ Further Review	Completed or CDP*	Summary Comments
TV-008	Technology Validation: Fuel Cell Bus Evaluations <i>Leslie Eudy; National Renewable Energy Laboratory</i>	3.8	X			The reviewers commented that the project was well designed, proving critical to the wide-scale adoption of fuel-cell-powered buses, and providing valuable insights for both U.S. Department of Energy (DOE) project managers and transit fleet operators. It was suggested that performance and reliability comparisons with previous generation buses, as well as bus deployments already performed or underway in Europe, should also be considered.
TV-016	Stationary Fuel Cell Evaluation <i>Chris Ainscough; National Renewable Energy Laboratory</i>	3.3	X			The reviewers noted that this relatively new addition to the Technology Validation portfolio takes advantage of previously developed and effective approaches. It was noted that results should be compared not only to DOE targets, but also to results for other conventional and emerging prime power technologies. Reviewers suggested that evaluation of stationary fuel cells should be expanded to other states, even if the evaluation includes only those projects that provide incentives for stationary fuel cells. Focusing data collection on specific system sizes and expanding analyses to include data on fuel cell maintenance, degradation, and reliability were also suggested.
TV-018	Hydrogen Recycling System Evaluation and Data Collection <i>Rhonda Staudt; H2Pump</i>	3.3	X			The reviewers commented that developing a system that will reclaim hydrogen from industrial waste is an innovative technology that addresses on-site renewable hydrogen creation and warrants validation. It was noted that some plan to recover schedule slippage is needed, as the go/no-go decision point and data collection were behind schedule. The reviewers requested more details on the cost per kilogram of hydrogen supplied. While hydrogen recycling could be an attractive business proposition for a subset of industrial hydrogen users, uncertainties exist regarding how much of the future demand for hydrogen could be met by this method, and reviewers felt that the potential is limited.

Project Number	Project Title <i>Principal Investigator Name &amp; Organization</i>	Final Score	Continue	Discontinue/ Further Review	Completed or CDP*	Summary Comments
TV-019	Hydrogen Component Validation <i>Kevin Harrison; National Renewable Energy Laboratory</i>	3.4	X			The reviewers expressed the opinion that the National Renewable Energy Laboratory's (NREL's) testing and analysis is valuable in accelerating commercialization of near-commercial technologies. Reviewers suggested that other manufacturers and component types could also be investigated, and that attention should be given to comparing results with DOE goals and targets. The reviewers noted that it may be desirable to more aggressively market NREL's component validation capabilities to industry so that they can take advantage of NREL's testing prior to demonstrating their new products or components to customers.
TV-020	Validation of an Advanced High-Pressure PEM Electrolyzer and Composite Hydrogen Storage, with Data Reporting, for SunHydro Stations <i>Larry Moulthrop; Proton OnSite</i>	3.3	X			The reviewers noted that the project fits well with DOE goals and is expected to lower costs with improved and more efficient components, as well as the potential to speed permitting-related approvals. Reviewers noted good collaborations with component suppliers and users, but also that expansion of the evaluation to include other fueling stations, organizations, and technologies should be considered. Reviewers suggested that the project should thoroughly evaluate how the advanced components being validated affect the costs of delivered hydrogen and ensure appropriate data is collected to support cost estimates.
TV-021	Forklift and Backup Power Data Collection and Analysis <i>Jennifer Kurtz; National Renewable Energy Laboratory</i>	3.6	X			Reviewers believed that NREL's business case analysis of the economic and operating performance of fuel cell forklifts and backup power systems has contributed to the commercial ramp-up of these systems. While detailed data were presented for forklift systems, reviewers suggested some additional analysis and information on backup power systems. Reviewers strongly suggested that this project should be continued beyond its proposed end date in order to establish a long-term performance record for these systems and to portray trends over several years.

\*Congressionally directed project (CDP)

## Safety, Codes and Standards

Project Number	Project Title <i>Principal Investigator Name &amp; Organization</i>	Final Score	Continue	Discontinue/ Further Review	Completed or CDP*	Summary Comments
SCS-001	National Codes and Standards Deployment and Outreach <i>Carl Rivkin; National Renewable Energy Laboratory</i>	3.3	X			Reviewers recognized this project as essential to the harmonization and development of codes and standards. Reviewers praised the coordination with code development organizations (CDOs) and standards development organizations (SDOs) and the value of the work being done in California. However, reviewers stated that the project focus, approach, and plan should be improved by incorporating clear, significant deliverables and associated timelines as well as metrics for tracking outreach efforts. In addition, the project scope should be expanded to address a range of needs such as codes and standards for hydrogen quality, metering, and certification of components and systems.
SCS-002	Component Standards Research & Development <i>Robert Burgess; National Renewable Energy Laboratory</i>	2.8	X			Reviewers acknowledged the importance and need for this project in advancing hydrogen infrastructure and codes and standards development and implementation. Specific strengths cited included the project's strong coordination and effective flow of information between SDOs, CDOs, and national/international laboratories. However, reviewers identified the need for stronger collaboration and coordination with industry as well as outreach to help transfer knowledge. Reviewers would also like to see a better defined project scope and clearer milestones to better evaluate the project.
SCS-004	Hydrogen Safety, Codes and Standards: Sensors <i>Eric Brosha; Los Alamos National Laboratory</i>	3.3	X			Reviewers recognized the strong coordination with industrial partners and overall project management and execution. However, reviewers noted concerns regarding the project's ability to deliver sensors that meet the specified targets. Reviewers also cited some uncertainty regarding industrial partners' ability to commercialize the technology. The reviewers suggested future work that includes the investigation of cross-sensitivity to methane (CH <sub>4</sub> ); the development of durability, maintenance, and manufacturing requirements; and manufacturing, maintenance, and other cost estimates and targets for relevant applications.

Project Number	Project Title <i>Principal Investigator Name &amp; Organization</i>	Final Score	Continue	Discontinue/ Further Review	Completed or CDP*	Summary Comments
SCS-005	R&D for Safety, Codes and Standards: Materials and Components Compatibility <i>Aaron Harris; Sandia National Laboratories</i>	3.6	X			Reviewers commended the communication with industry and the quality of the data and analytical methods. Stronger direct support to industry would strengthen this project, along with additional collaboration with other government-funded related research. Improved testing capabilities such as testing at -50°C would build credibility for embrittlement testing and would strengthen this project. Reviewers suggested further harmonization between SAE International and the Canadian Standards Association, along with more publications of research including preliminary results and conclusions to enable better review and feedback for future work.
SCS-007	Hydrogen Fuel Quality <i>Tommy Rockward; Los Alamos National Laboratory</i>	3.4	X			Reviewers praised the focus, dedication, and alignment of the project work with near-term real-world needs. This work is seen as a key success and important stepping stone toward implementation of hydrogen fuel quality standards. Reviewers noted a shortage of resources and industrial partner support for accelerating commercialization of the in-line analyzer. Reviewers also cited competing technical interests and the lack of analysis as well as cost data on contaminant levels as a project weakness. Reviewers suggested reexamining the project scope to include the investigation of the cost effectiveness of the technology and collaboration with an industrial partner to advance commercialization efforts of the in-line gas analyzer.
SCS-010	R&D for Safety Codes and Standards: SCS Project Overview - Hydrogen Behavior <i>Aaron Harris; Sandia National Laboratories</i>	3.2	X			Reviewers emphasized the project's strong research and experiments in validating data and models on H <sub>2</sub> release behavior. Strengths also include research collaborations and international harmonization efforts. However, the complexity of the project requires better efforts to simplify/clarify the objectives and communicate progress and future plans to project managers and the general public. Reviewers suggested the addition of underground storage into the fuel storage matrix and the need for more frequent and widespread publication and outreach, including coordination with International Organization for Standardization (ISO) TC 197.

Project Number	Project Title <i>Principal Investigator Name &amp; Organization</i>	Final Score	Continue	Discontinue/ Further Review	Completed or CDP*	Summary Comments
SCS-011	R&D for Safety Codes and Standards: SCS Project Overview - Risk <i>Aaron Harris; Sandia National Laboratories</i>	3.2	X			Reviewers recognized this project for its strong technical capabilities, thoroughness, and scientific basis, which is critical for enabling the siting of hydrogen projects, specifically refueling stations. The ability to compare risk with other industries is also a major improvement. However, reviewers expressed concern over the robustness of underlying assumptions and complexity of the toolkit that may lend itself to mis-use. Reviewers recommended considering applications for evaluating the risk associated with equipment or processes, along with incorporating stakeholder input to help shape future work.
SCS-019	Hydrogen Safety Panel and Hydrogen Safety Knowledge Tools <i>Nick Barilo; Pacific Northwest National Laboratory</i>	3.6	X			Reviewers noted the project’s strengths in sharing safety information and providing guidance and tools to increase awareness for industry. The safety panel was also highlighted for its collaboration and for providing a critical service to the community. However, reviewers identified the need to involve third-party certifiers and improve the coordination between the safety panel and safety planning in projects funded by the Fuel Cell Technologies Office. Reviewers suggested continued feedback to SDOs and that developing a comprehensive strategy around mobile platform applications will continue to build on the success of such safety knowledge tools.
SCS-021	NREL Hydrogen Sensor Testing Laboratory <i>Bill Buttner; National Renewable Energy Laboratory</i>	3.3	X			Reviewers applauded the work to understand the needs of industry and the effective collaboration with international partners. This work was also recognized for enabling sensor developers to improve sensors and measure progress toward goals. However, reviewers noted the importance of having a clear context, purpose, and goal for developing sensors to address the critical needs facing the deployment of hydrogen and fuel cell technologies. Reviewers recommended clear messaging about the role of sensors in achieving safety levels defined in codes and standards and suggested investigating the use of wide area detection and contact sensing technologies for early detection of H <sub>2</sub> leaks.

\*Congressionally directed project (CDP)

## Market Transformation

Project Number	Project Title <i>Principal Investigator Name &amp; Organization</i>	Final Score	Continue	Discontinue/ Further Review	Completed or CDP*	Summary Comments
MT-004	Direct Methanol Fuel Cell Material Handling Equipment Deployment <i>Todd Ramsden; National Renewable Energy Laboratory</i>	3.2			X	Reviewers noted that the hydrogen infrastructure cost barrier was definitely addressed, showing that a methanol refueling system is a small fraction of that for hydrogen; however, the direct methanol fuel cell (DMFC) lift truck power system durability is an issue that requires a complete evaluation. Reviewers recommended involving more than one vendor in the project.
MT-006	Fuel Cell Combined Heat and Power Commercial Demonstration <i>Kriston Brooks; Pacific Northwest National Laboratory</i>	3.6	X			Reviewers commented that the project is well planned, milestones are being met, and the analysis is useful. Reviewers also noted that various user types help to define the potential market better, although some market examples such as hospitals need much higher power levels. The lack of information on technical improvements needed should be addressed in the future.
MT-007	Landfill Gas-to-Hydrogen <i>Shannon Baxter-Clemmons; South Carolina Hydrogen and Fuel Cell Alliance</i>	2.8	X			While reviewers agreed that this application and project objectives are of great value, this project is significantly behind schedule due to technical problems. The project team has been unable to resolve the nitrogen diluent in the gas composition. The reviewers noted that while this problem is not a showstopper, it needs to be addressed with outside expertise. Reviewers stated that this project should continue to completion because the objectives hold great promise for turning landfill gas into usable fuel.
MT-008	Hydrogen Energy Systems as a Grid Management Tool <i>Mitch Ewan; Hawaii Natural Energy Institute</i>	3.2	X			Reviewers stated that the project presents a good opportunity for public acceptance of hydrogen fuel because the hydrogen is entirely from a renewable source, in this case geothermal power. Reviewer comments were also positive regarding the number of collaborators and stakeholders in industry and government along with resource leveraging. One reviewer noted the lessons learned after the project's completion would be of high value to similar projects. Reviewers also commented that the project focus needs to be narrowed to reduce project risks.
MT-011	Ground Support Equipment Demonstration <i>Jim Petrecky; Plug Power</i>	3.2	X			Reviewers supported the project's approach in that it was modeled after successful material handling equipment (MHE) deployment projects. Reviewers positively noted that the expansive team and stakeholder involvement aligned with the Market Transformation program objectives. Reviewers were concerned that the schedule was very aggressive but noted that concrete go/no-go decision milestones will minimize risks. One reviewer stated that the market size may be too small and that other applications should be brought in.

Project Number	Project Title <i>Principal Investigator Name &amp; Organization</i>	Final Score	Continue	Discontinue/ Further Review	Completed or CDP*	Summary Comments
MT-012	Fuel Cells as Range Extenders for Battery Electric Vehicles <i>Aymeric Rousseau; Argonne National Laboratory</i>	3.1			X	Reviewer opinions varied widely from the project being unnecessary to extremely valid and useful for electric vehicle technologies. Reviewers stated that the results and data presented were valid for extending zero emission vehicle range and of great relevance. Results from the completed study should be used to guide future work in this area.

\*Congressionally directed project (CDP)

## Systems Analysis

Project Number	Project Title <i>Principal Investigator Name &amp; Organization</i>	Final Score	Continue	Discontinue/ Further Review	Completed or CDP*	Summary Comments
AN-030	Worldwide Status of Hydrogen Fuel Cell Vehicle Technology and Prospects for Commercialization <i>David Greene; Oak Ridge National Laboratory</i>	3.5			X	Reviewers commented that this analysis project was very relevant to the Fuel Cell Technologies Office (FCTO) goals and objectives and made good progress. They commended the project for being comprehensive and providing the necessary evaluation of the technology status. The collaboration used in the project was excellent. The project findings should be incorporated in FCTO's program assumptions.
AN-031	Siting Strategies for Early Hydrogen Refueling Infrastructure in California: Learning from the Gasoline Experience <i>Michael Nicholas; University of California, Davis</i>	3.1	X			Reviewers commented that the project has made excellent progress. Reviewers felt that the project's strength stems from the field of resources and collaboration. The project is very relevant to the analysis of infrastructure development and more emphasis should be placed on market deployment and the interaction with vehicle deployment. Reviewers suggested future studies should focus on the minimum number of fueling stations needed for the early market vehicle rollout.
AN-032	Design and Economics of an Early Hydrogen Refueling Network for California <i>Joan Ogden; University of California, Davis</i>	3.4	X			Reviewers commented that this analysis project is very relevant to FCTO goals and objectives and made significant progress. The project's findings will contribute to understanding near-term hydrogen infrastructure costs and the appropriate level of support. The collaboration used in the project was excellent but should be expanded to include other countries that are installing infrastructure. The project could be expanded to include investigating impacts of low station utilization.
AN-033	Analysis of Optimal On-Board Storage Pressure for Hydrogen Fuel Cell Vehicles <i>Zhenhong Lin; Oak Ridge National Laboratory</i>	3.1	X			Reviewers observed the project approach was sound and straightforward, with good focus on analysis. The project provides vital information on station development and deployment and consumer value of fuel cell electric vehicles (FCEVs) relative to range and fuel cost trade-offs. They commended the project for the collaboration with industry and academia. The project is in the initial phases and has made modest-to-good progress and should continue to incorporate new cost data for other fueling pressures. The project should incorporate industry input on costs associated with modular station design. The project should include an "annoyance factor" of having to refuel more often with lower-pressure fuel.

Project Number	Project Title <i>Principal Investigator Name &amp; Organization</i>	Final Score	Continue	Discontinue/ Further Review	Completed or CDP*	Summary Comments
AN-034	Life Cycle Analysis of Hydrogen On-Board Storage Options <i>Amgad Elgowainy; Argonne National Laboratory</i>	3.2	X			Reviewers continue to commend this project for the excellent ongoing progress and relevance for life cycle assessments. The project should include more collaboration with industry to vet the results. Reviewers thought this project had the strength of being built on the Greenhouse Gases, Regulated Emissions, and Energy Use in Transportation (GREET) model architecture for providing life cycle analysis capabilities for onboard storage. Reviewers suggested that a broader context of storage options for vehicles be considered.
AN-035	Employment Impacts of Infrastructure Development for Hydrogen and Fuel Cell Technologies <i>Marianne Mintz; Argonne National Laboratory</i>	3.2	X			Reviewers concluded that the JOBS model is crucial for evaluating the impact of fuel cell technologies on job creation and provides a broader understanding of the role fuel cell technologies can play in the U.S. economy. Reviewers acknowledged the impressive list of stakeholders and collaborators for the project. They recommended the model be expanded to include hydrogen infrastructure and FCEV deployments as well as for the manufacturing of solid oxide fuel cells because they are now in production.
AN-036	Pathway Analysis: Projected Cost, Well-to-Wheels Energy Use and Emissions of Current Hydrogen Technologies <i>Todd Ramsden; National Renewable Energy Laboratory</i>	3.3	X			Reviewers observed that this project had an excellent choice of comparison technologies and models and is relevant to the FCTO goals. They acknowledge the project has good collaboration from a diverse set of stakeholders. The project could be strengthened by adding definition of the technology time frame, methodology of model validation, and future technologies.
AN-037	Hydrogen from Biogas: Resource Assessment <i>Genevieve Saur; National Renewable Energy Laboratory</i>	3.4	X			Reviewers commented that waste to fuel is relevant to solving environmental problems and reducing greenhouse gas emissions. The approach was clear and addressed renewable resource assessment. The project has made good progress. Moving forward, work should compare cleanup costs associated with hydrogen generation from wastes and correlate biogas resources with regional analysis.
AN-038	Global Hydrogen Resource Analysis (Hydrogen Implementing Agreement, Task 30A) <i>Tom Drennan; Sandia National Laboratories</i>	3.1			X	The reviewers commented that the project approach needs to ensure greater rigor in the methodology and consistent inputs from different countries. The project has made good progress but has exhibited limited quality assurance of the analytical tool. The project had good collaboration from a large array of countries but the effectiveness of the collaboration was not clear. The relevance of the project needs more explanation and demonstration. The reviewers concluded that the project needs to be completed and the results disseminated.

Project Number	Project Title <i>Principal Investigator Name &amp; Organization</i>	Final Score	Continue	Discontinue/ Further Review	Completed or CDP*	Summary Comments
AN-039	Life Cycle Analysis of Water Use for Hydrogen Production Pathways <i>Amgad Elgowainy; Argonne National Laboratory</i>	3.2	X			Reviewers commented that the project approach is clear and adequate to address a critical issue for future energy, including hydrogen. The project is in the initial phases and has few accomplishments at this point. The project will benefit from stakeholder and academic collaboration. Water availability and usage for energy generation is an important issue and the GREET model offers a high value for comparative life cycle analysis of water usage.
AN-040	Analysis of Fuel Cell Integration with Biofuels Production <i>Mark Ruth; National Renewable Energy Laboratory</i>	2.9			X	Reviewers commented the project approach was clear and the analysis was thorough. The project was well executed and is complete. The collaboration was limited but could have benefited from inclusion of industry stakeholders. The study was valuable to understand the impacts of integrating fuel cells in a bio-refinery.
AN-042	Hawai'i Hydrogen Initiative (H2I) Financial Scenario Analysis <i>Michael Penev; National Renewable Energy Laboratory</i>	3.5			X	According to reviewers, the project and analysis was well designed and utilized existing tools to conduct the scenario evaluations. The approach was adequate for the project scale and integrates other models for the evaluation. The analysis draws on contributions from a diverse set of stakeholders. Significant progress has been made in evaluating the infrastructure for Hawai'i. Additional scenarios should be explored that include an optimistic case. The model developed and analysis conducted for Hawai'i serves as a good structure and baseline for other different regions of the country.
AN-043	Analysis of Community Energy <i>Darlene Steward; National Renewable Energy Laboratory</i>	3.3			X	Reviewers commented that the project approach was satisfactory and progress was adequate. The project has benefited from a diverse group of stakeholders, but more regional data should be used to account for seasonal and geographic differences. The reviewers mentioned that the project was relevant to managing renewable power resources at a local level. Application of additional industry review, actual equipment cost input, and location data would benefit this project.

\*Congressionally directed project (CDP)

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## Introduction

The fiscal year (FY) 2013 U.S. Department of Energy (DOE) Hydrogen and Fuel Cells Program Annual Merit Review and Peer Evaluation Meeting (AMR), in conjunction with DOE's Vehicle Technologies Office AMR, was held from May 13–16, 2013, at the Crystal City Marriott and Crystal Gateway Marriott in Arlington, Virginia. This report is a summary of comments by AMR peer reviewers about the hydrogen and fuel cell projects funded by DOE's Office of Energy Efficiency and Renewable Energy (EERE). Projects supported by other DOE offices (including the Office of Science [Basic Energy Sciences] and ARPA-E) in areas relevant to hydrogen and fuel cells were also presented at the FY 2013 AMR. DOE uses the results of this merit review and peer evaluation, along with additional review processes, to make funding decisions for upcoming fiscal years and help guide ongoing performance improvements to existing projects.

The objectives of this meeting include the following:

- Review and evaluate FY 2013 accomplishments and FY 2014 plans for DOE laboratory programs; industry/university cooperative agreements; and related research, development, and demonstration (RD&D) efforts
- Provide an opportunity for stakeholders and participants (e.g., fuel cell manufacturers, component developers, and others) to provide input to help shape the DOE-sponsored RD&D program in order to address the highest-priority technical barriers and facilitate technology transfer
- Foster interactions among the national laboratories, industry, and universities conducting RD&D.

The peer review process followed the guidelines in the *Peer Review Guide* developed by EERE. The peer review panel members, listed in Table 1, provided comments about the projects presented. Panel members included experts from a variety of backgrounds related to hydrogen and fuel cells, and they represented national laboratories, universities, various government agencies, and manufacturers of hydrogen production, storage, delivery, and fuel cell technologies. Each reviewer was screened for conflicts of interest as prescribed by the *Peer Review Guide*. A complete list of the meeting participants is presented as Appendix A.

**Table 1: Peer Review Panel Members**

No.	Name	Organization
1	Abdel-Baset, Tarek	Chrysler LLC
2	Adzic, Radoslav	Brookhaven National Laboratory
3	Ahluwalia, Rajesh	Argonne National Laboratory
4	Ahmed, Shabbir	Argonne National Laboratory
5	Ainscough, Chris	National Renewable Energy Laboratory
6	Antoni, Laurent	Commissariat A l'Energie Atomique (CEA)
7	Antos, George	National Science Foundation
8	Araghi, Koorosh	National Aeronautics and Space Administration
9	Ardo, Shane	California Institute of Technology
10	Autrey, Thomas	Pacific Northwest National Laboratory
11	Balbuena, Perla	Texas A&M University
12	Balema, Viktor	Sigma-Aldrich
13	Baturina, Olga	U.S. Navy, Naval Research Laboratory (former)
14	Beattie, Paul	Ballard Power Systems
15	Bender, Guido	National Renewable Energy Laboratory
16	Benjamin, Thomas	Argonne National Laboratory
17	Birdsall, Jackie	Toyota Engineering and Manufacturing America
18	Bonner, Brian	Air Products and Chemicals, Inc.
19	Bordeaux, Christopher	Bordeaux International Energy Consulting LLC
20	Borup, Rod	Los Alamos National Laboratory
21	Bouwkamp, Nico	California Fuel Cell Partnership
22	Bowden, Mark	Pacific Northwest National Laboratory
23	Bowman, Robert	Oak Ridge National Laboratory
24	Boyd, Robert	Boyd Hydrogen LLC
25	Brett, Lois	Consultant
26	Brosha, Eric	Los Alamos National Laboratory

No.	Name	Organization
27	Brown, Craig	National Institute of Standards and Technology
28	Burgunder, Albert	Praxair, Inc.
29	Cai, Mei	General Motors, Research & Development Center
30	Cairns, Julie	CSA Group
31	Campbell, Stephen	AFCC Automotive Fuel Cell Cooperation Corporation
32	Cargnelli, Joe	Hydrogenics
33	Centeck, Kevin	TARDEC
34	Chahine, Richard	Hydrogen Research Institute, Institut de recherche sur l'hydrogene
35	Choudhury, Biswajit	DuPont Fuel Cells
36	Christensen, John	Consultant - U.S. Navy, DOD-DLA (retired)
37	Cole, Brian	U.S. Army RDECOM CERDEC
38	Collins, William	United Technologies (retired)
39	Conti, Amedeo	Nuvera Fuel Cells, Inc.
40	Creager, Stephen	Clemson University
41	Curtin, Dennis	DuPont (retired)
42	Dale, Nilesh	Nissan
43	Datye, Abhaya	University of New Mexico
44	Davis, Benjamin	Los Alamos National Laboratory
45	De Castro, Emory	BASF Fuel Cell, Inc.
46	Dedrick, Daniel	Sandia National Laboratories
47	Dinh, Huyen	National Renewable Energy Laboratory
48	Dixon, David	University of Alabama
49	Dobbins, Tabbetha	Rowan University
50	Dornheim, Martin	Helmholtz Zentrum-Geestadt
51	Duenas, Terrisa	NextGen Aeronautics
52	Ehlers, Peter	CSA Group
53	Erdle, Erich	EFCECO, Erdle Fuel Cell & Energy Consulting
54	Esposito, Dan	National Institute of Standards and Technology
55	Eudy, Leslie	National Renewable Energy Laboratory
56	Ewan, Mitch	University of Hawai'i, Manoa
57	Fan, Chinbay	Gas Technology Institute
58	Farese, David	Air Products and Chemicals, Inc.
59	Fenske, George	Argonne National Laboratory
60	Funk, Stuart	LMI
61	Gangi, Jennifer	Fuel Cells 2000
62	Gennett, Thomas	National Renewable Energy Laboratory
63	Gervasio, Don	University of Arizona
64	Giron, Enrique	Fuel Cells and Hydrogen Joint Undertaking
65	Gittleman, Craig	General Motors, Research & Development Center
66	Graetz, Jason	HRL Laboratories
67	Grassilli, Leo	Consultant - Office of Naval Research
68	Greene, David	Oak Ridge National Laboratory
69	Gross, Karl	H2 Technology Consulting LLC
70	Gross, Tom	Energy Planning and Solutions (Consultant)
71	Grot, Stephen	Ion Power
72	Gu, Wenbin	General Motors
73	Gupta, Ram	National Science Foundation
74	Hall, Karen	Technology Transition Corporation
75	Hamilton, Cyd	U.S. Department of Energy
76	Hamilton, Jennifer	California Fuel Cell Partnership
77	Hardis, Jonathan	National Institute of Standards and Technology
78	Harris, Aaron	Sandia National Laboratories
79	Harvey, David	Ballard
80	Hays, Charles	National Aeronautics and Space Administration, Jet Propulsion Laboratory
81	He, Wensheng	Arkema, Inc.
82	Hennessey, Barbara	U.S. Department of Transportation

No.	Name	Organization
83	Herbert, Thorsten	NOW GmbH
84	Hicks, Michael	H2 PowerTech
85	Hirano, Shinichi	Ford Motor Company
86	Holladay, Jamie	Pacific Northwest National Laboratory
87	Jacobson, David	National Institute of Standards and Technology
88	James, Brian	Strategic Analysis, Inc.
89	Jaramillo, Thomas	Stanford University
90	Jarvi, Tom	Sun Catalytix Corporation
91	Jensen, Craig	University of Hawai'i, Honolulu
92	Jensen, Torben René	Aarhus University
93	Josefik, Nick	U.S. Army Corps of Engineers (USACE-DOD)
94	Junge, Axel	General Motors, Research & Development Center
95	Kasab, John	Ricardo
96	Keller, Jay	Sandia National Laboratories
97	Kerr, John	Lawrence Berkeley National Laboratory
98	Knights, Shanna	Ballard Power Systems
99	Kocha, Shyam	National Renewable Energy Laboratory
100	Kongkanand, Anusorn	General Motors Corporation
101	Kopasz, John	Argonne National Laboratory
102	Koros, William	Georgia Institute of Technology
103	Kraigsley, Alison	National Institute of Standards and Technology
104	Kurtz, Jennifer	National Renewable Energy Laboratory
105	Lakshmanan, Balsu	General Motors Corporation
106	Leachman, Jacob	Washington State University
107	Leduc, Guillaume	Fuel Cells and Hydrogen Joint Undertaking
108	Lieberman, Robert	Intelligent Optical Systems
109	Linkous, Clovis	Youngstown State University
110	Lipp, Ludwig	FuelCell Energy, Inc.
111	Markovic, Nenad	Argonne National Laboratory
112	Maroni, Victor	Argonne National Laboratory
113	McConnachie, Jonathan	Exxon Mobil
114	McGrady, Sean	University of New Brunswick
115	McKone, Thomas	Lawrence Berkeley National Laboratory
116	Melaina, Marc	National Renewable Energy Laboratory
117	Merritt, James	U.S. Department of Transportation
118	Miller, James	Argonne National Laboratory
119	Minh, Nguyen	General Electric Global Research Center
120	Mittelsteadt, Cortney	Giner, Inc./Giner Electrochemical Systems, LLC
121	Moen, Chris	Sandia National Laboratories
122	Moffat, Thomas	National Institute of Standards and Technology
123	Moreland, Gregory	SRA International, Inc.
124	Motyka, Ted	Savannah River National Laboratory
125	Moulthrop, Larry	Proton OnSite
126	Mukerjee, Sanjeev	Northeastern University
127	Mukundan, Rangachary	Los Alamos National Laboratory
128	Myers, Deborah	Argonne National Laboratory
129	Nicholas, Mike	University of California, Davis
130	Oesterreich, Bob	Air Liquide Industrial
131	Ogden, Joan	University of California, Davis
132	Ohma, Atsushi	Nissan Motor Company
133	Olson, Gregory	Consultant – Sentech
134	Ott, Kevin	Los Alamos National Laboratory (retired)
135	Owejan, Jon	State University of New York
136	Padró, Catherine	Los Alamos National Laboratory
137	Parks, George	FuelScience LLC / Phillips 66
138	Paster, Mark	Consultant – Independent
139	Penev, Michael	National Renewable Energy Laboratory
140	Perret, Robert	Nevada Technical Services, LLC

No.	Name	Organization
141	Perry, Mike	United Technologies Research Center (UTRC)
142	Petrovic, John	Petrovic and Associates
143	Pivovar, Bryan	National Renewable Energy Laboratory
144	Podolski, Walt	Argonne National Laboratory
145	Polevaya, Olga	Nuvera Fuel Cells, Inc.
146	Protopappas, Peter	Navigant Consulting
147	Rambach, Glenn	SiGNa Chem
148	Ramsden, Todd	National Renewable Energy Laboratory
149	Richards, Mark	Versa Power Systems
150	Rinebold, Joel	Connecticut Center for Advanced Technology, Inc.
151	Rossmeyssl, Neil	U.S. Department of Energy, EERE
152	Sattler, Christian	German Aerospace Center (DLR)
153	Schlasner, Steven	University of North Dakota, EERC
154	Schneider, Jesse	BMW of North America, LLC
155	Siegel, Don	University of Michigan, Ann Arbor
156	Simmick, James	BP America
157	Skolnik, Ed	Energetics Incorporated
158	Sofronis, Petros	University of Illinois, Urbana-Champaign
159	Soto, Herie	Shell Hydrogen LLC
160	Stamenkovic, Vojislav	Argonne National Laboratory
161	Steen, Marc	European Commission, Joint Research Centre
162	Steinbach, Andy	3M
163	Stolten, Detlef	Forschungszentrum Jülich GmbH
164	Sutherland, Ian	General Motors Corporation
165	Swider-Lyons, Karen	U.S. Navy, Naval Research Laboratory
166	Thomas, C.E. (Sandy)	Clean Car Options
167	Trocciola, John	SRA International, Inc.
168	Ulsh, Michael	National Renewable Energy Laboratory
169	Vanderborgh, Nicholas	Los Alamos National Laboratory (retired)
170	Veenstra, Mike	Ford Motor Company
171	Voecks, Gerald	CalTech
172	Vora, Shailesh	National Energy Technology Laboratory
173	Wachsman, Eric	University of Maryland
174	Wagener, Earl	Tetramer Technologies
175	Wagner, Frederick T.	General Motors Corporation (retired)
176	Waldecker, James	Ford Motor Company
177	Walk, Alex	SGL Group
178	Warren, Charles David	Oak Ridge National Laboratory
179	Weber, Adam	Lawrence Berkeley National Laboratory
180	Wei, Max	Lawrence Berkeley National Laboratory
181	Wessel, Silvia	Ballard
182	Wheeler, Douglas	DJW Technology LLC
183	Williams, Mark	National Energy Technology Laboratory
184	Wilson, Mahlon	Los Alamos National Laboratory
185	Wolak, Frank	FuelCell Energy, Inc.
186	Woods, Stephen	National Aeronautics and Space Administration
187	Yang, Joyce	U.S. Department of Energy, EERE
188	Yuzugullu, Elvin	SRA International, Inc.
189	Zhu, Yimin	Silicon Energy Storage

### Summary of Peer Review Panel's Crosscutting Comments and Recommendations

AMR panel members provided comments and recommendations regarding selected DOE hydrogen and fuel cell projects, overall management of the Hydrogen and Fuel Cells Program, and the AMR peer evaluation process. The project comments, recommendations, and scores are provided in the following sections of this report, grouped by program area. Comments about program management are provided in Appendix B.

## Analysis Methodology

A total of **118** projects were reviewed at the meeting. As shown in Table 1, **189** review panel members participated in the AMR process, providing a total of **752** project evaluations. These reviewers were asked to provide numeric scores (on a scale of 1–4, with 4 being the highest) for five aspects of the work presented. A sample evaluation form is provided in Appendix C. Scores and comments were submitted using laptops (provided on-site) 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 not reviewed, is provided in Appendix D.

Scores were based on the following five criteria and weights:

- Score 1: Approach to performing the work (20%)
- Score 2: Accomplishments and progress toward overall project and DOE goals (45%)
- Score 3: Collaboration and coordination with other institutions (10%)
- Score 4: Relevance/potential impact on DOE program goals and RD&D objectives (15%)
- Score 5: Proposed future work (10%).

For each project, individual reviewer scores for each of the five criteria were weighted using the formula in the box below to create a final score for each reviewer for that project. The average score for each project was then calculated by averaging the final scores for individual reviewers. The individual reviewer scores for each question were also averaged to provide information on the project’s question-by-question scoring. In this manner, a project’s final overall score can be meaningfully compared to that of another project.

$$\text{Final Overall Score} = [\text{Score 1} \times 0.20] + [\text{Score 2} \times 0.45] + [\text{Score 3} \times 0.10] + [\text{Score 4} \times 0.15] + [\text{Score 5} \times 0.10]$$

A perfect overall score of “4” indicates that a project satisfied the five criteria to the fullest possible extent; the lowest possible overall score of “1” indicates that a project did not satisfactorily meet any of the requirements of the five criteria.

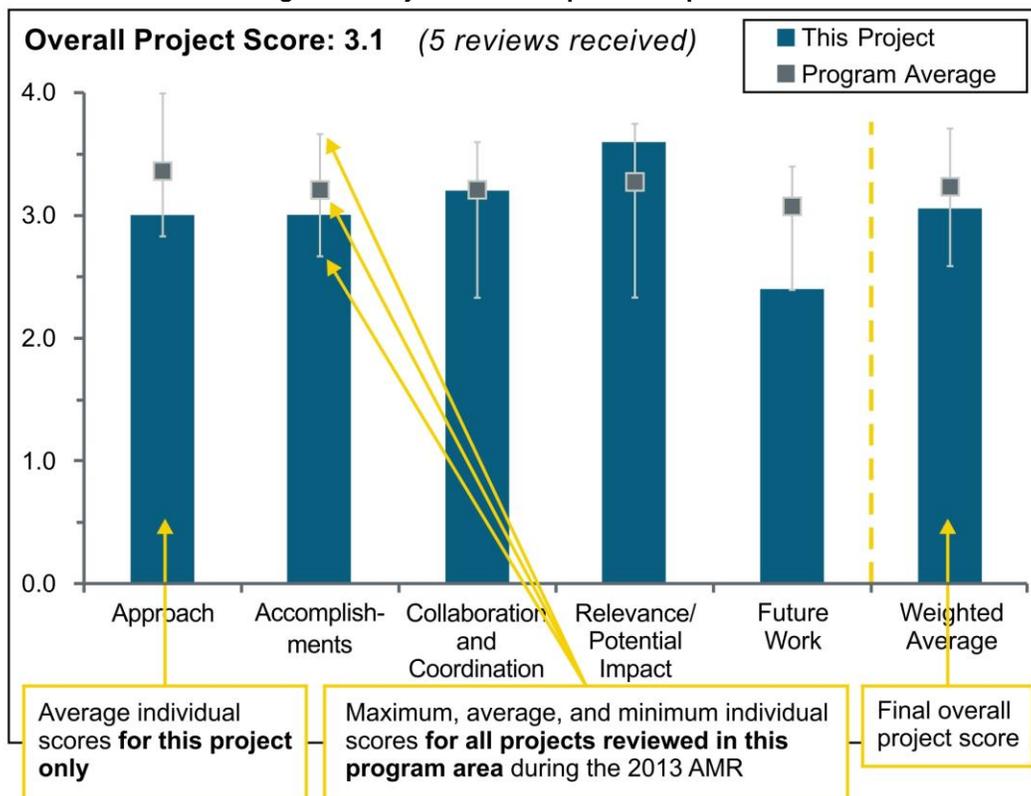
Reviewers were also asked to provide qualitative comments regarding the five criteria, specific strengths and weaknesses of the project, and any recommendations relating to the work scope. These comments were also entered into the online, private database for easy retrieval and analysis.

## Organization of the Report

The project comments and scores are grouped by program area (Hydrogen Production and Delivery; Hydrogen Storage; Fuel Cells; Manufacturing R&D; Technology Validation; Safety, Codes and Standards; Market Transformation; and Systems Analysis) in order to align with the Fuel Cell Technologies Office’s planning scheme. Each of these sections begins with a brief description of the general type of research and development or other activity being conducted. Next are the results of the reviews of each project presented at the 2013 AMR. The report also includes a summary of the qualitative comments for each project, as well as a graph showing the overall project score and a comparison of how each project aligns with all of the other projects in its program area. A sample graph is provided in Figure 1.

Projects are compared based on a consistent set of criteria. Each project has a chart with bars representing that project’s average scores for each of the five designated criteria. The gray vertical hash marks that overlay the blue bars represent the corresponding maximum, average, and minimum scores for all of the projects in the same program.

Figure 1: Project Score Graph with Explanation



For clarification, consider a hypothetical review in which only five projects were presented and reviewed in a program area. Table 2 displays the average scores for each project according to the five rated criteria.

Table 2: Sample Project Scores

	Approach (20%)	Accomplishments (45%)	Collaboration and Coordination (10%)	Relevance/Potential Impact (15%)	Future Work (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
Maximum	3.6	3.7	3.5	3.4	3.4
Average	3.3	3.2	3.1	3.0	3.1
Minimum	3.0	2.6	2.7	2.7	2.9

Using this data, the chart for Project A would contain five bars representing the values listed for that project in Table 2. A gray hash mark indicating the related maximum, minimum, and average values for all of the projects in Project A’s program area (the last three lines in the table above) would overlay each corresponding bar to facilitate comparison. In addition, each project’s criteria scores would be weighted and combined to produce a final, overall project score that would permit meaningful comparisons to other projects. Below is a sample calculation for the Project A weighted score.

$$\text{Final Score for Project A} = [3.4 \times 0.20] + [3.3 \times 0.45] + [3.3 \times 0.10] + [3.2 \times 0.15] + [3.1 \times 0.10] = 3.3$$

## 2013 — Hydrogen Production and Delivery Summary of Annual Merit Review of the Hydrogen Production and Delivery Program

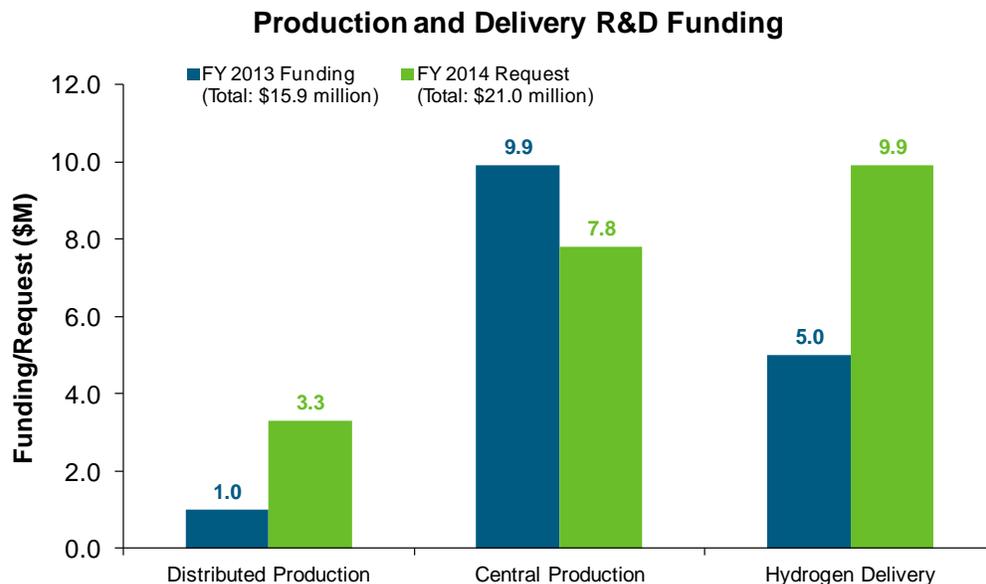
### Summary of Reviewer Comments on the Hydrogen Production and Delivery Program:

This review session evaluated hydrogen production and delivery research and development (R&D) activities in the U.S. Department of Energy (DOE) Fuel Cell Technologies Office (FCTO) in the Office of Energy Efficiency and Renewable Energy. The hydrogen production projects reviewed represented a diverse portfolio of technologies to produce hydrogen from renewable energy sources. Production project sub-categories included water electrolysis, solar-driven thermochemical cycles, photoelectrochemical (PEC) direct water splitting, and biological hydrogen production. The hydrogen delivery projects reviewed included R&D for low-cost pipeline materials; pipeline and forecourt compression, including electrochemical and cryo-compression technologies; and delivery cost analyses.

The reviewers recognized the production and delivery portfolios as focused, effective, and well managed, and the projects as well aligned with DOE goals and objectives. Reviewers commented positively on the progress made by the projects in the past year and noted the many beneficial collaborations between project partners and with outside organizations. They also emphasized the need for continued cost modeling of production and delivery technologies to identify and address cost barriers. Reviewers also stressed the need for balance between short-, mid-, and long-term technologies in the portfolios, and for more attention to mid-term goals, targets, and deployments.

### Hydrogen Production and Delivery Funding by Technology:

The fiscal year (FY) 2013 appropriation for the Hydrogen Production and Delivery program of the FCTO was \$15.7 million. Funding was distributed 68% to 32% between hydrogen production and hydrogen delivery, respectively; this is approximately the same distribution used in FY 2012. Production funding is increasingly focused on long-term, renewable pathways such as PEC, biological, and solar-thermochemical hydrogen production. While this emphasis will continue in FY 2014 as part of the \$21 million budget request, it is anticipated that there will also be new R&D starts addressing short- to mid-term technologies in production and delivery. The delivery portfolio emphasis in FY 2013 was on reducing near-term technology costs such as those associated with tube trailers and forecourt compressors, and identifying additional low-cost early market delivery pathways that are viable. This emphasis will continue in FY 2014.



### Majority of Reviewer Comments and Recommendations:

Fifteen projects were reviewed, receiving above-average to high scores (3.0–3.6) with an average score of 3.3. The scores are indicative of the technical progress that has been made over the past year.

**Biological Hydrogen Production:** Five projects in biological hydrogen production were reviewed, with an average score of 3.3. Projects in this area included efforts to improve the performance of algal, cyanobacterial, and bacterial microorganisms that produce hydrogen through splitting water or fermentation of biomass. Reviewers cited a number of achievements, including 1) light-induced hydrogen production by algal cells expressing a bacterial hydrogenase at oxygen levels that suppress the normal algal hydrogen production, 2) effective combination of different methodologies and modifications to improve cyanobacterial systems, and 3) deletion of a metabolic pathway that could compete with fermentative hydrogen production. However, they also expressed concern that there could be difficulty with scaling up these types of systems to industrial scale and questioned the ability of the modified strains to thrive under bioreactor conditions. Key recommendations were to seek collaborations and to identify more specific and quantitative targets for intermediate steps in the different projects for this longer-term pathway.

**Electrolysis:** Presentations or posters were given for seven projects (including one new Phase I and four Phase II Small Business Innovation Research [SBIR] projects) addressing low-cost, high-performance hydrogen production; renewable energy storage; grid integration (reviewed in the Technology Validation session); and home refueling. Because most of the projects were either just starting or in their last year, or reviewed in another session, only one electrolysis project—an SBIR Phase II project addressing high-efficiency electrocatalysts for alkaline membrane electrolysis—was reviewed in this session. This project received a final score of 3.0. Reviewers praised the efforts to use less-expensive materials to reduce the cost of electrolyzers. However, it was noted that the Ru- and Ir-based pyrochlore catalysts under consideration may not provide enough of a cost benefit when compared to traditional precious metal catalysts. Reviewers suggested reducing efforts in catalyst development in order to focus on other areas of research, such as membrane performance and durability. Carrying out a Hydrogen Analysis model (H2A) cost analysis was also recommended.

**Hydrogen Delivery:** Five projects were reviewed in the area of hydrogen delivery, receiving an average score of 3.4. Projects were praised by reviewers for good organization, collaboration, and return on investment. It was recommended that all projects update and expand cost and system analysis by adding more factors, gathering more data from stakeholders, and using updated information from the Hydrogen Delivery Scenario Analysis Model (HDSAM) and H2A analyses. Project-specific suggestions for improvements were also made, including improving system engineering (e.g., improvements in welding) and testing (e.g., using extreme conditions) and preparing for demonstration technologies that have reached the appropriate stage of research. The cost analyses were noted as important in determining the potential of the projects for reaching DOE targets.

**Photoelectrochemical Hydrogen Production:** Five oral presentations and four poster presentations were given in the area of materials R&D for solar hydrogen production via PEC water-splitting. Many of the PEC projects are ending in 2013, and most have been reviewed numerous times since their inception. Two ongoing PEC projects were reviewed, receiving an average score of 3.3. Reviewers felt that projects in this area were well aligned with DOE objectives, with a focus on developing the most promising PEC material systems and prototypes. They acknowledged notable accomplishments in enhanced durability in the promising III-V semiconductor materials under investigation in these projects. Projects were rated highly for advancing the state of the art in theoretical understanding and experimental characterization of PEC interfaces, developing innovative surface treatments for extending PEC durability, and effective collaborations with the PEC Working Group. Recommendations for future work included stronger emphasis on demonstrating the extended durability of high-efficiency III-V devices under realistic on-sun conditions, further consideration of alternative lower-cost material systems, and expanded collaborative efforts. Reviewers also noted that continued refinement of R&D priorities based on performance and cost analysis is needed.

**Solar-Driven High-Temperature Thermochemical Production:** Presentations or posters were given for five solar-driven, high-temperature thermochemical hydrogen production projects—two addressing two-step, high-temperature reaction cycles, and three addressing hybrid (multi-step, including an electrolysis step) reaction cycles. The latter projects are ending in 2013 and were not reviewed. The two reviewed projects received an average score

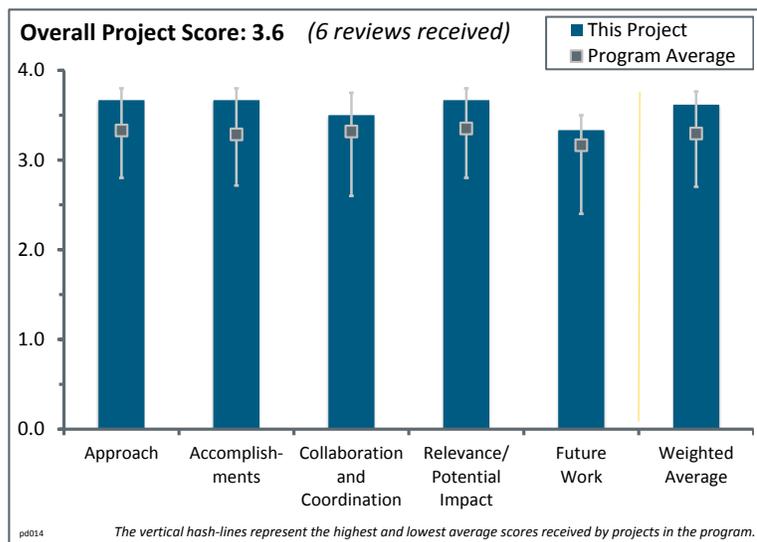
of 3.3. Reviewers praised the innovative approaches and achievements in evaluation of kinetics, analysis of performance requirements, and materials selection and design for the perovskite and hercynite reaction cycles. Suggestions for both projects included increasing attention to reactor design, scale-up and testing, and H<sub>2</sub>A cost and performance analysis.

## Project # PD-014: Hydrogen Delivery Infrastructure Analysis

Marianne Mintz; Argonne National Laboratory

### Brief Summary of Project:

This project strives to provide a platform for comparing alternative hydrogen delivery component and system options to reduce the cost of delivered hydrogen. The H2A Delivery Scenario Analysis Model (HDSAM) provides a modeling structure to automatically link and size components into optimized pathways to satisfy requirements of market scenarios and computes component and system costs, energy, and greenhouse gas emissions. The scope of fiscal year 2013 activities included incorporating the SAE J2601 refueling protocol in the modeling of hydrogen refueling stations, evaluating the role of high-pressure tube trailers in reducing refueling station capital, and updating estimates for the hydrogen delivery cost and contribution of refueling station components.



### Question 1: Approach to performing the work

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

- This appears to be a robust approach.
- It is excellent that the work centers on use of practical infrastructure that exists or is about to be commercialized.
- The models created to evaluate hydrogen delivery pathways are essential to the effort to evaluate the options for greenhouse gas (GHG) reduction using hydrogen as a fuel. The outreach to industry, technical teams, and other national laboratories is exemplary.
- The development of a rigorous thermodynamic tank fill model will enable a more detailed understanding of the fill process. The use of modeling to examine multiple forecourt configurations has identified promising new options to reduce delivery cost.
- The barriers are well defined along with the partners and the funds necessary to overcome the barriers. There are three national laboratories and industry partners. It is unclear if the team looked at other performance models being developed overseas.
- It is not obvious who sets the priorities for analysis. It is not clear how the model is addressing industry needs.
- It is unclear if there really is a lack of analysis in this area. The industry appears one step further on the way to standardization.

### Question 2: Accomplishments and progress toward overall project and U.S. Department of Energy (DOE) goals

This project was rated **3.7** for its accomplishments and progress.

- This is truly outstanding work by the Argonne National Laboratory (ANL) team.
- It is essential to incorporate SAE J2601 as soon as possible; otherwise the results are of questionable value.
- The results of the high-pressure tube trailer work show a clear path to lowering forecourt costs. This project has delivered a very good return for a \$300,000 investment.

- The work performed to date is a practical assessment of the industry's progress and the anticipated pathways.
- The supply side may need to be reconsidered as the demand side is adjusted over the next three, five, and ten years.
- Although the industry and stakeholders apparently provided input on the direction of this effort and what delivery options to include, it is unknown (level of certainty) if the investigated delivery pathways will be used by industry. In addition, it is not clear if this pathway is realistic due to the property size of existing gas stations (the footprint available to add hydrogen station equipment) and the separation distances required by building/station codes and standards (set by the National Fire Protection Association).

### Question 3: Collaboration and coordination with other institutions

This project was rated **3.5** for its collaboration and coordination.

- The project team is doing a nice job socializing their analysis with peer organizations and sourcing data from organizations that currently or will soon operate in this space.
- The collaboration between ANL, Pacific Northwest National Laboratory, and the National Renewable Energy Laboratory is excellent. This reviewer attended the DOE-sponsored Hydrogen Compression, Storage, and Dispensing (CSD) Cost Reduction Workshop and therefore may be more aware of the collaboration than the other reviewers.
- There is apparent interaction with other national labs and industry stakeholders, although the role of the other national labs is not always clear. Regarding the hydrogen production companies as industry stakeholders, there should be an effort to approach and include their suppliers (and potential suppliers) to get more reliable cost information.
- It is unclear how much the industry is involved and if it is involved through the U.S. DRIVE Technical Teams. It is unclear what "regular interaction" means.
- This project has limited formal collaboration, but this has not adversely affected the program. Significant work has been done with industrial entities to obtain and validate cost and performance data.
- The team is getting support from the industry and developers to optimize pathways. The modeling needs to be continually revised as markets change to optimize station configuration. The work is based on SAE J2601. However, the SAE J2601 committee may be considering changes in fiscal year 2014.

### Question 4: Relevance/potential impact on advancing progress toward DOE research, development, and demonstration (RD&D) goals

This project was rated **3.7** for its relevance/potential impact.

- The hydrogen pathway work is very important, and the focus on compressor cost and technology is clearly identified by the work of this team.
- This project can help to set concrete priorities for future research and development projects, but it is unclear how this process works.
- Accurate modeling is essential for the program to guide research and ensure that research dollars are spent effectively.
- This work is considered critical to making sure the delivery models are in line and able to optimize equipment configuration as industry approaches the introduction of hydrogen refueling requirements.
- This project is providing the "checks and balances" for technologies and systems being considered to service the fuel cell electric vehicle (FCEV) market. The relevance is very high, and the potential impact will hopefully be in line with the industry's evolution.
- As this is a modeling effort, it will help with decision making, but it is not clear what the industry response will be based on the findings. In addition, it is unclear what the overhead margins are for station equipment because of the small number of suppliers. It is good to see an evaluation of the number of cascade tanks and the effect on station cost.

### Question 5: Proposed future work

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

- The future work is necessary.
- The future work matches well with the new areas in the research portfolio.
- This project needs to continue with the analysis phase to consider energy requirements.
- It is not quite clear how the future work is defined nor if there will be any work on the cryo-pump within the liquid delivery options. SAE J2601 is essential, but it is not clear if there will also be recommendations on potential changes to this standard.
- This project should consider the cost of underground hydrogen storage, as it is already becoming increasingly difficult to find properties that can house hydrogen station equipment, especially considering the current small capacity/size of proposed stations compared to what is expected for full commercialization.
- The key issues that need to be incorporated into future H2A and HDSAM model revisions include the following:
  - The large-diameter 160 bar low-pressure steel storage tubes shown in the configuration model are not commercially available.
  - The models show single compressors that can go from 20 bar to 950 bar, and these, too, are not commercially available; hence the need to break compression into two steps from 20 to 500 bar and then 500 to 950 bar.
  - The models show 875 bar as the maximum pressure out of the compressor, but that is not enough to achieve 700 bar fueling. The current technology is 950 bar type with four composite tubes. The models do not yet include the cycle life of high-pressure tubes or methods to optimize the station cost with respect to the tube cycle life. This is more of a factor for steel tubes than composite tubes, but all high-pressure tubes have cycle life “issues.”

#### Project strengths:

- This project is strong.
- This project has a strong techno-economic analysis.
- This project has a strong scientific partnership and a very comprehensive tool.
- The inclusion of industry and stakeholder input in both the review and focus of the research is a strength of the project.
- The development of the models to analyze hydrogen delivery infrastructure is critical to support the deployment of hydrogen-fueled FCEVs, which offer both zero tailpipe emissions and lower total well-to-wheel emissions compared to any other fast-fill vehicle fuel technology.
- The project should review the model’s analysis and validation to ensure the scenario conditions are realistic and the permutations are in agreement. Refining the tube trailer configuration is providing good insight as to the cost of their use for hydrogen delivery. Physical loss projections may need to be re-evaluated.

#### Project weaknesses:

- The low level of funding limits capabilities.
- The model is as strong as the data provided by stakeholders.
- This project needs more funding to enable the team to consider all supply options.
- The industry collaboration is not transparent. With regard to that, the industry relevance is also hard to judge.
- This project needs to document and publish the findings and expand the effort model with future technologies.
- The only project weaknesses are associated with some of the assumptions made in the Nexant report years ago, which have been carried forward in the HDSAM and H2A models. This must be addressed in the future work.

**Recommendations for additions/deletions to project scope:**

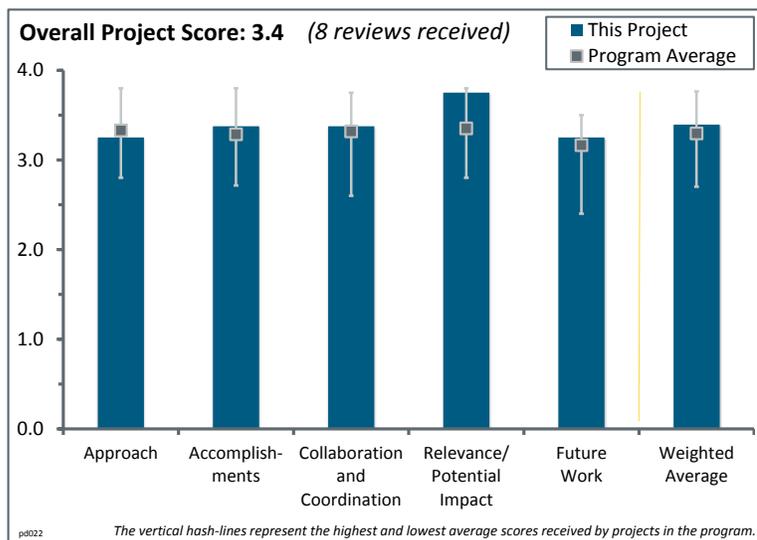
- It is not clear what will happen if the dispensing temperature based on SAE codes changes.
- This project should have stronger technical recommendations towards industry, maybe through a definition of baseline / standard stations. This project should include an ionic compressor and cryo-pump in the analysis. It is not clear if there any considerations for mobile refueling hardware.
- It would be great to see a comparison of the compressed natural gas (CNG) and liquefied natural gas (LNG) fueling pathways to the various hydrogen (and FCEV) pathways. There are a lot of fugitive emissions associated with LNG transfer (over 20% losses between liquefier transfer to tanker, transfer to LNG station bulk tank, and final transfer of LNG to the vehicle). These GHG emissions are not well known and do not (yet) get the same scrutiny as the hydrogen production and delivery pathways.
- The project should look into the cost and economics of underground storage (both bulk and small-scale), including the impact of decreased pre-cooling requirements on the dispensed cost of hydrogen.
- This project should model the impact of the cost and durability of 35 and 70 MPa nozzles (and hoses) on the annual operating cost of hydrogen stations, considering that 70 MPa nozzles currently cost ~\$10,000/unit, rebuilds are very costly, and nozzles are not very robust when dropped. The project should compare this to gasoline nozzles (~\$300/unit) and CNG nozzles.
- This project should explore if station operators really use a temperature and pressure communication signal to fill hydrogen vehicles.
- This project should explore what ideal station sizes are at different SAE J2601 filling temperatures (economy, efficiency, cascade size, etc.).
- The project should be careful not to get too wrapped up with modeling all aspects of J2601 in different parts of the station system. All stations that fill FCEVs will need to be J2601 compliant, and the current J2601 modeling team already has a hard time modeling this for the revision of the J2601 Technical Information Report (2010).
- This project should consider an evaluation of the annual operating cost at different station sizes (currently quoted operation and maintenance costs appear to be high).
- It is unclear if these models consider continuously running compressors. Apparently, the frequent start/stop events have a significant impact on durability/lifetime, and this could be an option to consider in addition to the economics/efficiency of the number of cascade tanks.

## Project # PD-022: Fiber-Reinforced Composite Pipelines

Thad Adams; Savannah River National Laboratory

### Brief Summary of Project:

Composite pipeline technology has the potential to reduce installation costs and improve reliability for hydrogen pipelines. Advantages of using fiber-reinforced polymer (FRP) include excellent burst pressure ratings, superior chemical and corrosion resistance, and reduced installation costs with spooling. The goals of this project are to provide test data to support a technical basis for using technology in hydrogen service and to integrate FRP into the ASME B31.12 Hydrogen Piping and Pipeline Code by 2015. This project performed fatigue testing in FRP at various pressures in fiscal year (FY) 2013.



### Question 1: Approach to performing the work

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

- The approach was well laid out and seems well designed. The key is getting ASME involved and using natural gas experience to help.
- The program continues to address the technical concerns associated with placing fiber-reinforced piping in hydrogen service, which is being coordinated in parallel with safety, codes, and standards development.
- The contractor performed good engineering practices, fatigue testing under several pressure conditions, and a fatigue cycle test as outlined in the FY 2012 forward work and FY 2013 progress report.
- This is excellent work for the level of funding provided. The scope of the work should be expanded to include a greater number of environmental stressors and conditions, such as moisture, temperature extremes, more flaw sizes, flaw orientation, etc. The work should also be expanded, not only to address how to test pipes but also to figure out how to overcome the shortcomings identified and design better pipes.
- This is a great, clever, low-cost alternative to metal pipes, and it is excellent that this project is concurrently funded with the metal pipeline project, as this is the most pragmatic approach to total success. The approach is to conduct standard fatigue tests of FRP under pressure. This is a well-defined, readily achievable objective, but also may be the key problem with the project. The scope is very limited to ideal conditions and does not completely replicate the extreme conditions that FRP will face when implemented. A key focus of the work needs to be accelerated testing in extreme conditions. Many advantages to FRP are cited, including limited joints, the ability to manufacture it onsite, low embrittlement, etc. A key addition to this list could be safety at puncture from reduced spark ignition. This should be tested against standard metal pipes, as it could be a significant selling point.
- The management of the project is very good. The project is well organized and follows a written FRP live management plan, an important tool for a multi-year project. The goals are credible and aligned with the U.S. Department of Energy goals. The team has managed to keep the project moving forward, despite funding fluctuations, and have identified some engineering issues (e.g., O-ring extrusion). While the ultimate goal of the project is the applied engineering development of a product standard, the project needs to have more scientific depth, especially coming from a national laboratory. It would be valuable if the team added the goal of a peer-reviewed archival publication (more than an ASME report) so their study does not get lost over time.

- The approach used by the project is indeed a pipeline management plan. The issues of service degradation and design margins have already been addressed, and now the project focuses on quantifying the degradation mechanism(s) in an effort to describe the fatigue life of the structure as a function of hydrogen pressure. The identification of delaminating and fiber cracking is the key to ascertaining fatigue resistance. In this regard, the design of the fatigue pressure versus the cycles-to-failure diagram is an important tool that can help, in collaboration with other ASME codes and standards, to design safe operation performance maps. With regard to the O-ring failure, the association of the failure and extrusion with the asymmetry of the loading seems to set the direction to mitigate the problem, given that any hydrogen effects have been ruled out.
- It appears that over the course of this project, including the work done at both Savannah River National Laboratory (SRNL) and Oak Ridge National Laboratory (ORNL), sufficient testing of commercially available FRP pipelines has been done to allow their proper design and use for hydrogen transport under codes and standards that will now be completed by ASME. It would be better if all the key tests and test results were presented in a concise manner and conclusions drawn as to the acceptability of FRP pipeline for hydrogen transport and whether any additional testing is required. The list of testing categories is provided but with no summary of the results and conclusions. Hydrogen leak rates from FRP pipelines have been measured and appear reasonably low. However, it is not clear from the presentation if acceptable hydrogen leak rates from FRP pipelines have been established and who should set these leak rates. Fatigue testing has been done, but it is not clear if this was done at all the appropriate frequencies and stress levels. In prior years, SRNL developed an FRP life management plan that guides what testing needs to be done. SRNL is writing a very complete report on all the testing that has been done, which should greatly aid the writing of FRP pipeline for hydrogen transport codes and standards by ASME.

## Question 2: Accomplishments and progress toward overall project and U.S. Department of Energy (DOE) goals

This project was rated **3.4** for its accomplishments and progress.

- The project's barriers and goals are well defined and are being met.
- Progress appears good, but the real test will be the actual acceptance by ASME, which is a pass/fail point.
- The team accomplishments demonstrated the ability to overcome several technical challenges that were directly targeted at the DOE goals.
- Given the goals stated for the project, the team is making good progress and following their plan. It is not clear how their work affects the cost of pipelines other than enabling an alternative to higher-cost steel. They are definitely on track to meet the standards goal, as evidenced by progress on developing fatigue failure data and their leadership on the ASME B31.12 committee to codify the results.
- This year, fatigue testing was completed on unflawed FRP pipelines that also included metallic joints. The leakage through the joint was identified as caused by insufficient O-ring design and material choice. A remedy was provided but not tested. The team wrote a thorough report on all the testing that has been done in prior years; the FY 2014 testing will be added to the report. This report should greatly aid the writing of the new codes and standards for FRP pipeline hydrogen transport.
- Observing how the project evolved over the years, one can safely state that significant progress has been made. In fact, the design of the initial diagram of the fatigue life of the FRP is a solid indicator of the progress made. The completion of the FRP testing report is another indication that the project's results can be discussed by ASME for codification and the setting of standards. In addition, this report provides a thorough review of the literature and the testing protocols. As such, it constitutes a valuable resource for future advancements in the field of FRPs.
- The project has accomplished its goals, but those goals should be expanded for more rigorous environmental stressors and a wider range of flaw sizes. The response of the composite will be sensitive not only to the flaw size but also to flaw orientation. The latter was not tested.
- It is shocking to see that this project is in its seventh year. It has achieved approximately half the rate of progress that would be expected. It is unclear why the project got to its sixth year before beginning pressurized fatigue testing. Ratings aside, the progress is definitive and demonstrates clear accomplishment towards DOE's objectives of reducing cost while maintaining safety.

**Question 3: Collaboration and coordination with other institutions**

This project was rated **3.4** for its collaboration and coordination.

- The researchers are following the most appropriate path to have this work turned into a test standard.
- The team demonstrated good coordination and collaborations among multiple organizations and institutions (e.g., ASME).
- This exhibits good teamwork among project partners that involve industry, government laboratories, and codes and standards.
- The collaboration appears very good, especially with ORNL and ASME. It would be good to have more manufacturers represented, and maybe the direct participation of more natural gas entities.
- Continuous interaction and exchange with ASME is very important for the project's results to be assessed from a technology standpoint. The listed collaboration with ORNL is not clear.
- There appears to be excellent collaboration with ASME on this project, which should greatly assist the writing of codes and standards for FRP pipeline for hydrogen transport service. There appears to be very good collaboration with FRP pipeline manufacturers. There is no mention of collaboration with the DOE Hydrogen and Fuel Cell Pipeline Working Group. This project is a member of that working group and should be collaborating with the other members on a more routine basis.
- This team has built just the right partnerships for the scope and funding level of this project. They have engaged the ASME B31.12 code committee and provide leadership. The team has an industrial supplier for FRP and shares engineering information. They have leveraged expertise in material systems at other federal laboratories. The one concern is that they are working with only one industrial supplier, which limits the diversity of fatigue failure information they are developing. It is not good to develop a product standard based on the system of only one supplier. The project would have to receive more resources in order to expand the testing base.
- There are no partners from academia included in the effort. This is particularly surprising given the potentially large scope of environments the piping will be exposed to, and the relatively straightforward nature of the fatigue tests. University partners could be contracted to accomplish these tasks, and a student could be trained to enter the workforce (win-win). Given the limited budget of this project, though, partnership with academia on a yearly basis may not be feasible. The partners are located primarily in the South. Given the geographical variability of this problem, it makes sense to have partners in other regions of the country. The partnership with ASME is strong and a key benefit. Much of the work completed here is applicable to general FRP use and not limited to hydrogen.

**Question 4: Relevance/potential impact on advancing progress toward DOE research, development, and demonstration (RD&D) goals**

This project was rated **3.8** for its relevance/potential impact.

- This is a critical step in providing a hydrogen delivery system.
- Pipelines play a significant role in hydrogen transfer, which has been identified in the DOE Fuel Cell Technologies (FCT) Office goals.
- DOE considers FRPs to be a cost-effective delivery pathway. As such, FRPS are a key technology that needs to be well understood with regard to reliability and safety. The project's results are helping to advance precisely this goal. The same holds for the project's research on O-rings, which are part of the structure.
- If the capital cost of hydrogen pipelines could be significantly reduced, hydrogen pipeline transport could be a low-cost option for hydrogen delivery and help enable meeting the FCT Office's cost targets. FRP pipeline holds that promise. This would be a key enabler of using hydrogen as a major energy carrier with very low-carbon emissions.
- Despite pipeline hydrogen distribution being envisioned as a longer-term hydrogen supply pathway, this fundamental understanding, development, and industry safety acceptance of lower-cost FRP will be valuable in supporting early market initiatives.
- This research is of benefit to general FRP use and is not limited to hydrogen. The development of a new ASME standard for hydrogen use in FRP is highly relevant. A direct comparison of the cost of FRP versus

metal pipelines was not presented and would make the case for relevance simple. It may be that this slide was included in the early years of the project. If not, it is a serious concern that this comparison has not yet been made.

- This project will be important only to the extent that there is a concentrated area of usage that is sufficient to support the investment in a pipeline network. This is likely to be quite far in the future, but it is a good building block. The project is excellent in the long term, but maybe only fair in the short term. The cost reduction will be important, but it is not clear how much FRP will actually reduce overall cost. The installation cost will be lower, but it is not clear what percentage this comprises of the overall cost, including overhead, permitting, rights of way, etc.

### Question 5: Proposed future work

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

- The proposed future work is a good plan to enable the use of FRP pipeline for hydrogen service.
- The work proposed is appropriate, but there needs to be more emphasis on optimizing the composite technology to design better pipes.
- The future work identified by the team demonstrates pathways to complete additional fatigue and rupture tests and complete codification into ASME standards.
- Completing FRP codification into ASME B31.12 would be a major accomplishment of this project and is within sight.
- If ASME is convinced that this is an appropriate item to add to their code set, that is excellent progress and should validate the technical approach.
- The team is following their FRP life management plan.
- Research has been proposed to determine the variability in the fatigue data by varying the loading ratio to  $R=p_{min}/p_{max}$ . This will allow the project to correlate the dependence of hydrogen-induced degradation in terms of parameters whose influence is known to be very important in the field of fatigue and in the absence of hydrogen, and perhaps will help draw conclusions on the nature of the failure mechanism(s).
- The proposed future work is non-specific, likely owing to problems during the early years in appropriately scoping the project. It is not clear what conditions will cause the FRP to fail and what factors primarily contribute to the cost. Identifying these clearly will help to scope the necessary extreme environment tests that need to be conducted and the components that need to be improved. The prevailing approach seems to be “try it and see,” and in the seventh year, that impression is frustrating. The accelerated lifetime tests are very relevant and a logical next step. The additional fatigue testing with Fiberspar absolutely needs to include testing pipe samples in use in various areas around the country, including very different environments. This project should try to find conditions that cause the FRP to fail. Only then can the limits be known that should become standards.

### Project strengths:

- This project has a good management plan, leadership on ASME B31.12, and structural design.
- The team exhibited great engineering practices with intensive levels of testing and coordination with ASME.
- Involvement of ASME early in the process to get buy-in was good, along with involvement of Fiberspar and the material testing.
- Integration with standards committees and manufacturers and understanding hydrogen delivery needs and industry are strengths of this project.
- This project has excellent, carefully controlled laboratory experiments. These form a foundation to compare to extreme environment tests. This is excellent work with standards development and the close partnership with ASME.
- This project appears to have outstanding project leadership, and the project team is successfully addressing the previously identified barriers of FRP pipeline for hydrogen service. Based on the work conducted to date, the team recognizes the need for additional fatigue testing and stress rupture testing.
- This project aims to collect the data needed to ascertain reliable and safe operation of FRPs in the presence of hydrogen. The development of the fatigue safety diagrams is a project strength because it helps elucidate

the integrity of the FRPs and therefore their judicious use for hydrogen transport. The proposed approach to develop inspection criteria for the failure of O-rings also serves the project objectives. Overall, the project is focused, and this in itself is a unique strength.

- If the capital cost of hydrogen pipelines could be significantly reduced, hydrogen pipeline transport could be a low-cost option for hydrogen delivery and help enable meeting the Program's cost targets. The FRP pipeline holds that promise. This would be a key enabler of using hydrogen as a major energy carrier with very low-carbon emissions. The team wrote a thorough report on all the testing that has been done in prior years and will add the FY 2013 testing to the report. This report should greatly aid the writing of codes and standards for FRP pipelines for hydrogen transport. There appears to be excellent collaboration with ASME on this project, which should also greatly assist the writing of codes and standards. There appears to be very good collaboration with FRP pipeline manufacturers.

### Project weaknesses:

- This project needs deeper material science and archival publications.
- It is not clear if the team considered alternative O-ring materials.
- Hydrogen permeation at different working pressures was not investigated or addressed by the contractor.
- There are too few environmental stressor variations. There is a lack of recognition of the importance of flaw orientation on the mechanical behavior of composite materials.
- The presenter specifically said, "No impact on varying pH was detected." However, slide 26 states that "[in] extreme values of pH some impact could be seen." This direct discrepancy, with a non-specified value of impact, is a concern. The proposed future work is non-specific, which is likely because of problems with appropriately scoping the project in early years. It is not clear what conditions will cause the FRP to fail or what factors primarily contribute to cost. After seven years, one would expect at least a bullet on these issues.
- It would be much better if all the key tests and test results were presented in a concise manner and conclusions were drawn on the acceptability of FRP pipeline for hydrogen transport and whether any additional testing is required. The list of testing categories is provided but with no summary of the results and conclusions. There is no mention of collaboration with the DOE Hydrogen and Fuel Cell Pipeline Working Group. This project is a member of that working group and should be collaborating with the other members on a routine basis.
- By testing only one company's product, it is not clear that the project addressed the potential failure issues of other manufacturers. The project should consider that one company may have specific know-how that another does not. It is not clear if the mechanical fittings will ever be acceptable for direct burial, especially at high pressure and with the test results. There are already some restrictions in this regard in codes, and it is unclear if it is practical in the long term based upon historical leakage and the test results that already show issues. The focus has been as much on the O-ring and mechanical connection as the pipe. While these are needed, it distracts from the fundamentals of the pipe itself.
- The main weakness of the project is the lack of fundamental understanding on how fatigue advances delamination and failure in the presence of hydrogen. This is a weakness because unless we understand the parameters governing this failure mechanism, the project results may be specific only to the pipelines tested under the given flawed geometry and loading conditions. The reference to the fact that a Fiberspar pipe section in Alberta, Canada, meets the factory specifications on burst pressure and glass transition is not rigorous scientific evidence. It is not known whether the loading frequency, the loading ratio, etc. in Alberta are the same as those for hydrogen transport in the United States. The association of the O-ring failure with the material hardness was an unclear point during the project presentation. In fact, the reviewer does not understand why hardness is associated with the extrusion of the O-ring.

### Recommendations for additions/deletions to project scope:

- The project's scope and funding should be increased to include more test conditions and flaw orientations.
- A general understanding of the quality of commercially available FRP material would be good for establishing the likelihood of material flaws.
- The project should add research and/or shift efforts to avoiding underground mechanical joints, which are too prone to failure and leakage.

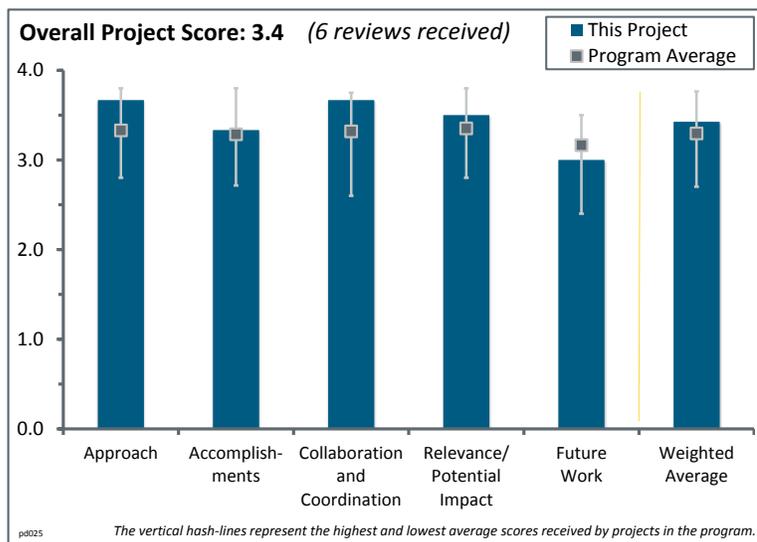
- Hydrogen permeation is a major concern, especially at high pressure. The project team should consider addressing and evaluating hydrogen permeation through the material, especially at mechanical coupling joints.
- With the baseline and ideal laboratory measurements nearing completion, the researchers must find the limits to the technology due to extreme environmental variability. The only way to ensure safety is by carefully locating and quantifying the limits, then making sure the FRP is not installed in conditions that could approach these limits. Modeling should have been completed early on in the project to identify the most sensitive environment sources of degradation. As it stands now, the researchers are stuck with a “try it and see” approach. After seven years, that approach seems unsound; however, the project must go on, given the importance and established investment.
- It seems that third-party damage is an important cause for FRP failure. Hence, a protocol to assess this is required. It is not clear from the project’s presentation how a water environment affects the performance of the FRPs. If the presence of epoxy will mitigate the issue, it is not clear what happens if the integrity of the epoxy layer is disrupted. Apart from the load ratio  $R$ , the loading frequency needs to be investigated as well.

## Project # PD-025: Hydrogen Embrittlement of Structural Steels

Brian Somerday; Sandia National Laboratories

### Brief Summary of Project:

This project measured the fracture thresholds and fatigue crack growth of steel hydrogen pipelines to demonstrate the reliability and integrity of steel hydrogen pipelines for cyclic pressure applications. Hydrogen embrittlement was accommodated by measuring fracture properties in hydrogen following the ASME B31.12 design standard. An analytical model was developed to quantify the inhibiting effects of oxygen on hydrogen-accelerated fatigue crack growth, including variables such as load-cycle frequency and oxygen concentration. This model may provide insight into the effects of gas impurities on hydrogen-accelerated fatigue crack growth for mixed natural gas plus hydrogen.



### Question 1: Approach to performing the work

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

- This project is making continued good progress on long-term goals. It seems to focus on key items, such as welding.
- Understanding and possibly mitigating the effect of hydrogen embrittlement on steel pipelines is a good objective.
- The team demonstrated good engineering practices, fatigue testing, effects of cracks, crack propagation, and understanding the effects of oxygen on hydrogen embrittlement.
- This was a solid, outstanding all-around presentation of the approach. This is a textbook example of taxpayer funding well spent. Moreover, DOE's dual-front funding approach of existing technologies likely to carry hydrogen and next-generation technology (another program) is the most pragmatic way to prevent an accident.
- The barriers are discussed and partially addressed. It is not clear whether the research team studied modern X-65 steels or older (1970s) X-65 steels. They do have different microstructures. The project should interface with Oak Ridge National Laboratory (ORNL) in regards to their friction stir welding research efforts. There should also be more work on the migration of oxygen impurities and other contaminants from natural gas that act as a catalyst or a contaminant at the crack tip.
- The focus of this project is to fully understand hydrogen embrittlement in steel pipelines so that they can be properly designed for safety and reliability. The key remaining issues to address in this effort include fatigue crack growth in the presence of gas impurities, such as oxygen, and the nature of hydrogen embrittlement in welds. The project is taking an outstanding approach to researching these issues. It is using state-of-the-art experimental techniques and equipment to measure fatigue crack growth rates under fatigue conditions in the presence of hydrogen at pipeline operating pressures. It is combining this with theoretical models that can explain the observed behavior and testing these models. It is now also using density functional theory (DFT) to predict the impact of various gas impurities on hydrogen embrittlement. The combination of these approaches is providing remarkable insight into the nature of hydrogen embrittlement that will enable appropriate design of steel pipelines for hydrogen transport.

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**Question 2: Accomplishments and progress toward overall project and U.S. Department of Energy (DOE) goals**

This project was rated **3.3** for its accomplishments and progress.

- This is decisive proof of a physics-based model showing validation with carefully taken measurements.
- The team's accomplishments demonstrated several technical challenges that were directly targeted at DOE's goals.
- The accomplishments are good, but there is too much focus on inhibitors that might have limited practical value.
- There is conclusive evidence that low-cost additives to steel pipelines can significantly reduce embrittlement and, therefore, pipeline cost.
- This project strongly supports long-range goals and objectives of the DOE Hydrogen and Fuel Cells Program (the Program). The progress achieved over the past year is discussed. This project will need to expand the work scope to include higher strength and modern steels, including weld consumables and processes that may help meet the future projected cost requirements.
- Considering the funding level for fiscal year (FY) 2013, this project has made excellent progress. It expanded the model being used to predict fatigue crack growth behavior in the presence of gas impurities in the hydrogen. The model predictions with oxygen fit the observed behavior extremely well. This year, the project also included the use of DFT to be able to predict the impact of impurities other than oxygen. Fatigue crack growth rates are now being measured on various parts of welds. The results are remarkably consistent considering the experimental challenge of the non-homogeneities present in welds. This is due to outstanding experimental technique.
- It does not seem like a year's worth of work was done since last year's presentation. A model has been developed, but that should not have taken a year. It would have been good to see greater progress over this time.

**Question 3: Collaboration and coordination with other institutions**

This project was rated **3.7** for its collaboration and coordination.

- This is a textbook example of good collaboration and coordination.
- This project has good coordination with a large consortium of investigators. Participation by Dr. Petros Sofronis at the University of Illinois makes this possible.
- The team demonstrated excellent coordination and collaborations among multiple organizations and institutions.
- This project has good collaboration and an open process with others. The key stakeholder is the U.S. Department of Transportation (DOT), and they are engaged.
- The collaboration on research efforts is underway with ORNL and there was some mention of the National Institute of Standards and Technology (NIST). This project needs to look at an expanded model for fracture properties recently developed by NIST-Boulder.
- This project is part of the DOE Pipeline Working Group. This group consists of all of the Program-funded projects on hydrogen pipelines and other organizations. This encompasses national laboratories, Secat, Inc., Exxon Mobil, the University of Illinois, NIST and ASME. This group meets at least once per year to share results and provide insights into each other's work. The experimental work done at Sandia National Laboratories (SNL) is done in true seamless partnership with the theoretical modeling work at the University of Illinois. This partnership is resulting in remarkable data and understanding of the hydrogen embrittlement of steels. The people at SNL and the University of Illinois are also members of the International Institute for a Carbon Neutral Society funded by Japan. This presents the potential for additional collaboration on hydrogen embrittlement of steels being done at Kyushu University in Japan.

**Question 4: Relevance/potential impact on advancing progress toward DOE research, development, and demonstration (RD&D) goals**

This project was rated **3.5** for its relevance/potential impact.

- This project targets the key weakness of steel pipelines for hydrogen transport.
- Pipeline is one of the most significant methods for hydrogen transport, and this has been identified in Program goals.
- This project will likely lead to economical additives for hydrogen pipelines that inherently limit embrittlement.
- Steel is the material of choice for all existing hydrogen pipelines, so steel is very relevant to industry and the future growth of hydrogen as a fuel; however, widespread pipelines are not needed until the economics of hydrogen can be justified.
- The work described appears to be in line with the project goals and objectives. This work is seen as critical to the Program and could potentially provide significant advancements toward verifying pipeline safety with the delivery of hydrogen. The failure prediction models under refinement have the potential of using other components within the fuel cell system.
- This project will enable the safe and reliable design of steel pipelines for the routine transport of hydrogen under the expected condition of oscillating pipeline pressures. This may be the least expensive method of transporting large amounts of hydrogen long distances when hydrogen is a major energy carrier. The current projected cost for the transport of hydrogen by steel pipelines is too high for rapid and significant penetration of hydrogen as an energy carrier, unless the cost of fossil fuels increases further. It is not clear how the results of this project could be applied to reduce the cost of hydrogen transport in steel pipelines.

**Question 5: Proposed future work**

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

- There should be less focus on inhibitors.
- This project needs to focus on friction stir welding to determine and demonstrate the lower-cost approach for safely transporting hydrogen.
- The future work identified by the team demonstrates pathways to complete additional fatigue crack growth measurements at both girth weld and seam welds, and additional pipeline steel testing.
- It would be good to see a greater rate of accomplishments from the project by (1) using the model to study other mechanisms of crack growth impeding other species, (2) looking at different steel compositions, and (3) using friction stir welding and studying differences in weld vulnerabilities.
- The future work includes gathering the needed data on fatigue crack growth rates for both girth and seam welds, as well as steels other than X52. It is not clear how the work done to date or the future work might address the high costs of hydrogen transport in steel pipelines.
- The most robust solution to embrittlement problems faced by pipeline operators needs to include a portfolio of remediation steps. The researchers have identified promising passive additives to economically accomplish this goal. A potential extension could include active crack remediation steps, for example, determining at what point during crack initiation the surface can be refinished or coated to remedy the crack to extend pipeline life without replacement. The presence of both oxygen and water could also be an interesting follow-up study.

**Project strengths:**

- This project targets the key weakness of steel pipelines for use with hydrogen.
- One strength is the principle investigator, who made a very “SMART” (Specific-Measurable-Attainable-Realistic-Timely) presentation.
- This project uses great engineering practices, along with modeling and collaborations with national laboratories and academia.
- This project has good basic research. Understanding the effect of impurities is also useful, albeit maybe not a practical consideration.

- The collaboration across several federal laboratories and agencies provides excellent use of funds and knowledge. Partnering with industry as well as codes and standards committees and groups is seen as a good, sound investment of research and development resources.
- The project is taking an outstanding approach to research fatigue crack growth rates in steel pipelines in the presence of hydrogen, including in the presence of gas impurities. It is using state-of-the-art experimental techniques and equipment to measure fatigue crack growth rates. It is combining this with theoretical models that can explain the observed behavior and testing of these models. The project is now also using DFT to be able to predict the impact of various gas impurities on hydrogen embrittlement. The combination of these approaches is providing remarkable insight into the nature of hydrogen embrittlement that will enable the appropriate design of steel pipelines for hydrogen transport. This project will enable the safe and reliable design of steel pipelines for the routine transport of hydrogen under the expected condition of oscillating pipeline pressures. This may be the least expensive method of transporting large amounts of hydrogen long distances when hydrogen is a major energy carrier. The experimental work performed at SNL is done in true seamless partnership with the theoretical modeling work at the University of Illinois. This partnership is resulting in remarkable data and an understanding of the hydrogen embrittlement of steels.

#### Project weaknesses:

- It is a stretch to find a weakness in this project. The difficulty of this project is low enough that a university could accomplish the same work, probably at a lower cost, and train students in the process. This could potentially be a better use of taxpayer funds. If students were trained during the program, it was not mentioned, and they were trained indirectly. The energy labs exist to do the big, dangerous, and expensive work that nobody else can. However, Somerday is doing a better job than most university faculty could, so he is the right person for the job.
- There was a poor rate of progress on objectives in 2013. This project needs to step up progress.
- To better evaluate the effects of hydrogen on crack growth, the principle investigator should look at recent developments in the crack growth models developed at NIST-Boulder for hydrogen-induced cracking.
- As much as modeling is important to gain an analytical understanding of a material's behavior, it still needs to be verified by actual testing. More testing needs to be done, especially on hydrogen dissociation in oxygen-rich environments.
- The focus on impurities acting as an inhibitor is interesting, but it is unclear if it can be used as a reliable method in practical use to guarantee safe performance. Also, the project must consider those impurities compared to SAE J2719 to make sure that they are even possible while meeting the required specifications.
- The current projected cost for the transport of hydrogen by steel pipelines is too high for rapid and significant penetration of hydrogen as an energy carrier using steel pipelines for hydrogen transport, unless the cost of fossil fuels increases further. It is not clear how the results of this project could be applied to reduce the cost of hydrogen transport in steel pipelines.

#### Recommendations for additions/deletions to project scope:

- This project should accelerate the work on objectives.
- This project should consider alternate welding methods and figure out/recommend a means of lowering the cost of steel pipelines.
- This project should attempt to determine how its results might be applied or extended to reduce the cost of transporting hydrogen in steel pipelines by better pipeline design, alternative steel compositions, or lower-cost welding.
- This project should have a joint discussion with ASME B31.12 code committees, SAE J260, NIST-Boulder, the ORNL friction stir welding research team, and the DOT Pipeline and Hazardous Materials Safety Administration to jointly develop a research and development plan to address the remaining issues.
- A potential extension could include active crack remediation steps, for example, determining at what point during crack initiation the surface can be refinished or coated to remedy the crack to extend pipeline life without replacement. The presence of both oxygen and water could also be an interesting follow-up study.
- Although steel pipelines provide significant advantages over competing technologies, they still require a significant number of girth welds. The welding process needs to be done onsite during the installation, and

its quality is directly impacted by the environment. More work and research needs to be done to further understand those impacts.

## Project # PD-028: Solar-Thermal Redox-Based Water Splitting Cycles

Al Weimer; University of Colorado

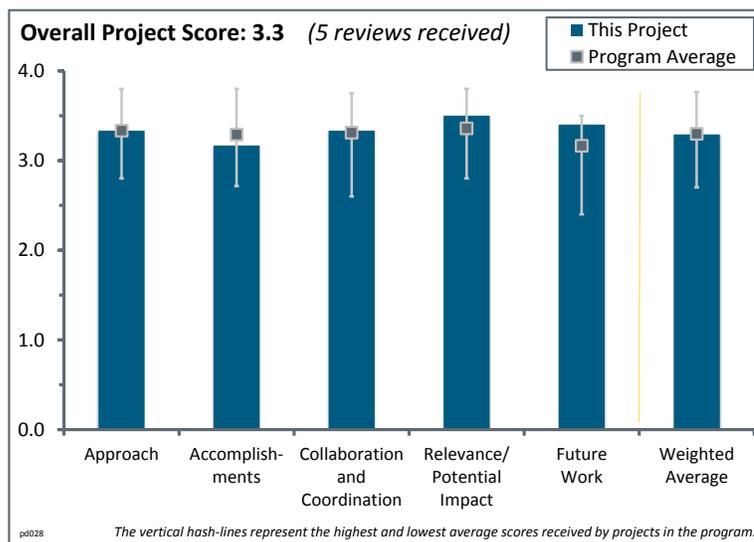
### Brief Summary of Project:

The objective of this project is to develop and demonstrate robust materials for a two-step thermochemical reduction-oxidation (redox) cycle that will integrate easily into a scalable solar-thermal reactor design and achieve the U.S. Department of Energy (DOE) cost targets for solar hydrogen. The project also develops steady-state and dynamic models of a multi-tube solar receiver to identify parameters controlling receiver efficiency, identify optimal tube/cavity configurations and solar flux input, and quantify the impacts of isothermal operation on receiver efficiency.

### Question 1: Approach to performing the work

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

- The project is doing excellent work on an innovative idea.
- This is a good practical approach to developing redox kinetics and materials selection.
- Evaluating the hercynite cycle materials and evaluating the effects of increased pressure and temperature on the reaction rates is a good approach towards meeting the main objectives of this project.
- The project focuses on a key factor to overcome the gap between the theoretical efficiency of thermochemical hydrogen production and the state of the art. A significant part of the provided solar energy is needed to reheat the redox material after water is split to remove the oxygen by working isothermally. This solves another problem of such high-temperature (HT) reactions; thermal stresses are minimized, possibly leading to much longer lifetimes of the components. The concept to identify an appropriate class of oxides and the development of appropriate structures is not likely to be improved.
- The project compared the hercynite isothermal process with the temperature swing performance of hercynite, cerium oxide (CeO<sub>2</sub>) and zirconium-doped CeO<sub>2</sub>, with a claim of superior hercynite isothermal performance using increased water vapor partial pressure. It is difficult to distinguish the operational or cost implications of this approach. Additionally, the penalty of simultaneous oxygen and hydrogen production was unclear. Isothermal reactor operation was not clearly explained, so it was difficult to discern the benefits or disadvantages of the isothermal approach beyond the claim of superior performance. The focus on isothermal swing process would benefit greatly by better exposition of system-level benefits beyond the material response to HT fluctuation.
- The material advantages of hercynite over modified cerias may be illusionary. The data are presented on a gram activity basis, but the density of ceria is approximately twice that of hercynite, which may minimize apparent activity differences on a volumetric basis. If ceria is both the active phase and support versus the hercynite on inert alumina, less hercynite is in the reactor relative to ceria, which further debits hercynite. One of the proposals for using hercynite in a particle flow reactor is to use atomic layer deposition to coat alumina nanospheres. Particle flow is likely to cause attrition, which would slowly abrade the outer-surface hercynite from the alumina core over many cycles, in addition to the slow loss of material that may result from the reaction cycle. The isothermal reactor performance of hercynite is excellent and represents a true and potentially significant advantage of the hercynite material that should continue to be pursued.



**Question 2: Accomplishments and progress toward overall project and U.S. Department of Energy (DOE) goals**

This project was rated **3.2** for its accomplishments and progress.

- This project has made good progress in understanding redox reaction rates.
- Good progress was presented on this project, including the benefits provided by the zirconium-doped CeO<sub>2</sub> and the effects of the increased water pressure on the hydrogen production rates.
- The demonstration of decent hydrogen production during isothermal cycling and the impacts of operating pressure and temperature performance of the hercynite are encouraging. The 150-cycle activity maintenance of the hercynite material appears promising. Use of the hercynite material in an isothermal reactor system appears feasible.
- Significant developments in performance could be achieved, and some are already reported. The methodology of the project has the potential to overcome key barriers leading to substantially higher process efficiencies and component lifetimes. Therefore the project also has the potential to significantly lower the cost for thermochemical hydrogen production.
- The progress of the hercynite cycle research and development (R&D) and its focus on critical performance metrics has been good. Among the missing ingredients are a system definition and system performance analysis using the Hydrogen Analysis (H2A) version 3 tool. It would seem that the many years of metal oxide thermochemical redox R&D would pay off with understanding and tools, permitting more rapid turn-around of material and system performance metrics.

**Question 3: Collaboration and coordination with other institutions**

This project was rated **3.3** for its collaboration and coordination.

- As can be seen from the results, the project has had a great deal of collaboration.
- Each partner serves a unique function and appears able to provide the team with the necessary skills and equipment.
- There seems to be reasonable collaboration between the researchers of this work and both the National Renewable Energy Laboratory and Sandia National Laboratories.
- The collaboration within the project is logical and necessary. By integrating world-leading knowledge on the high-flux irradiation of solar receiver–reactors and on laser-assisted stagnation flow reactors, the project goals seem to be achievable, and the results will be of very high quality.
- The collaboration metrics are outstanding, but the coordination metrics are poor based on the significantly divergent approaches to meeting common program objectives exhibited by the collaborating partners. Some of this is clearly a consequence of maintaining teams without a competitive solicitation of new projects, but the question remains whether the DOE Hydrogen and Fuel Cells Program would be better served by a more coordinated effort.

**Question 4: Relevance/potential impact on advancing progress toward DOE research, development, and demonstration (RD&D) goals**

This project was rated **3.50** for its relevance/potential impact.

- This project is very relevant to DOE's hydrogen production R&D objectives for the longer-term central hydrogen production targets.
- The relevance of the project is very high, as it might solve one of the key problems of two-step thermochemical cycles: the intermittent heating between the two steps. The impact in achieving higher efficiencies is therefore significant. Additionally, material issues of HT cycling will be minimized, probably leading to extended lifetimes of the components.
- HT thermochemical systems are incredibly complex, with very demanding operating conditions. This particular thermochemical program appears to offer a two-step isothermal cycle in a fixed-bed reactor, which is as simple as such a system can be. The potential for success appears higher than numerous alternative HT thermochemical processes explored in the past.

- It would have been good to see more progress on reactor design and analysis using H2A.
- Sufficient uncertainties remain for hercynite performance in both temperature swing and isothermal performance that prevent this project from moving into the “outstanding” category. Those uncertainties are largely reflected by operational uncertainties associated with both the emergent reactor design and the degree of simultaneous oxygen and hydrogen production.

### Question 5: Proposed future work

This project was rated **3.40** for its proposed future work.

- The proposed plan should enable continued progress and development of the hercynite system.
- The proposed work will add great value to this work, especially the inclusion of H2A analysis for the isothermal redox processing.
- The project has progressed in a logical manner. The future work should include dealing with steam flow variation and modifications to eliminate the variability mentioned. Scale-up issues with packed bed design should be understood.
- The proposed future work is the logical continuation of this outstanding project. The proposed task will make it possible to prepare more reactive particles and to demonstrate the technology under concentrated solar radiation.
- Much of the proposed future work addresses the completion of work reported in this review. However, the proposed future work also addresses the development of material for incorporation in a particle flow reactor. No benefits of this divergent approach were addressed.

### Project strengths:

- This project is very relevant to DOE’s longer-term hydrogen production pathways.
- The project is carried out by a world-class team of scientists. The partners create a strong synergy within the project. The project is well linked to other projects and teams in the same research area.
- Good data were gathered for developing rate expressions, there was good collaboration between labs and partners, and good work was done on optimizing materials for redox.
- This project has experienced researchers that have developed an effective plan to capitalize on the unique features of the hercynite system, which offers operating advantages over alternative HT thermochemical systems.
- The project is a very innovative attempt at solving one of the key issues to achieving close-to-theoretical efficiencies of thermochemical hydrogen production and reducing the temperature gap between the two steps.
- This project has clear technical proficiency and clear progress toward significant hydrogen production via both temperature swing and isothermal redox of hercynite. High-efficiency cycle performance was estimated. Cycle performance was demonstrated on different test beds.

### Project weaknesses:

- Not enough time was spent on reactor design and scale-up. The steam flow variation should have been addressed sooner.
- Hercynite, with its constant reaction back and forth into separate components, may offer integrity challenges that will only be apparent after prolonged HT operation.
- The reactor technology being used is straightforward and probably the right choice for carrying out this project. However, there are more advanced reactor concepts under development that might be suitable to achieve an additional raise in the efficiency of the process.
- This project has inadequate design and analysis (probably due to insufficient funds, but also possibly due to the lack of focus on program objectives). The collaborating partners continue to move along divergent paths, thereby diluting progress toward the program objectives. The justification for simultaneous development of a particle flow reactor was not clear.

**Recommendations for additions/deletions to project scope:**

- This project should implement an effective effort in design and performance analysis of a reactor and should work to accelerate the progress toward a cycle performance assessment via H2A v.3. The project should define the benefits/disadvantages of varying water vapor partial pressure to achieve higher performance rates. Also, investments required for implementing a particle reactor flow concept need to be justified.
- The existing connection with other teams should be used to combine all developments in two-step thermochemical cycles as well as on materials on reactor technology.

## Project # PD-035: Semiconductor Materials for Photoelectrolysis

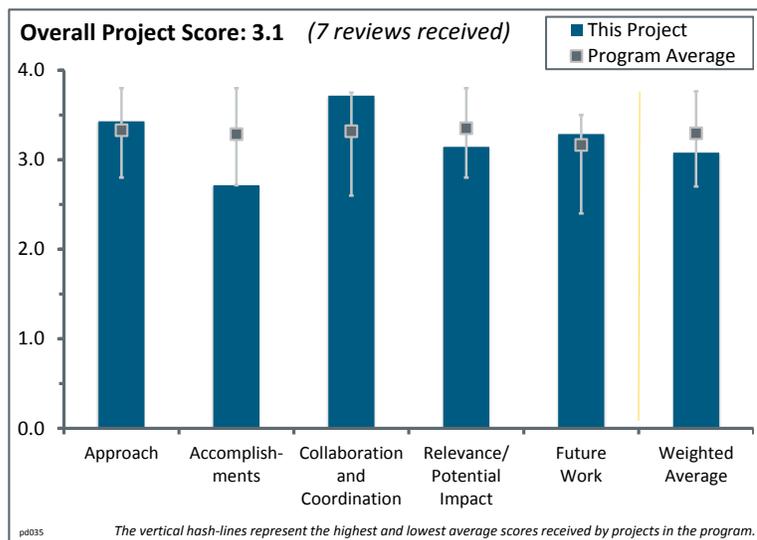
Todd Deutsch; National Renewable Energy Laboratory

### Brief Summary of Project:

The objective of this work is to develop semiconductor material devices that can split water into hydrogen and oxygen spontaneously upon illumination with a minimum of 10% efficiency. The main focus this past year has been to develop state-of-the-art III-V materials that meet the U.S. Department of Energy's (DOE's) near-term efficiency targets, and to optimize surface treatments for these materials that promote durability.

### Question 1: Approach to performing the work

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



- This project has done good work on material evaluation and surface treatments. The team seems to have a good understanding of surface treatment conditions.
- The approach to the work performed in this project is in line with that of the Office of Energy Efficiency and Renewable Energy (EERE) Photoelectrochemical (PEC) Working Group's three-pronged approach to developing efficient and stable photoelectrode materials. Attempting to stabilize highly efficient (but previously unstable) materials is an important area of research.
- As long as the gallium-based III-V tandem electrode is the most efficient PEC system and the only one that has delivered greater than 10% solar-to-hydrogen (STH) conversion efficiency, it deserves a spot in the Hydrogen Production program portfolio, and somebody needs to be working on it. This project is a reasonable mix of developing new materials and optimizing existing ones.
- This group is clearly addressing one of the three major PEC approaches of the PEC Working Group. The project team is candid about barriers to success, such as irreproducible results from metal impurities. The nitridation technique is well-designed and feasible, and the efforts of this group are clearly integrated with others, as evidenced by the Partners and Acknowledgments slides. The project is also taking a multipronged approach to this challenge by studying a variety of aspects in parallel, which is a good research model.
- The National Renewable Energy Laboratory (NREL) continues to focus on improving the durability of their champion III-V semiconductor material. The continued development of these materials is critical to the ultimate success of photoelectrochemical hydrogen production. In parallel, NREL is also giving thought towards how these materials will ultimately look at the system level and is developing the appropriate characterization techniques to further this goal.
- This is a broadly collaborative and coordinated project that has made significant progress in two of the five technical targets in the 2012 Fuel Cell Technologies Office Multi-Year Research, Development, and Demonstration Plan (MYRDDP). The approach is somewhat diluted by widely divergent pathways and material choices among the partners, with little justification for continuing some of those pathways beyond completing existing efforts to seek incremental improvements/understanding. The two technical targets with significant progress are STH efficiency and hydrogen production rate; both of these advances are based on a single expensive material and device concept. It appears that the approach could be significantly improved by greater investment in the discovery of less-expensive highly photoactive materials and alternative design/synthesis pathways to achieve equivalent progress in hydrogen production cost, solar interface, and electrode cost per TPD (metric tons per day) hydrogen. Such investments could possibly be

implemented without unrealistic funding increases by better focusing and coordinating the many PEC Working Group members.

- The team should look at the economic and environmental sustainability before devoting too much effort to the material. Of special concern is the CO<sub>2</sub> footprint of gallium and indium.

### **Question 2: Accomplishments and progress toward overall project and U.S. Department of Energy (DOE) goals**

This project was rated **2.7** for its accomplishments and progress.

- The primary accomplishment achieved this year appears to be the elucidation of problems with reproducibility in the nitrogen ion treatment of GaInP<sub>2</sub> photocathodes, due in large part to help from the surface characterization team at the University of Nevada–Las Vegas (UNLV). Progress was also made in the development of other III-V materials and in setting up an outdoor PEC testing platform.
- NREL has addressed the durability of their electrode materials via the formation of surface nitrides. There was some degree of ambiguity regarding the efficiency of nitride incorporation; however, Dr. Deutsch is now confident that they have identified the path forward via co-implantation with a dilute co-dopant. Due to provisional patent protection, the nature of this dopant was not revealed. An advanced characterization system was prototyped to perform sophisticated PEC measurements under outdoor sun illumination. Publishing a manuscript on standardized PEC testing and reporting is a very important part of the process, as it mandates that independent researchers perform their measurements and calculations such that meaningful information can be extracted to provide effective comparisons between different material classes and fabrication techniques.
- The general PEC hydrogen production program advanced significantly this past year by demonstrating performance and durability feasibility with at least one device and material configuration. This is an outstanding accomplishment and should serve to focus future work on the discovery of similar materials and designs that could surmount remaining barriers to accelerate achievement of program objectives. It is noteworthy that collaborators providing highly sophisticated material characterization and related *ab initio*/molecular dynamics simulations were central to validation of the reported advanced performance. Another achievement in the form of technology-enabling efforts allowed the prediction and demonstration of at least one material corrosion pathway, which could help with the discovery of interface stabilization processes for other materials and device designs. The collaborative project completed its multi-year standardized protocols and reporting methodology effort, which should help to reconcile many other reports of performance.
- This group has achieved a high-efficiency Group III-V PEC system that exceeds DOE's near-term PEC efficiency targets, but the group has had few advances since the system was first demonstrated in 1998. Their small advances since 1998, especially in surface protection, have demonstrated progress toward DOE goals.
- There has been an impressive improvement in photoelectrode durability via nitrogen doping of the surface through ion implantation. There is some concern about the methodology, though. By imposing an external bias, there may be a cathodic protection effect that serves to reduce corrosion from what it would be in the solar-driven system. That might explain why greater durability was demonstrated at higher current density (i.e., greater applied voltage). Eventually, these results should be corroborated by illuminating the isolated cell and letting the cell voltage and current float as the system evolves. Achieving 24 hours of stability is good news, but it is still well short of the 1000 hours ultimately required. Clearly it is time to push beyond and determine what the new stability limits are. Adding bismuth took 0.06 eV off the bandgap energy. That is better than nothing, but it is not clear how much more can be expected. Perhaps the theoretical justification as to what gains could be expected should be revisited and given more prominence.
- It would have been good to see more work done on durability and on-sun testing.

### Question 3: Collaboration and coordination with other institutions

This project was rated **3.7** for its collaboration and coordination.

- NREL clearly provides coordination and leadership to the other PEC Working Group members.
- The NREL group has very good collaborations with the PEC Working Group, which includes a multitude of complementary expertise, including synthesis, modeling, and characterization.
- This project is actively engaged through synergistic collaborations with a number of partners, especially the PEC theory and surface characterization groups.
- The work done by UNLV was critical to optimizing surface treatment. This is a good demonstration of collaboration in all areas.
- This group definitely interacts with other groups to publish papers on experimental techniques, technoeconomic analysis, and general research. This is clearly evidenced by the Partners and Acknowledgments slides. The group utilizes extensive computational modeling support from one DOE EERE-funded principal investigator and surface characterization from another.
- This is a highly collaborative project and participates in the PEC Working Group that meets regularly to discuss process options and report progress. Inclusion of sophisticated characterization and simulation teams has proven its value and should be emulated, where appropriate, within other Hydrogen Production and Delivery program efforts. Coordination of this effort should be improved to accelerate the progress toward meeting the technical targets in the 2012 MYRDDP. Changing specific tasks among partners in the PEC Working Group could be disruptive and might lead to the replacement of some partners, but the project should continue to seek project constructs that appear to follow the most promising pathway.

### Question 4: Relevance/potential impact on advancing progress toward DOE research, development, and demonstration (RD&D) goals

This project was rated **3.1** for its relevance/potential impact.

- Being able to directly couple solar to water splitting is the key to improved STH efficiency.
- This group is targeting a Type-IV system, which could be cost-competitive with natural gas-derived hydrogen in the long term.
- The work that NREL conducts is extremely relevant to the current DOE objectives for PEC hydrogen production. They are moving the technology forward towards meeting future DOE milestones.
- The project is well focused on program objectives and success in material discovery and synthesis accompanied by device designs. Enabling cost-effective fabrication and manufacturing would provide an attractive option to solar-powered hydrogen production.
- This project is well aligned with DOE's objectives. Even if III-V semiconductors are not ultimately a low-cost hydrogen-generating PEC technology, the ability to achieve high STH efficiency with today's III-V technology is very useful for addressing device-level challenges and stability at high current densities associated with the EERE PEC efficiency targets.
- This project and the PEC program as a whole could be cut tomorrow and have little impact on the foreseeable future of implementing of hydrogen and fuel cell technology. There are many other ways to supply hydrogen more cheaply than PEC. However, most of them exploit nonrenewable resources and do not prepare us for a sustainable energy future. Even within the program, PEC has to share the limelight with solar thermochemistry and photobiology. Nevertheless, DOE needs to bet some money on PEC, and a few million dollars a year on the possibility that technical advances can enable hydrogen production cheaper than photovoltaic (PV)-electrolysis is a worthwhile wager.

**Question 5: Proposed future work**

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

- The investigators understand what has been accomplished and what the next round of experiments should be.
- The general proposed future work is fine. Although not explicitly stated, there needs to be a narrowed task for applying the good nitriding process to a high-efficiency tandem cell and validating that process by reporting a superior result to the previous 12% STH efficiency from a decade ago.
- Overall, the future work plans are appropriate. Determining if the application of a nitrogen ion treatment to other III-V surfaces (and beyond) should be a priority, as should the determination of Faradaic efficiency during stability tests to alleviate concerns about surfactant interference. Outdoor testing with 10 times the concentration and light-cycling will also be of great use to the PEC community.
- This reviewer did not highlight any decision points but clearly laid out the proposed future work. The breadth of this proposed work is sufficient enough so that if some aspects struggle or become slowed, others can become the focus. This multi-pronged approach is advantageous in that the overall project and goals do not stall.
- The proposed work builds carefully on the success demonstrated this past year and is certainly focused on two of the three undemonstrated technical targets. Nevertheless, some thought should be given to alternative materials should it prove impractical to develop cost-effective synthesis and manufacturing processes to implement designs that could meet STH efficiency targets.
- This project needs to focus more on on-sun trials.

**Project strengths:**

- The leading PEC cell system for hydrogen production is continuing to improve. It is the flagship project for the PEC program.
- This is a nice, broad approach to understanding materials and surface treatments using expertise from various resources. This project seems to be on track.
- This project has outstanding technical proficiency, outstanding collaboration, outstanding facilities, and outstanding interactions with similar groups that are outside the inner circle of collaborators.
- The team and collaborations are very strong and experts in PEC, and this group has clearly identified a tractable problem to investigate using the wealth of resources afforded to them. Their approach is solid and, should large breakthroughs be discovered, there is a strong chance of realizing a cost-effective and scalable technology.
- The GaInP<sub>2</sub> remains the leader of high-performance PEC materials. Primarily through NREL, a wealth of knowledge on using this material for PEC has been accumulated over the past 15 years that is valuable toward further development. The recent results identifying the requisite co-dopant for effective nitriding validates the efficacy of the larger PEC working group towards solving outstanding issues in a collegial manner.
- This project has good synergy between theoretical, characterization, and materials experts. The extensive experience in III-V PV materials and PEC development makes NREL well suited for carrying out research focused on the task of stabilizing high-efficiency photoelectrode materials. NREL's current role as cell test and certification center for the PV field makes it a logical choice to assume this role for the evolving PEC field.

**Project weaknesses:**

- More focus needs to be placed on durability and on-sun trials.
- This project has insufficient investment in alternative pathways in the event of a failure of the current material focus.
- This project should be careful not to overstep milestones and perform experiments that provide a valid assessment of the state of the art.
- It appears that significant time was consumed figuring out the reproducibility issues associated with the nitriding treatment, and it still remains unclear if nitriding the III-V surface is a viable long-term option.

The absence of Faradaic efficiency measurements is a notable weakness of this project, given that its primary objective is to investigate the stability of these materials.

- This group generates hydrogen and oxygen in one vessel and does not report Faradaic yields. As such, the photoelectrodes may be reducing oxygen instead of protons, and thus the observed current and efficiencies may be artificially inflated. Another weakness is the group's use of expensive hydrogen evolution electrocatalysts (i.e., platinum) and oxygen evolution electrocatalysts (i.e., RuO<sub>2</sub>). The group must start addressing catalyst requirements and investigate alternative electrocatalysts that are more abundant and could be scaled to the terrawatt scale. The authors should clearly identify when a three-electrode or two-electrode measurement is used, as well as all of the experimental conditions used for each IV plot, including the potential where water splitting occurs.
- At some point, every materials-intensive project needs to have the capability to generate material in appreciable quantities. Although NREL has III-V fabrication capabilities, it appears from the review that this is more of a foundry-type relationship, with limited materials available for PEC. From the 2012 DOE Hydrogen and Fuel Cells Program Annual Merit Review, the proposed future work indicated that there would be an evaluation of dual (stacked/side-by-side) systems that were not highlighted in this review. It is unclear if this was abandoned or completed. In some ways, there appears to be a passivity towards the effort (i.e., NREL will characterize materials that come their way and generally support the larger community). There needs to be a sense of urgency towards finishing the III-V work.

#### Recommendations for additions/deletions to project scope:

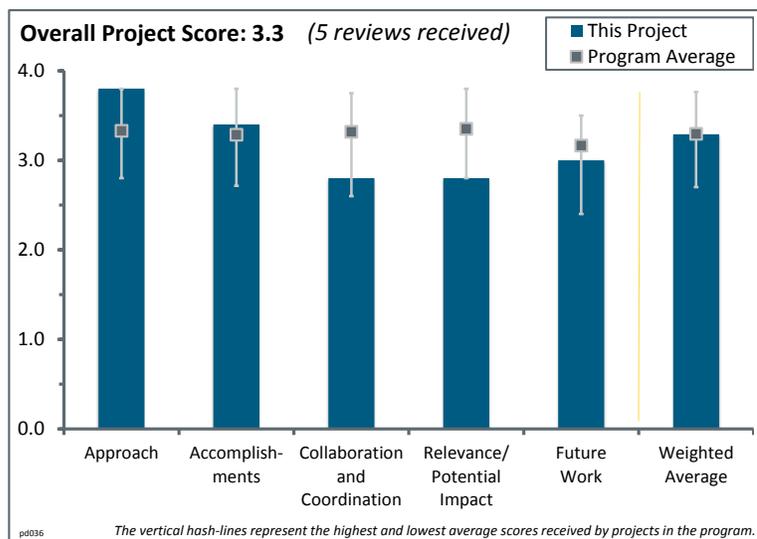
- At this point in the project, there really should be a singular goal. This project should apply all the hard work from the previous few years and fabricate a fully functioning, nitrided tandem that exceeds previous performance metrics. This is important for the overall validation of current and past efforts and gives credibility to the potential for future success.
- While it is certainly a worthwhile venture, too much effort is focused specifically on understanding and demonstrating passivation of a single material (GaInP<sub>2</sub>) by a single nitridation process (nitrogen ion implantation), a finding that was presented last year. This approach should be extended to other materials to view how universally useful the nitrogen ion treatment may be for III-V materials. Given that investigating stability is a primary objective of this project, accurate determination of the Faradaic efficiency (in the presence and absence of surfactant) and minor corrosion rates should be a priority.
- Evaluating PEC system stability is important, but the stability should also be assessed with day–night variations. The group's proposed on-sun testing should surely include multiple day tests where the system is bathed in hydrogen and oxygen at night. Some corrosion/passivation processes occur under conditions in which the sun is not shining and the PEC device is bathed in hydrogen and oxygen to reverse bias the cell. It is imperative that the project researchers begin to address these issues. As such, they must employ a separator (e.g., Nafion or a very fine, small frit) in PEC measurements to separate their hydrogen and oxygen reaction products. Then, when the sun goes down, they should assess their system stability in the presence of these gases. Another possibly useful condition to evaluate is in neutral pH with a large buffer concentration; there the III-V material should only passivate and not corrode, resulting in a stable electrode.
- This project should continue characterization and simulation studies of semiconductor–electrolyte interfacial phenomena for better understanding of electrochemical and corrosion processes. This project should encourage PEC Working Group members to evaluate the opportunities for closer coordination and teaming for III-V materials discovery and performance testing. This project should also encourage fundamental science agencies to invest in continuing an *ab initio*/molecular dynamics approach to interfacial behavior studies, including development/incorporation of quantum dynamic modeling of energy states in liquids. This project seeks broader collaboration with materials synthesis/fabrication specialists and continues or expands upon relationships with device manufacturing institutions.

## Project # PD-036: Maximizing Light Utilization Efficiency and Hydrogen Production in Microalgal Cultures

Tasios Melis; University of California, Berkeley

### Brief Summary of Project:

The objective of this project is to improve the sunlight-utilization efficiency of photosynthesis in microalgae by up to 300%, which will improve hydrogen or fuels production in microalgae and cyanobacteria by about the same percentage. Research proceeds on the truncated light-harvesting antenna (TLA) concept, which minimizes the light-harvesting antenna size of the photosystems to prevent early light-saturation of photosynthesis and the associated wasteful dissipation of absorbed sunlight. Genes and associated molecular mechanisms that confer a TLA property in the TLA3 strain of *Chlamydomonas reinhardtii* are identified, and protocols are developed for the targeted truncation of the light-harvesting antenna size in cyanobacteria.



### Question 1: Approach to performing the work

This project was rated 3.8 for its approach.

- The researcher has demonstrated that the gene replacement approach to the size reduction of antenna structures has general applicability in both algae and cyanobacteria.
- The approach has been methodical and step by step. The work in *Chlamydomonas* was carried to completion. The knowledge learned is being applied in the cyanobacteria system in a clear and deliberate manner.
- The identification and cloning of genes involved in truncated antenna size in microalgae and cyanobacteria is impressive. The work accomplished in the Melis lab is impressive and fits well with the work of Weyman et al. The approach is very robust.
- The success of the approach adopted and the techniques applied by this project to address antenna reduction in green microalgae provides great confidence that similar success will be achieved with cyanobacteria. A slide showing  $\Delta cpc$  transformants indicates some change has already occurred. More quantitative information as to the extent of the effect would be appreciated in next year's presentation.
- In 2012 and 2013, this project reduced the antenna size, but it is not clear what the direct result has been.
- In a bioreactor, it was always assumed by the team of principal investigators (PIs) that a family of microalgae is needed across the cross section of the reactor to get the best solar utilization. Therefore, algae in the middle of the reactor would have a larger antenna than those on the exterior surfaces to have the most favorable average solar utilization for hydrogen production. Now it appears that the intent is to produce a monoculture all with the same antenna size. Except for the science, the approach does not show how this will produce the levels of hydrogen needed at a cost that is practical and able to meet any of the targets, or with a higher efficiency. Based on reviewer comments from the 2012 DOE Hydrogen and Fuel Cells Program Annual Merit Review, it appears the approach for stable mutants is to incubate and continuously replace TLA mutants with new strains. It is not apparent this will be an economical approach, and it is not addressed as part of this work or any of the analysis activities.

## Question 2: Accomplishments and progress toward overall project and U.S. Department of Energy (DOE) goals

This project was rated **3.4** for its accomplishments and progress.

- The project completed the objective to reduce the antenna size with the potential to improve photosynthetic efficiency. It is not clear if this mutant strain can improve hydrogen yields or system efficiencies to meet the DOE targets.
- Cyanobacteria were successfully modified to eliminate blue receptors of the antennae through methods previously used on algae. Cyanobacteria with reduced antenna size were first produced about 10 years ago, so the general accomplishment is not new.
- The increased utilization efficiency above what was expected is excellent, as is the elucidation of the mechanisms of TLA2 and TLA3 function in the light-harvesting-complex-protein assemblage. The characterization in cyanobacteria is another example of impressive accomplishments.
- This project exhibits commendable progress. Unlike the original green microalgae work, which had well-documented, explicit targets over time that were achieved well ahead of schedule, the targets for the cyanobacteria work are not as obvious. For example, it is unclear if there is a target date for the transformation go/no-go decision. In the absence of targets, this reviewer will assume worst-case timing comparable to the microalgae work. On that basis, this work appears to be on schedule.
- Neglecting the issue of project duration, the accomplishments of the *Chlamydomonas* system have taken this task to completion. The antenna adjustment in cyanobacteria work has begun, and initial pigmentation arguments suggest that the concept is operational. There remains a significant amount of work to be done in the cyanobacterial system. A question is whether the effort is diluted by attempting to explore the extended photosynthetically active radiation (ePAR) concept at the same time.

## Question 3: Collaboration and coordination with other institutions

This project was rated **2.8** for its collaboration and coordination.

- Collaboration and cooperation between the Melis and other laboratories seems strong, and the topics overlap to produce a sum greater than their parts.
- Some collaboration exists primarily on education and supplying strains, but there is no indication of collaboration on the use of bioreactors to determine a more real-life trial on its stability and production capability.
- This project and presentation seem to be pretty much stand-alone. There was not much evidence of actual collaboration or input from collaborators.
- The researcher is capable of conducting the work with minimal input from outside groups, so lower levels of collaboration are not necessarily hindering the project. Nation Renewable Energy Laboratory (NREL) researchers and others are making use of the advances and were described as being offered advice on implementation.
- As was true for the microalgae work, this cyanobacteria project appears to be state of the art with little or no need for collaboration. The beneficiaries of collaboration with this project appear to be other collaborators, not this project.

## Question 4: Relevance/potential impact on advancing progress toward DOE research, development, and demonstration (RD&D) goals

This project was rated **2.8** for its relevance/potential impact.

- This project directly and effectively addresses the “light utilization efficiency” barrier (2012 Fuel Cell Technologies (FCT) Office Multi-Year Research, Development, and Demonstration Plan [MYRDDP], barrier number AN). This and prior work could have a substantial effect on photobiological efficiency of the production of various products in addition to hydrogen.
- Antenna size modification will be necessary in all algae and cyanobacteria organisms to achieve commercial fuel production levels. The technique has general applicability and is not limited to hydrogen-

producing organisms. However, this technique must be combined with significant advances in other aspects of cell modification to achieve DOE hydrogen production goals.

- While hydrogen production is certainly relevant, the rate at which progress is being made argues against the project as being critical to the program. As part of a go/no-go, the PIs should be expected to evaluate the best results that they think will be achieved, and decide the project's ultimate fate based on this production expectation. Assuming an argument can be made to continue, the PIs should estimate how close they are to completion and estimate realistic timelines.
- The PI has stated this work links with other efforts at NREL and the J. Craig Venter Institute, but the PI does not show how they are linked or if any outcome in terms of production yield has been observed. The one data point referenced is from 2010, which used a mutant that had 50% of the control. If that was such a significant yield increase, it is unclear why the lab did not stop there and do more bioreactor testing to determine if it was replaceable. The PI has said this is very time-consuming work requiring many hours of laboratory time. For such an effort, there should have been some attempt to show higher yields and more mutant stability, instead of just stating that six other groups have formed due to this PI's efforts, especially with the laboratory in Australia.
- The lack of fitness evaluations is a concern for the potential impact. To knock out such a large portion of the photosynthesis complex and consider it unlikely to inhibit organismal production is not a scientifically sound approach. Predictions appear to be formulated based on assumptions without testing. To test organismal fitness or assess basic physiological responses of TLA mutants would be simple and inexpensive. Certainly, the collaborating laboratories would be able to do such a test. These are basic and critical assumptions needed to meet the desired FCTO MYRDDP goals. The organisms need to survive and thrive.

### Question 5: Proposed future work

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

- The plan is adequate. The question on ePAR remains.
- The proposed cyanobacteria work appears to be very achievable and well focused on barrier AN.
- The general ePAR idea is sound, but the proprietary limits on divulging actual approaches limit the reviewer's ability to evaluate the effectiveness of the idea.
- Most of the future work should be based on determining the stability and replication potential of the mutants in a mass culture situation, before additional genetic mutation work is agreed upon. This project should develop a more accurate predictive model based on hydrogen production levels or efficiencies with the TLA strains.
- The future direction appears to be an assessment of stability and fitness according to the slides, which would address the concerns previously raised by this reviewer concerning lack of fitness evaluations. The PI's response to audience questions regarding organismal fitness and physiological response to TLA was insufficient, which was a concern. If the future studies as indicated in the presentation include fitness and physiological measures (in all four future subtopics), then the score of this reviewer would change from three to four. Assumptions are insufficient to meet the long-term DOE goals.

### Project strengths:

- The scientific approach is well thought out and has been adequately conducted. It has taken some time, but the work is perhaps quite difficult.
- This project is tackling big problems of general use to the entire community of photobiological fuel production, not just hydrogen.
- This project completed the proposed work and provided strains to other organizations for testing. A project strength is the multi-culture tests that the PI has said are in progress.

### Project weaknesses:

- As new approaches are tried to enhance light utilization in algae and cyanobacteria, collaboration may be useful but potentially limited by the researcher's proprietary concerns.

- There is no direct link to see if these mutants can be integrated into a biological system to produce hydrogen to meet the MYRDDP cost targets and efficiency goals.
- It is taking a long time to come to some conclusions. The estimates of final attainment and percentage of achievement would allow some assessment of whether this project should begin its second decade. It is not clear if the approach will be adequate to achieve the top targets in terms of hydrogen production.

**Recommendations for additions/deletions to project scope:**

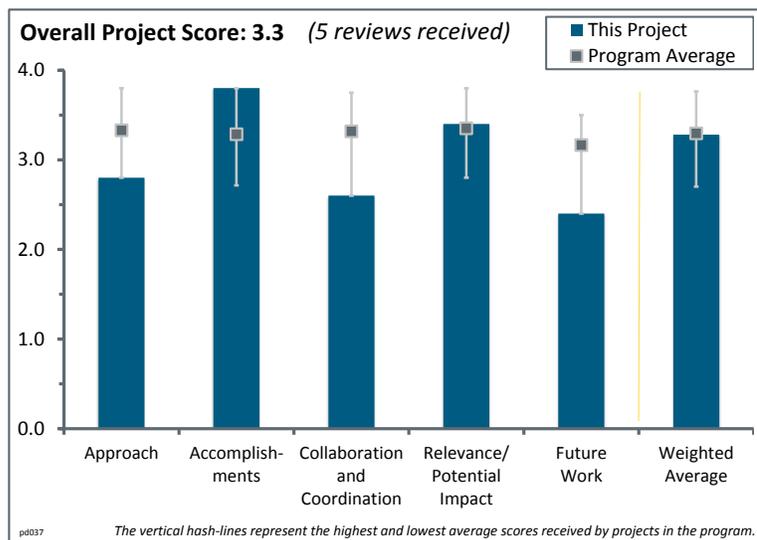
- This project should decide to put ePAR on hold for now, as it appears to dilute the effort.
- This project should complete a thorough characterization of the mutants' ability to survive a mixed culture environment, produce hydrogen with a reasonable yield, and survivability with the wild type in a bioreactor before committing funds for more genetic engineering.

## Project # PD-037: Biological Systems for Hydrogen Photoproduction

Maria Ghirardi; National Renewable Energy Laboratory

### Brief Summary of Project:

Photobiological water splitting coupled to hydrogenase-mediated hydrogen production has the potential to convert about 10% of incident solar energy into hydrogen. Various barriers have been identified as currently limiting green algal hydrogen production, including the oxygen sensitivity of the hydrogenase enzyme, the competition for reductant with CO<sub>2</sub> fixation and cyclic electron flow, the down-regulation of photosynthesis due to non-dissipation of the proton gradient and state transitions, and the low light-saturation of photosynthesis. The general goal of this project is to develop photobiological systems for large-scale, low-cost, and efficient hydrogen production from water.



### Question 1: Approach to performing the work

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

- The approaches utilized have successfully met the project goals in terms of product and timeliness.
- The approach to generating hydrogen production in green algae seems reasonable. The presenters have knocked out the native hydrogenase and added an oxygen-tolerant clostridial hydrogenase (PsaD-CaI). While the rate of hydrogen production is much lower in the mutant system, the mutant is able to generate small amounts of hydrogen in the presence of oxygen.
- This project is well focused on addressing the “rate of hydrogen production” and “oxygen accumulation barriers” (barrier numbers AO and AN from the Fuel Cell Technologies (FCT) Office 2012 Multi-Year Research, Development, and Demonstration Plan [MYRDDP]). In the past, the existence of Task 2 has provided risk reduction and some flexibility. While sulfur deprivation (and its discontinuous nature) appears to be an inferior means of achieving hydrogen production compared to incorporating an oxygen-tolerant hydrogenase, it is unfortunate lack of funding eliminated Task 2 and its work related to the non-dissipated proton gradient and study of the long-term performance of immobilized culture.
- Adding an oxygen-tolerant hydrogenase to the algae is the straightforward part of the project. Connecting this hydrogenase to the cell supply chain so it can make hydrogen is a much harder long-term issue that must be addressed.
- The rationale for pursuing a parallel track with green microalgae is not very clear. Heterologous gene expression is what is being pursued, so the native number and complexity of genes in *Chlamydomonas* should not be a factor, unless gene knockouts are necessary. A better argument would be if *Chlamydomonas* is faster growing, less susceptible to predators/competitors, easier to manipulate genetically, or more robust in outdoor conditions.

## Question 2: Accomplishments and progress toward overall project and U.S. Department of Energy (DOE) goals

This project was rated **3.8** for its accomplishments and progress.

- This project completed the milestone on light-dependent expression of clostridial hydrogenase (PsaD-CaI) successfully and on time. This appears to be a technical breakthrough. The assays for oxygen tolerance were well done and showed promising results in atmospheric concentrations of oxygen.
- The successful transfer of clostridial hydrogenase into the algae is impressive. The confirmation of a uniform population using the green fluorescent protein (GFP) assay is well done. The ability of the mutant to produce small amounts of hydrogen in the presence of oxygen is a major achievement. The presenter's plan to boost production by using a stronger promoter is sound.
- The researchers succeeded in putting the oxygen-tolerant hydrogenase into a cell and reported 2% of the rate of hydrogen production of the wild type. Part of this activity was retained in the presence of oxygen relative to the wild type, which is encouraging. This work is foundational and only the first step. Years of additional work in a myriad of areas on cell modification will have to be combined to reach DOE's targets.
- Steady progress has been made with significant accomplishments, such as the CaI transformant and subsequent quantification of light-induced hydrogen photoproduction, and recognition of heterogeneous strain communities on GFP plates. The techniques are classical and have been used for some time, but they are not easy, nor are they always readily accomplished. This explains the 12 years invested to produce this sequence of accomplishments.
- Commendably, the project successfully introduced a bacterial hydrogenase into a photosynthetic alga, induced expression, and observed light-dependent hydrogen production in the presence of oxygen. The project recovered a high-producing strain after significant heterogeneity appeared. And, despite cancellation, Task 2 demonstrated continuous operation of immobilized cultures for 1,440 hours, 70% to 90% of the time; however, hydrogen production rates were only 0.5% to 10% of initial rates.

## Question 3: Collaboration and coordination with other institutions

This project was rated **2.6** for its collaboration and coordination.

- This project has effectively leveraged Office of Science funds to develop a more sensitive assay; however, owing to budget constraints, partnerships with some collaborators were lost. Long-term partnership with the Melis lab appears to be unaffected.
- This project had to drop collaborators because of a lack of funding. This project started working with a new group in France that has a mutant that shows promise in terms of addressing Task 2 (ATP synthase mutant).
- This project has lost partners because of a funding decrease. The partners appeared to perform valuable functions, and their loss means that useful avenues will not be studied. This project has begun working with a new team in other areas, but not in the area of lost collaboration.
- The loss of Task 2 appears to have reduced the project's level of collaboration and capabilities. The results of this research have been communicated through several publications and conferences (including international conferences).
- The reduction in collaboration is the fault of funding shortages. The reviewer wonders if collaborations are not possible without providing funding. Certainly money "greases the wheels," so to speak, but collaborations with other funded laboratories conducting similar work must be possible. People were presenting such work at the 2013 Hydrogen and Fuel Cells Program Annual Merit Review. The principal investigator (PI) has indicated that conversations with industrial partners are ongoing. Industry people working in the general field of algal photosynthesis would probably be amenable. Some of these musings were effectively addressed by the PI, who indicated potential collaborations with a group in France who are working on a mutant with the same effect as a proton decoupler, thereby addressing some of the issues lost in the Russia collaboration.

**Question 4: Relevance/potential impact on advancing progress toward DOE research, development, and demonstration (RD&D) goals**

This project was rated **3.4** for its relevance/potential impact.

- A photosynthetic algae strain that produces hydrogen has much potential and should be pursued.
- The research appears to be at an early technology readiness level, so it is unclear how these research results will translate into larger production scales.
- The relevance of this process to providing hydrogen to hydrogen fuel cell systems is not questionable. Other energy supplies are complicated by their environmental footprint. The utilization of photobiological systems does not suffer the same issues and thus is a long-term solution rather than a “bridge” solution. The PI has addressed the FCT Office MYRDDP.
- This work should identify the issues surrounding photobiological hydrogen production in algae, but in and of itself will not meet the long-term DOE goals. However, this work is necessary if the goals are to be met in the future.
- Acquiring a productive green algae that (1) possesses an oxygen-tolerant hydrogenase, (2) has a more efficient reduced antenna, and (3) is capable of dissipating the related proton gradient would be a significant stride for the biological hydrogen production pathway.

**Question 5: Proposed future work**

This project was rated **2.4** for its proposed future work.

- The proposed future work builds on past accomplishments and is the logical continuation of the work in progress.
- The proposed future work, in terms of combining the genetic mutations into a production strain, is the logical next step.
- The work is novel, and the accomplishments are significant. It is also recognized that because the work is novel and the techniques are time-consuming, 12 years of investment is warranted; however, the goals for the future seem less than ambitious.
- The proposed work is a logical extension from the present position. The team needs to sit down and analyze why the hydrogen production rate is so low and how to make the most significant advance. It is unclear what the limiting factor is for hydrogen production in the algal system with the oxygen-tolerant hydrogenase—probably a connection with the cell supply chain. It is unclear if this proposed work maximizes the connection or if other directions are more promising.
- This reviewer did not see a defined plan to improve the recombinant hydrogenase activity, aside from testing the stronger promoter. Furthermore, it will be important to determine if increased hydrogen production will have a negative effect on the cells or if the cells will maintain the promoter/hydrogenase genes over a relevant time scale.

**Project strengths:**

- This is an excellent team capable of unraveling the issues of hydrogen production in algae.
- This project is well conceived and executed. The challenges and complexity are identified and addressed (e.g., the heterogeneous community on the GFP plates). The lab has made significant contributions to moving this science forward.
- Green algae that can be used for hydrogen production has a lot of promise in the biofuels industry. This project has already achieved a great milestone in generating small amounts of hydrogen in a prokaryotic system.

**Project weaknesses:**

- It is not clear whether the project is addressing the biggest issue, versus more tractable issues.
- There does not seem to be a strong plan for increasing hydrogen production and confirming that higher levels of hydrogen will not have a negative effect on the cells.

- This is not a project weakness, but a funding question. It is unclear why basic science, such as this, and all the projects presented during this review period are not funded by the DOE Offices of Basic Energy Sciences (BES) or Biological and Environmental Research (BER). This may simply reflect the reviewer's lack of knowledge of DOE funding decisions and guidelines. The weakness is the speed with which the work is progressing.

**Recommendations for additions/deletions to project scope:**

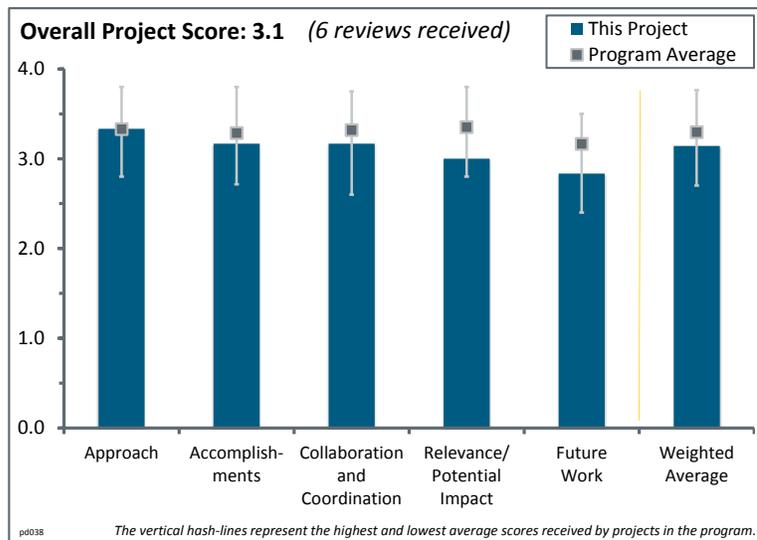
- Additional work should be done to confirm that the hydrogenase system will be maintained over a relevant time scale in a working system. It is unclear how the presenters will confirm that the hydrogenase genes/promoters will not be mutated over time.
- This project should develop collaborations, which will increase the speed of the task accomplishments. The project should explore the physiological constraints of ATP synthase under variable growth conditions and explore the phenotypic variation resulting; identify barriers to hydrogen production over time, which seems to be, in part, strain-specific; and generally push the expectations in the proposed future research.

## Project # PD-038: Fermentation and Electrohydrogenic Approaches to Hydrogen Production

Pin-Ching Maness; National Renewable Energy Laboratory

### Brief Summary of Project:

The objective of this project is to develop direct fermentation technologies to convert renewable lignocellulosic biomass resources to hydrogen. The project addresses techno-economic feasibility of hydrogen production via biomass fermentation in three tasks. Task 1 uses cellulose in lieu of sugars and optimizes parameters in sequencing fed-batch bioreactors to lower feedstock costs. Task 2 is aimed at improving hydrogen molar yields by developing genetic tools to block competing pathways. Task 3 integrates a microbial electrolysis cell (MEC) reactor with fermentation to improve hydrogen molar yield.



### Question 1: Approach to performing the work

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

- The coupled system approach is unique and appears to be advantageous, thanks to unit operational synergies. This approach appears to produce high theoretical hydrogen molar yield and may be more near-term to scale-up compared with photo-biological approaches.
- By including the MEC reactor, the researchers seem to be maximizing the potential hydrogen production. The genetic approaches to creating strains that increase hydrogen production are sound. The assumption that knocking out the ethanol pathway will result in more hydrogen production might not be valid but needs to be tested.
- This program has an effective three-pronged approach: modify conventional bioreactors to address demands of a unique system, alter synthetic organisms to achieve hydrogen production from cellulose, and create a new electrochemical reactor for hydrogen production from the biological hydrogen production effluent. The MEC reactor system appears applicable to biological effluent in general, but it is not limited to hydrogen producers and may warrant its own program depending on advancement.
- The project is well focused on barriers AX, AY, and AZ in the Fuel Cell Technologies Office 2012 Multi-Year Research, Development, and Demonstration Plan, i.e., hydrogen molar yield, feedstock cost, and systems engineering. The potential to attain a yield of 11.6 moles hydrogen/mole sugar is impressive, and the approach being pursued provides confidence that a significant improvement beyond 4 moles hydrogen/mole sugar is achievable.
- The linkage between tasks and where the whole project is going is not clear. Lignocellulose is the apparent target feedstock, but it is not very prominent in the plans. This project is also apparently slow-moving overall.
- The focus of this work should be on the conversion of sugar to hydrogen and all the issues dealing with this fermentation process. Since a great deal of this work is aligned with the U.S. Department of Energy (DOE) Bioenergy Technologies Office (BETO), many of the pretreatment issues, barriers, and equipment costs have already been addressed. For example, clean, low-cost, cellulosic-based glucose from an integrated biorefinery (IBR) could be made available cheaply so the research team can focus on the fermentation improvements needed. The equipment like Cellunators™ for optimum mixing and cell disruption has been developed and scaled to commercial size. The processes to remove inhibitors, such as acetic acid and

formic acid, have been implemented and can be applied. These types of technologies can be easily adapted to this application for the fermentation process to be economical.

### Question 2: Accomplishments and progress toward overall project and U.S. Department of Energy (DOE) goals

This project was rated **3.2** for its accomplishments and progress.

- The project experienced a breakthrough in terms of making genetically tractable *Clostridium thermocellum*. The project appears to have met other milestones on time.
- This project completed some milestones ahead of schedule. This project has many promising tasks and has already demonstrated some. The accomplishments by both the National Renewable Energy Laboratory (NREL) and Pennsylvania State University (Penn State) teams are impressive.
- This project successfully modified the fermenting apparatus for consistent feed delivery. The increase in hydrogen production rate via process variables was a useful demonstration. Last year, the 2013 hydrogen production goal was 4 moles hydrogen/mole glucose; this appears to be the 2015 goal now. Knocking out the formate pathway was a good step in organism modification. The MEC work was an excellent proof-of-principle demonstration.
- The increased hydrogen yield was very good for this approach. This approach may not be reasonable, especially to develop a proprietary plasmid that eliminated the formate pathway. Based on the system economics, by-products are attractive ways to reduce the cost of hydrogen if the yields for the primary pathway are reasonable. Formate can yield other attractive products with a higher value. Based on the molar yields and rate increases on direct fermentation, these seem sufficient for a process system. The complexity of creating plasmids is an interesting science, but it is unclear why it is needed here. It is unclear if the process should focus on fermentation of good hydrogen yields or concentrate on hydrolysis and saccharification. Hydrogen generation in an MEC reactor was very good, but it was not apparent if preliminary economics were conducted to identify barriers the technology must overcome to be feasible.
- Task 1 has resolved an issue with sub-optimal hydrogen production rates by decreasing the fermentor hydraulic retention time, but it will ultimately have to address inefficiencies of handling larger liquid volumes. Task 2 has developed a mutant in which the pyruvate–formate pathway has been knocked out and demonstrated it several months ahead of schedule. The mutant appears to produce significantly more ethanol and marginally less pyruvate than the wild type. Task 3 has begun processing a more realistic wastewater stream and identified issues with protein treatment. Task 3 has devised a very novel approach to eliminate a conventional power source for the electrochemical cell; this effort does not appear to address program barriers as directly as development of the electrochemical cell.
- The progress and accomplishments do not seem major for the project duration. The progress seems slow.

### Question 3: Collaboration and coordination with other institutions

This project was rated **3.2** for its collaboration and coordination.

- The project exhibits good collaboration on all fronts to reduce duplication and increase performance.
- The coordination between NREL and Penn State appears to be excellent. An additional collaboration with a team in Canada did not produce measurable results but was valuable to the presenter in terms of knowledge gained.
- The three different collaborators appear to provide distinct services that will advance the program and enable the accomplishment of the project's goals. This was the best apparent collaboration of any project this reviewer reviewed that day.
- Task 3 linkage to the fermentative work has improved. The task is beginning to process more realistic fermentation wastewater and identify issues such as higher protein levels than were previously studied. Task 2 is now positioned for greater interaction with Task 1 by providing mutants for testing.
- The collaboration with Penn State is strong and synergistic. It is clear from the results so far that the efforts are well coordinated among the participating institutions. There was good leveraging of the Genome Canada relationship; however, the genetic engineering component may have benefitted from a collaboration with Dartmouth College (Lee Lynd) or Oak Ridge National Laboratory, which are both

proficient in working with *C. thermocellum* due to the Office of Science Bioenergy Research Science Center activity, of which NREL is a participating organization.

- This project seems like three separate projects with not much evidence of collaboration. It is not clear what the groups are gaining from each other.

### Question 4: Relevance/potential impact on advancing progress toward DOE research, development, and demonstration (RD&D) goals

This project was rated **3.0** for its relevance/potential impact.

- The combined approach of bioreactor, genetic engineering, and MEC research is an excellent way to maximize the output of the funding.
- This appears to be a feasible approach for hydrogen production, especially for grid-independent facilities that have a waste or lower-cost sugar stream to make hydrogen. This hydrogen can be used to hydrogenate and produce drop-in fuels, to run stationary fuel cells for auxiliary power units (APUs), or in local vehicle applications.
- Efficient fermentation of a less expensive feedstock through the application of an inexpensive process would be a significant step in achieving DOE targets.
- Owing to the relative ease in scaling and integrating these more “conventional” bioprocesses, it is likely that this approach will yield significant quantities of hydrogen in a shorter timeframe, which will aid in more realistic techno-economic evaluations of how this might affect cost goals by 2030.
- The relevance is likely there. However, the magnitude of the value to the overall DOE Hydrogen and Fuel Cell Program is questionable. Lignocellulose is mentioned but does not appear to be a focus.
- The general idea of producing hydrogen from cellulose is scientifically sound, but it is questionable for practical application. Taking a feedstock that can be readily converted into ethanol, a renewable liquid fuel product of high volumetric energy density at standard temperature and pressure that has an efficient delivery system, and making hydrogen instead with all the concomitant problems that result from a gaseous energy feedstock seems counterintuitive. Unless hydrogen can be produced significantly more efficiently than ethanol, or serve a unique function, it will not happen. Getting extra energy from a biological effluent in the MEC reactor may possess some merit, even if it is hydrogen.

### Question 5: Proposed future work

This project was rated **2.8** for its proposed future work.

- The proposed future work is a logical extension of ongoing research.
- The proposed work is a logical extension of the current progress and should allow the team to meet the project goals.
- The future plans appear to be building upon the progress to date and are likely to address the remaining barriers. The penalties of frequent liquid replacement in the bioreactors in terms of operating expenditures should be examined more closely in techno-economic models.
- The future work needs to be reevaluated for impact.
- This project demonstrated that deletion of the pyruvate-to-formate gene produces more ethanol, leading to a hypothesis that knockout of the ethanol production pathway will refocus the output to hydrogen, which may or may not be valid. This requires testing.
- It is not clear why this project does not focus on the fermentation to produce hydrogen and does not try, with limited funds, to scale the MEC reactor, eliminate the formate pathway, and develop new equipment to feed cellulosic slurries. If this process can produce multiple products and high hydrogen yields, it will have exceeded any of the accomplishments from the biological hydrogen production pathways. Then this project could collaborate more effectively with BETO to reduce or modify existing feedstock processes to reduce cost and improve the yields more.

### Project strengths:

- This is an excellent collaborative team that can work together to achieve goals.

- This project has good principal investigators (PIs) and organizations conducting research, and good fermentation yield.
- This project has strong collaborations. It combines multiple technologies to maximize hydrogen production. Overall, this reviewer was very impressed with the work and the level of coordination.

**Project weaknesses:**

- This project has too large a scope with limited resources.
- This is a very fragmented project. It is unclear what value each piece brings and when each section will reach an evaluation point.
- The MEC reactor could be considered a separate project altogether with its own set of difficulties that may warrant a larger effort once it is past the proof-of-principle stage and the preliminary economic analysis.

**Recommendations for additions/deletions to project scope:**

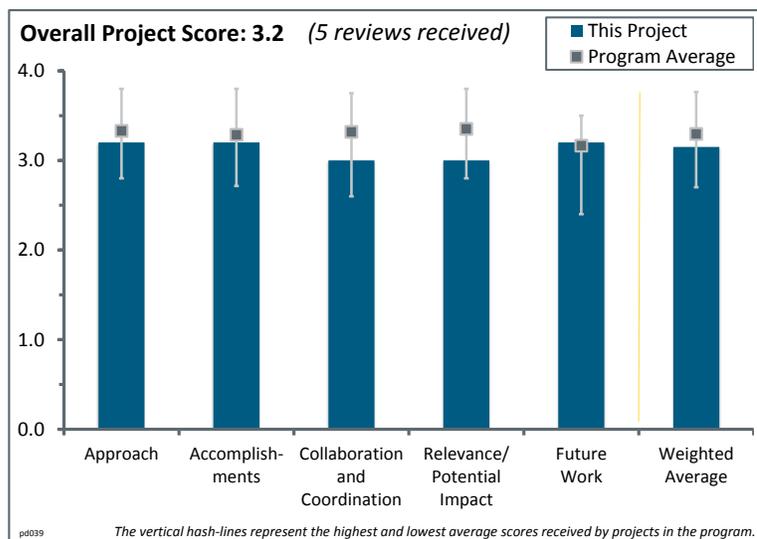
- There should be some firm targets for the project, and each task should be evaluated in light of them. The interactions between the PIs should be strengthened as necessary.
- The presenter stated that there is no competition between biofilm formation and clostridial cells; however, the presenters should include an evaluation of the biofilms in the MEC.
- Instead of focusing on traditional agricultural or woody biomass resources, this project should be exploring the *C. thermocellum* treatment of municipal solid waste and other organic wastes that might be co-located with wastewater treatment plants that may already be considering MEC technologies. This can bypass many feedstock availability issues. Also, since the carbon is supplied at such a low concentration (5 grams per liter per day under current experimental conditions), this technology could be especially amenable to dissolved organic carbons and cellulose from municipal liquid wastes.

## Project # PD-039: Hydrogen from Water in a Novel Recombinant Oxygen-Tolerant Cyanobacterial System

Phil Weyman; J. Craig Venter Institute

### 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. Current approaches to improve the system include (1) developing strategies for increasing expression and activity of the environmentally derived hydrogenase in cyanobacteria by changing the frequency and strength of promoters, testing a novel strategy for expression of hydrogenase, and altering the FeS cluster ligation to increase hydrogen evolution activity; and (2) developing strategies for increasing hydrogenase-ferredoxin interaction through construction of a ferredoxin-hydrogenase fusion protein that maintains activity.



### Question 1: Approach to performing the work

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

- This approach is systematic, thorough, clear, and logical.
- The approach is effective and has resulted in several new improvements in hydrogenase activity. Now the project needs to determine if these mutants perform when put into a large mixed colony.
- The presenters have incorporated multiple pathways to increase hydrogen production in the presence of oxygen, including increasing promoter strength, creating fusion proteins, and modifying different sites on the protein.
- This project has begun investigating the more limiting aspects of hydrogen production from cells, connecting the oxygen-tolerant hydrogenase enzyme to ferredoxins. The interaction of hydrogenase with the cell supply chain is a far more limiting factor on hydrogen production than the activity of the enzyme. Hopefully this work will illuminate the supply chain limitations on hydrogen production.
- IPTG induction is likely to be costly on large-scale systems. The project should look at copper-inducible promoters (Himadri Pakrasi). It is not clear why seawater would be the best metagenomic resource for oxygen-tolerant hydrogenases. Also, the screening criteria and rationale for the identification of the clones of interest were not explained to indicate what features in the sequence indicated promising activity. If those sequence features could have been predicted, then rational design of hydrogenases and targeted mutagenesis of the native hydrogenase could have been pursued in parallel.

### Question 2: Accomplishments and progress toward overall project and U.S. Department of Energy (DOE) goals

This project was rated **3.2** for its accomplishments and progress.

- These are very good accomplishments to achieve increased evolution of hydrogen.
- This project reached the January 2013 go/no-go milestone earlier than scheduled. The rate of evolution appears to be only a two-fold improvement; however, the hydrogenase activity could be higher when time is not taken into account. The ferredoxin hydrogenase fusion protein milestone appears to be on track.

- The presenters have demonstrated that, by combining extra promoters and a double substitution, they achieved a factor-of-five boost in hydrogenase output that is not oxygen-sensitive. The many different pathways to achieve the project goals have been evaluated, and go/no-go criteria have been clearly defined.
- The project achieved excellent progress, especially in light of the collaboration between Weyman and Maness. The tasks are mostly at 100% complete; those remaining are on track. The scaling-up question remains an issue, but at this basic exploratory stage, it seems a premature question (brought up by previous reviewers). This type of research, though it has applications, is fundamentally basic research and as such cannot be expected to scale up. The quantification of hydrogenase activity, identification of novel “maturation” genes, and other accomplishments are impressive.
- The increase of two times the in vitro hydrogen production from the combined system was nice, but the actual function in the working cell is what is important. It did illustrate how hard the problem of photo-biological hydrogen production actually is. The ferredoxin mutants were encouraging, but it is not clear how the project has gone far along the path of improving “hydrogenase-ferredoxin (Fd) electron transfer to enable 25-fold better Fd docking to the hydrogenase” (it was listed as 20% done). The real performance metric should be enhanced hydrogen production by XY% through this approach.

### Question 3: Collaboration and coordination with other institutions

This project was rated **3.0** for its collaboration and coordination.

- The collaboration with the National Renewable Energy Laboratory (NREL) appears to be fruitful; it led to ferredoxin troubleshooting and improvements.
- This is a good team with excellent principal investigators, and the partners communicated and worked together to validate performance.
- It seems the collaboration between Weyman and Maness has been productive and resulted in exceptional achievements in both projects presented at this review.
- The roles of collaborators were not clearly defined.
- Previously, the program had direct ties to NREL, but the project and NREL’s DOE Hydrogen and Fuel Cells Program Annual Merit Review presentations were separated this year with the implication that they still communicate. Researchers from the J. Craig Venter Institute (JCVI) are perfectly capable of pursuing this work, with or without external collaborators, and probably have colleagues with which to discuss approaches at JCVI.

### Question 4: Relevance/potential impact on advancing progress toward DOE research, development, and demonstration (RD&D) goals

This project was rated **3.0** for its relevance/potential impact.

- Creating a non-oxygen-sensitive hydrogenase system is very promising and would contribute well to DOE goals.
- Biological hydrogen production is an incredibly complex problem. This work is focused on identifying the issues that surround this problem. This work will not solve the problem directly but must be combined with numerous other advances in cell modification if the problem is to be solved in the next 20 years.
- Oxygen tolerance is critical for biological hydrogen production, and this project has made advances in the science. However, how much of an impact these improvements would yield has not been identified since there is no indication or reference to any economic analysis.
- There are no attempts at scalability, and the work appears to be on the “long-term” trajectory (more fundamental in nature) towards the biological hydrogen production cost goal of \$10/gasoline gallon equivalent (gge). This project has “quite a ways to go,” as stated by the PI himself.
- The impact on basic science will be significant because of the exploration of promoters, genome sequencing contribution, quantification of hydrogenase activity, and the identification of causal mechanisms. The contribution to hydrogen production looks promising, but at such an early stage, it seems impossible to predict how this will scale up to the production level. It is unclear what the issue will be with strain contamination. It is unclear what will happen to cellular or organismal fitness when engineered for increased hydrogen production.

**Question 5: Proposed future work**

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

- The ferredoxin coupling and making the final cyanobacterial strain are important and will be addressed.
- The plans build on previous accomplishments, but until all of the modifications are put into a strain, the actual improvement over any of the previous work will not be known.
- The presenters have clearly defined their pathways for moving forward, including the evaluation of promoter strength and using light to drive hydrogen production.
- It is not clear that proximity of the hydrogenase to ferredoxin is the rate-limiting step to hydrogen production. If that is the case, it would be nice to know what the theoretical maximum rate would be to measure progress.
- The future work builds on the lab's success (which is substantial), as well as the work of others, such as Maness. This collaborative atmosphere and previous success bode well for future success. The techno-economic analysis will help identify promising directions and allow those which lack promise to be discontinued, which is a sensible way to mitigate risk.

**Project strengths:**

- The researchers have the knowledge, skills, and equipment necessary to achieve the project milestones.
- This project is clearly defined by the project goals. The previous results have demonstrated the researchers' ability to achieve their goals.
- This project is well planned, has clear milestones, has achieved some milestones, has productive collaboration, and has abundant resources to work with.

**Project weaknesses:**

- There seems to be some overlap with the NREL group.
- All the work of this project might make only minimal direct progress toward the ultimate goal of practical biological hydrogen production. Interfacing the hydrogenase with the cell supply chain is difficult and unlikely to be maximized in the near future.
- The project has not considered scaling, and it is unclear if the researchers have examined the fitness consequences of their engineering. Many of the reviewer concerns from last year have been addressed, with the question of scaling up via *ex vivo* to *in vivo* experiments being one example. Many concerns have not been addressed, such as the potential role of additive or pleiotropic gene effects on the desired phenotype. It is unclear if "forward screening" mutagenesis is a non-starter. The gene stacking or redundancy may address some of these issues and others (e.g., Muller's ratchet).

**Recommendations for additions/deletions to project scope:**

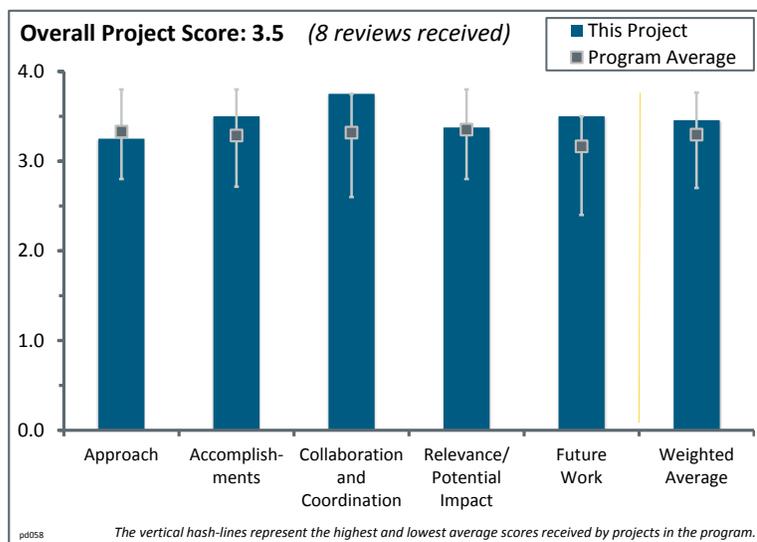
- This project should explore fitness under the parameters that are likely to be experienced by the organism in production.
- It will be important to measure other elements besides gene expression as controls for hydrogenase activities and parameters to modify for better activity. These can include protein folding assays, metabolic pathway optimizations (shutting down endogenous hydrogenases to elevate the relative levels of metal co-factors), optimizing localization of the protein, shutting down proteases, and other bioprocess engineering methods.

## Project # PD-058: Characterization and Optimization of Photoelectrode Surfaces for Solar-to-Chemical Fuel Conversion

Tadashi Ogitsu; Lawrence Livermore National Laboratory/National Renewable Energy Laboratory

### Brief Summary of Project:

The objectives of this project are to develop a theoretical tool chest for modeling photoelectrochemical (PEC) systems; compile a database of research publications on relevant photoelectrode materials; uncover key mechanisms of surface corrosion of semiconductor photoelectrodes; understand the dynamics of water dissociation and hydrogen evolution at the water-photoelectrode interface; evaluate the electronic properties of the surface and water-electrode interface; elucidate the relationship between corrosion and catalysis; and produce simulated x-ray spectra for interpretation of experimental results.



### Question 1: Approach to performing the work

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

- This project is doing good work, which can provide important molecular insight into the process.
- The approach is broad and attempts to address a wide range of issues regarding PEC systems.
- The molecular dynamic simulation remains an important tool, as it simultaneously addresses the barriers for durability and efficiency. By comparison to empirically derived data, the models can be validated and become more efficient as predictive tools.
- This research is highly complementary to experimental efforts within the PEC working group, which certainly play into the approach of this project. That being said, the overall project approach on slide 6 that illustrates how theoretical/modeling tools are used in modeling PEC systems (and how different modeling tools relate to each other) was not clear.
- The efforts to simulate and computationally model the surfaces of III-V semiconductors under conditions of catalysis are the major thrust. Although commendable, this seems like a gargantuan effort that may be too large of a scope for this project. Notwithstanding, this research is highly integrated with other U.S. Department of Energy (DOE) Office of Energy Efficiency and Renewable Energy (EERE) PEC hydrogen production efforts and supports empirical mechanisms.
- Aligning the project as supporting the National Renewable Energy Laboratory (NREL) effort on III-V tandem electrodes is valid. The advancement of the theoretical methods appears to agree fairly well with the experimental data, but the goal would be to advance its predictive power to where it could advise the experimentalists. It does not look like the capability is there yet.
- Using computational methods along with an understanding of the basic physics involved in PECs could be an important driver of future discoveries. An analog to this is the rapid, wide-scale screening of chemicals for drug discovery used in the pharmaceutical industry. Material screening is important, and if it can be done theoretically and computationally first, this could save a lot of time and money, accelerating the pace of discovery. This approach applied to PEC could help this field become commercially relevant, which it struggles to do at this point.
- This numerical work integrating molecular dynamics simulations using water with density functional theory (DFT)-based semiconductor energy states has permitted first-time description of various phenomena

occurring at the electrolyte–semiconductor interface. The development of PL<sub>2,3</sub>-edge spectra was compared with x-ray absorption spectroscopy (XAS) spectra and provided first-time experimental/theoretical state correlation and confidence in applications of DFT interface state calculations. A hole-trap corrosion mechanism that was proposed from numerical evidence and experimental evidence supported this hypothesis. Currently work is under way for further corroboration that could help find countermeasure treatments to stabilize the interfaces. This project is a collaboration with a much larger effort, but it has suggested some critical pathway solutions that might not have been discovered experimentally.

### **Question 2: Accomplishments and progress toward overall project and U.S. Department of Energy (DOE) goals**

This project was rated **3.5** for its accomplishments and progress.

- This project has done a great job identifying and describing the corrosion mechanism and beginning to understand how to move hydrogen production using various materials.
- Excellent progress is being made for the level of funding received. Elucidating the influence of water structure on photocatalytic mechanisms and photoelectrode stability is of tremendous importance to the PEC field.
- This project has accumulated an impressive number of papers related to PEC. It would be good to see more detail on what exact online collaboration tools are being used to disseminate relevant information to partners. The identification of corrosion mechanisms is an important result, given its detrimental effects on experimental work and progress on PEC material system stability and durability.
- There was a narrow spectrum of objectives commensurate with the funding levels. The project successfully tested the hole corrosion model against data from NREL. The validation of the model against previous NREL data proves the efficacy of these techniques and provides confidence for future results. The project is continuing to build the theory to match the data generated from surface characterization from the Heske group.
- The systems being studied are relevant to present technical challenges in the PEC program. The principal investigator (PI) is looking at implanted nitrogen and “unintended metals,” which are directly supportive of other research projects. The investigator reported fascinating results on the relative ability of InP to transport protons laterally across an adsorbed monolayer of water molecules compared to GaP. It is unclear if those results can be applied to GaInP<sub>2</sub>, or if that represents an entirely new level of difficulty in computation for which it is too early to tell. The project should also consider why, if the electrode is to perform in 3M H<sub>2</sub>SO<sub>4</sub>, it is important to have lateral transport of protons across the surface.
- A database of PEC-related research is in development and is currently archiving about 1,200 papers from which relevant information is shared with various PEC projects within the PEC Working Group. The hole-trap corrosion hypothesis has been confirmed by detailed interface characterization at both the University of Nevada–Las Vegas (UNLV) and the Advanced Light Source at Lawrence Berkeley National Laboratory. Further confirmation was found through experimental evidence at NREL, and that early work is being expanded in collaboration with the theoretical and material characterization groups. Finally, the simulation of proton transport mechanisms at water–semiconductor interfaces has illuminated catalyst roles in PEC hydrogen release and has identified potential mechanisms for corrosion-resistant properties discovery.
- It is unclear from the Milestones slide exactly how far this project has progressed because the milestones do not contain dates. Notwithstanding, the percentages complete seem rather large, but the body of work seems somewhat scant. This group reports results on proton transfers at interfaces and corrosion mechanisms/attenuation on III-Vs.

### **Question 3: Collaboration and coordination with other institutions**

This project was rated **3.8** for its collaboration and coordination.

- The collaborations appear to be clear, strong, and beneficial to all parties.
- Good collaboration is shown through technical accomplishments achieved this year.

- The PI is clearly trying to be supportive of PEC efforts elsewhere in the DOE Hydrogen and Fuel Cells Program.
- This project does a good job collaborating with the larger PEC Working Group and more specifically the NREL effort for III-V semiconductor material development and, additionally, the surface characterizations from the Heske group.
- This project has logical and productive collaborations with experimentalists within and outside of the PEC Working Group.
- This group clearly collaborates with others in the PEC Working Group. Recently, they extended their collaborative modeling efforts to copper-indium-gallium-diselenide (CIGS), initiated with the University of Hawaii and the University of Texas (UT), Arlington.
- This project is a wholly collaborative effort within the PEC Working Group, although only a few of the PEC projects have found ways to implement its supporting role. The coordination of theoretical/numerical effort with applied material needs has been outstanding. The additional coordination and collaboration with other theoretical groups has been initiated by this project in hopes of expanding both the level of effort and the numerical tools development.

#### **Question 4: Relevance/potential impact on advancing progress toward DOE research, development, and demonstration (RD&D) goals**

This project was rated **3.4** for its relevance/potential impact.

- Support for the Hydrogen and Fuel Cells Program is relevant to the extent that the entire PEC program is relevant.
- This project helps move PEC technology towards understanding how to improve solar-to-hydrogen (STH) efficiency to the required levels.
- Current state-of-the-art materials do not simultaneously possess both good PEC efficiency and accompanying stability. These types of models are therefore essential for future development.
- The work being performed in this project is of great scientific and practical performance to this field. Further development of these computational tools could be invaluable for achieving accurate high-throughput screening of the stability and photocatalytic activities of photoelectrode materials.
- This group is modeling the catalytic and stability effects of various semiconductors. This research will help support mechanisms in PEC devices, but it is on the fundamental end of the research continuum. This research synergizes well with the surface chemistry team at UNLV and PEC efforts at NREL.
- The objective of developing a theoretical tool chest for modeling PEC systems is important. A sharper understanding of the physical mechanisms involved can help steer experimental researchers in the right direction to arrive at meaningful results more quickly.
- As a stand-alone effort, this project would not provide directly relevant support to achieving the Hydrogen and Fuel Cells Program objectives. On the other hand, coordination of theoretical/numerical studies with applied research and development efforts has resulted in outstanding progress in both understanding and reducing obstacles to PEC. In this sense, the effort has outstanding potential for relevance and a potentially large impact.

#### **Question 5: Proposed future work**

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

- It is good to see an interest in transitioning to Approach Two materials.
- The proposed future work is presented but lacks specifics and dates; in addition, there is no mention of decision points.
- The future work is clear and topical. There should be more detail on the public dissemination of the physical model of PEC physics.
- The first three milestones relate to the stabilization of the III-V semiconductor via surface nitriding. The demonstration of durable III-V PEC materials would be a significant accomplishment, and these models may just offer the necessary insight to provide a pathway towards success.

- The proposed projects are appropriate, although the value of investing too much time in investigating CIGS-based photoelectrodes is questionable because of stability concerns. The proposed work on understanding how the water structure and associated proton mobility influence reaction mechanisms is a very timely and potentially important subject, as is the dynamic modeling of photoelectrodes under bias.
- The proposed future work is in strict coordination with the focus, reflecting requested simulations in support of current PEC projects. Continuing validation studies are essential, and these are reflected in the proposed work. CIGS is becoming a central material, and CIGS studies are reflected in the proposed work. The relationship between hydrogen evolution and corrosion is thought to be strong, and the effort is proposed in order to illuminate this process. Modeling interface materials under bias will be a unique achievement with potentially enormous implications to process understanding and control.
- There needs to be more effort on milestones four and five, which are critical in understanding how to push STH levels out and have a robust system. This project should continue to try to understand the GaP and InP variation and mechanism.

### Project strengths:

- The project, if successful, may set the groundwork for an accelerated discovery in PEC.
- This is a valid effort trying to adapt *ab initio* DFT molecular dynamics to the semiconductor/electrolyte interface.
- This project fits well with the overall fuel cell strategy. The project is developing a set of criteria to better understand the materials and the selection for PEC.
- This project has outstanding technical capabilities, facilities, and collaborative efforts.
- This research is highly collaborative and completes a strongly synergistic effort between surface/materials characterization, PEC function, and computational modeling/simulation.
- The development of corrosion models continues to improve and compare favorably to the empirical data. As general concepts are developed, they hopefully can be successfully parlayed to other promising PEC materials such as SiC and CIGS.
- The core competency of the PIs in applying *ab initio* DFT and molecular dynamics (MD) simulations to PEC systems is evident, and fruitful collaboration with experimental partners has been established.

### Project weaknesses:

- It is important that the modeling effort be widely available and vetted through experimental validation.
- It would be good to see more specific priorities on the future work and where the effort will be focused.
- The computational resources and level of effort are constrained by concerns over funding levels and continuity.
- Some of the proposed future work items are vague, and it seems like this project is pulled in many different directions.
- The predictive power appears great enough to simulate spectra fairly well, but the project may not yet be able to model a PEC system complex enough to explain experimental results.
- The latest results are not as impressive as those in the 2012 DOE Hydrogen and Fuel Cells Program Annual Merit Review report. The modeling effort is commendable, but it seems like a large and complex undertaking that may require additional team members and funding. It may not be worth adding this to the PEC hydrogen production portfolio.
- The scope of this project is well thought out and sufficiently narrow to maximize the probability of success. The models appear to be for binary InP and GaP when they need to be expanded for the GaInP<sub>2</sub> system and compared to empirical data from NREL.

### Recommendations for additions/deletions to project scope:

- This project should seek additional support from fundamental research agencies to expand the “influence region” of the simulations and to add quantum dynamics simulations to the liquid phase.
- This project can clearly identify milestone targets and systems to explore. There does not seem to be a clear path for the next step in the studies. Also, this project should include the specific next steps in the CIGS

collaboration. Major technical challenges and the proposed means to overcome them should be clearly spelled out.

- The science behind the photo-corrosion of a cathodically protected surface is quite interesting. As with any model, the efficacy needs to be proven against empirically derived data. This has been met with success for the binary InP and GaP system. There is a real opportunity to develop the theory against real experimental data on the GaInP<sub>2</sub> material, and in the short term, this should be a narrow focus. The nitrided surface provides a second opportunity to test the model with a more complex surface structure.
- Although the initial efforts have focused on just a few materials as computational methods are developed and refined, extension of this work across many materials, in conjunction with experimental efforts to demonstrate the potential predicative power of these modeling efforts, would be extremely powerful. This includes trends in surface catalytic activity, susceptibility to corrosion, and energy band alignment. To date, it seems that much of this work has been driven from the experimental side, but as modeling capabilities are refined (as it seems they have been), it would be nice to see the opposite occur. Similarly, close collaboration with experimental efforts to validate modeling results on the surface hydrogen bond network and photoelectrode operation under bias should be pursued.

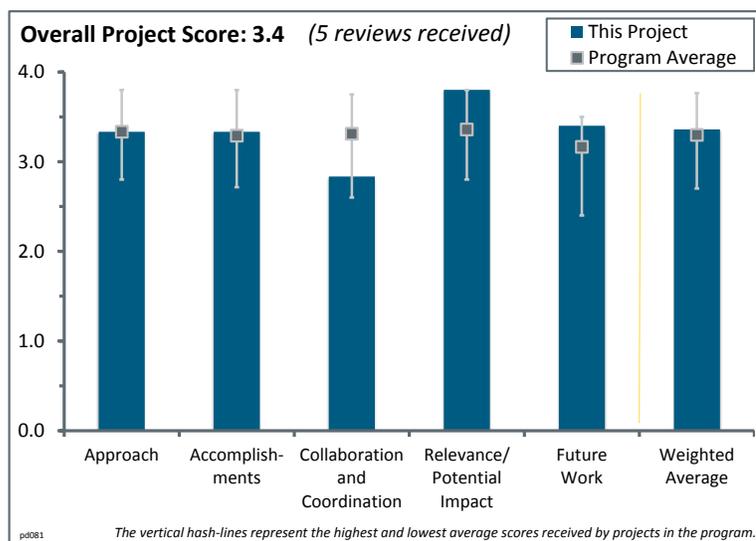
## Project # PD-081: Solar Hydrogen Production with a Metal Oxide-Based Thermochemical Cycle

Tony McDaniel; Sandia National Laboratories

### Brief Summary of Project:

The objective of this project is to develop a high-temperature solar thermochemical (STCH) reactor and redox materials for efficient hydrogen production based on a two-step, non-volatile metal oxide cycle. The 2012–2013 objectives include designing and assessing the feasibility of particle receiver–reactor concepts; discovering and characterizing suitable materials for two-step, non-volatile metal oxide thermochemical cycles; and constructing and testing reactor prototypes.

### Question 1: Approach to performing the work



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

- The approach seems to be very “Edisonian.” The project would benefit from investigating why certain perovskites behave the way they do.
- This project has made good progress on perovskite evaluation of redox kinetics and showed good progress on synthesizing targeted materials.
- The project addresses one of the crucial points for reaching the theoretical efficiencies of thermochemical hydrogen production. The use of a vacuum instead of flushing gases has the potential to achieve real breakthroughs, as well technical benefits, such as reducing the operational cost of the process. The approach to achieve this is excellent.
- The approaches presented in the project, including analysis of the hydrogen production cost using the Hydrogen Analysis version 3 model (H2A), materials discovery, and reactor design, are very effective for accomplishing the project objectives and the U.S. Department of Energy’s (DOE’s) targets for the STCH hydrogen production pathway in the longer term.
- The materials program is mining perovskites for new high-temperature STCH cycles and has rational scientific design principles to guide the search for useful perovskites. This is an excellent approach that moves away from the simple monometallic or bimetallic phases pursued in the past to find novel materials with optimum properties. The reactor program addressed a variety of issues, but not high temperature reactor operation. The other issues are unimportant if the reactor system does not operate at high temperature. For this reviewer, the materials approach earns a 4, and the reactor approach earns a 2, for an average of 3.
- This project has established a comprehensive approach to achieving program objectives and targets by integrating active materials discovery with receiver reactor design. Both of these tasks were thoroughly justified by outstanding analysis of performance requirements, including overall solar-to-hydrogen efficiency targets, requisite heat recuperation, and material thermochemical activity to meet those targets. The performance testing is either under way or planned for each of those critical issues, and alternative materials and design options have been planned in response to performance testing. A design concept for solar collection and concentration has been developed and offers a relatively inexpensive pathway to prototypical on-sun testing and demonstration.

### Question 2: Accomplishments and progress toward overall project and U.S. Department of Energy (DOE) goals

This project was rated **3.3** for its accomplishments and progress.

- More work needs to be done on materials discovery. It is not clear if a low-bed permeability can be maintained as the reactor is scaled up.
- The proposed reactor concept could feasibly solve the issue of avoiding flush gases and, therefore, raise the efficiency of the thermochemical hydrogen production significantly. Through the possible increase of efficiency, it seems realistic that DOE's goals for hydrogen production costs are achievable.
- There was good progress reported on this work. The hydrogen production cost analysis done on this project demonstrated that, for central hydrogen production (100,000 kg/day), the STCH pathway can meet DOE's ultimate cost targets. This project has made good progress on the materials discovery work.
- The materials portion of the program took a major leap forward this year with the discovery of a perovskite material that appears to perform substantially better than the CeO<sub>2</sub> standard with regard to oxygen capacity, oxygen mobility, and lower reduction temperature. The H<sub>2</sub>A analysis suggests the system is close to the 2020 DOE hydrogen cost target. The reactor system was demonstrated to have sufficient particle transport rates to cycle the process and adequate bed sealing to keep hydrogen and oxygen separate at low temperatures. After five years in the project, it is surprising that high temperature operation has not been demonstrated, although this aspect was described as a 2014 activity. In addition, a moving particle system will exhibit particle attrition; this issue and its impact on reactor system performance have not been studied.
- Outstanding progress was exhibited in receiver–reactor analysis and design, and prototype operational component testing is under way. At least two materials have been formulated for thermochemical activity testing, including one baseline material with enhanced performance via zirconium doping. A large class of perovskites was selected for the materials discovery effort, and the number of potential materials was significantly reduced by selecting materials with three characteristics for further investigation. Forty-five perovskite candidates have been synthesized for screening by thermogravimetric analysis for thermochemical activity and reaction kinetics studies.

### Question 3: Collaboration and coordination with other institutions

This project was rated **2.8** for its collaboration and coordination.

- There is not much evidence of collaboration during this phase.
- This project has good collaboration in the areas of materials discovery and on the economic analysis.
- It seems that the partners are very well connected. A clear synergy exists in the coordination of receiver–reactor development material issues and solar concentrator layout and development. All the tasks jointly used development models that predict the performance of the technology. Based on the presented results, the data used seems to be very reliable, and therefore the collaboration and integration seems to be close to perfect.
- The coordination between materials researchers and between reactor researchers separately appear robust. It is not clear how much interaction there is between the two groups, but it is clear that the new materials will feed into the test reactor program in the future.
- The project exhibits close cooperation with its partner, but the coordination of efforts by the partners is less than outstanding since each is pursuing a different class of materials and each appears to be planning distinct receiver–reactor designs. The partnership appears to be a result of necessity rather than a joint collaborative pursuit of the common overall program objective.

### Question 4: Relevance/potential impact on advancing progress toward DOE research, development, and demonstration (RD&D) goals

This project was rated **3.8** for its relevance/potential impact.

- The costs and work presented are in line with the overall goals of the program.

- This work is very relevant to DOE's research and development efforts and targets long-term central hydrogen production pathways.
- The project has a very high potential to substantially contribute towards achieving the DOE targets for renewable hydrogen production. It is likely that it will lead to significantly reduced hydrogen costs compared to the current state of the art.
- This program addresses the long-term goal of moving to renewable hydrogen sources in the 2020–2030 time frame. STCH approaches have fallen short in the past, and this effort seeks to combine a new reactor system for a two-step metal oxide cycle based on novel perovskite materials to overcome traditional obstacles. Both components of the system appear promising and show evidence that they possess superior attributes to competing STCH approaches.
- Uncertainty remains in terms of the level of perovskite thermochemical performance, but given the success in the materials discovery effort, this project will provide a viable solar-powered thermochemical hydrogen production path. Since perovskites are only one of many other materials options, the overall approach in this project offers considerable promise to achieving the ultimate STCH program goal.

### Question 5: Proposed future work

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

- The proposed future work is well conceived as a follow-up to current activities and is well focused on barriers targeted by current work.
- The project is very well focused. The next steps are logical. The project plan seems to be appropriate for effectively achieving the goals.
- The proposed work seems to be reasonable and provides a good plan for addressing the barriers associated with the STCH pathway. The continuation of the materials R&D work plus the sensitivity studies on the cost analysis will be of great value to this work.
- The team needs to focus on more materials discovery. The team seems to be placing too much emphasis on reactor details and design.
- The materials effort has only scratched the surface of perovskite potential, and continued efforts in the area as described in the plan are demanded. The reactor system must be tested at high temperature going forward to look at the effects of particle attrition on system performance and the impact on oxygen release and hydrogen production reactions. Even if the metal oxide changes over time, the physical impact of particles moving through the system and changing must be studied.

### Project strengths:

- This project has outstanding technical proficiency, facilities, and project work planning.
- The STCH hydrogen production pathway is highly relevant to DOE's efforts toward longer-term hydrogen production pathways.
- The current materials approach is excellent. The reactor system design promises peak performance. The team appears to have the resources to accomplish goals and is performing well.
- This project is taking a practical approach to reactor design. Good progress was made on the synthesis of candidate materials.
- The project is based on an excellent concept, tackling one of the key factors for reaching very high theoretical efficiencies of two-step thermochemical hydrogen production by avoiding additional gases. The partners are world-leading scientists, and the synergy between them is obvious.

### Project weaknesses:

- The collaboration with other researchers in the field is weak.
- This project must demonstrate high temperature operation of a reactor system prototype long enough for problems to develop. The problems may depend on the metal oxide chosen for the cycle.
- The presented simulations are based on solar dishes, which are inappropriate for the proposed technology. The concept of the proposed receiver–reactor seems to be feasible; however, moving parts at very high temperature with a temperature gradient over the moving parts is probably tricky to realize.

- It seems that maintaining particle size control is very important for the reactor to operate effectively. The durability of the material will be of key importance, as it is conveyed and continually cycled through the reactor. It was not apparent that any testing was being conducted to verify and ensure particle stability of the perovskite material under heat and impact, as will be the case in the actual process as the material moves through the auger.

**Recommendations for additions/deletions to project scope:**

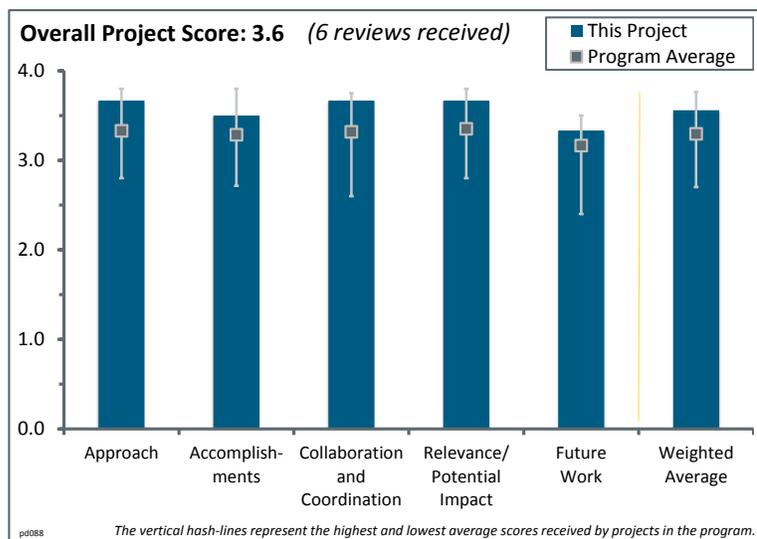
- The project should make a concerted effort to bring in other institutions and individuals to participate in a broader, well-coordinated effort.
- This project needs significant experimental reactor work at operating temperatures and a probabilistic assessment (using H2A analysis) to see the probability of the project meeting the targets. For instance, in the current assessment, the solar-to-hydrogen efficiency changes from 6.2% to 16.7%; it is unclear whether the probability of that actually happening is 10%, 50%, or 90%.
- H2A analysis should be performed for a solar tower/heliostat field arrangement and compared to analysis done for the solar dish scenario. The reflector geometry should be optimized by using ray tracing for a specific location over a full year to maximize the annual output of the system.

## Project # PD-088: Vessel Design and Fabrication Technology for Stationary High-Pressure Hydrogen Storage

Zhili Feng; Oak Ridge National Laboratory

### Brief Summary of Project:

The objectives of this project are to address the significant safety and cost challenges of the current industry standard steel pressure vessel technology and to develop and demonstrate the steel/concrete composite vessel (SCCV) design and fabrication technology for stationary storage of high-pressure hydrogen. Integrated vessel design and fabrication technology should use commodity materials (e.g., steels and concretes); mitigate hydrogen embrittlement to steels; and develop advanced, automated manufacturing of layered steel tanks.



### Question 1: Approach to performing the work

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

- This project is a very novel use of a combination of technologies (concrete and steel) to deliver a cost-effective storage system. There is a good focus on reducing the cost of the complete system.
- The approach the project team is taking is excellent. The long study and cost analysis phases seem to have allowed the project to develop such that the next phase (that includes fabrication) will benefit from findings that the team has developed over the past two years. The approach to developing an ASME code case is very good.
- The technical approach is excellent, but the presenter and project could make a stronger reference to the fact that layered steel tank technology is already in use at refineries for gaseous storage, per the presenter's feedback during the question and answer session. He addressed hydrogen permeation through different layers and venting this hydrogen off (low quantities at near-atmospheric pressure). Although the interior storage volume is currently calculated at room temperature, the project should consider what the realistic capacity is when system tanks are in operation in an underground concrete set-up, which is most unlikely to operate at room temperature. Compared to above-ground storage, this is a much more stable environment that could have a positive impact on the cost of hydrogen dispensed due to the decreased requirements for pre-cooling.
- This project covers low- (160 bar), moderate- (430 bar), and high- (820 bar) pressure storage operating regimes and efforts that should be focused on addressing industry needs within the range of moderate- to high-pressure storage. There were also a wide range of vessel designs, and it is unknown if site fabrication is required for the largest (564 kilogram) design.
- This project is an excellent and novel, low-cost concept for stationary storage. Since the material cost is often the most sensitive parameter, significant attention must be paid to minimize the use of expensive materials. Although this was considered—for example, in Cases One through Three—no effort was made to consider varying the steel wall thickness by component. For example, the steel layer in the center shell of Case Two does not need to be as thick as the heads. A slide showing simply how much money could be saved from varying the wall thickness in lower-stress regions of the structure should be presented. The “leak before failure” approach is much appreciated. Joule-Thomson expansive heating of hydrogen through small leaks/cracks needs to be considered, as this has been a cause of explosions.

- In regard to installation at the station, there are excavation issues, costs inclusive of excavation, and installation code cases. It is unclear what the value is in terms of station footprint reduction, how leakage through the permeation barrier gets measured, and if leakage is monitored throughout station life. It is also unclear what the process is for end-of-life remediation/disposal and if this is a mild or significant issue. Other issues that need to be better explained include the cycle life of the vessel; lifetime cost effects; the benefits this reinforcement method has over other techniques, such as carbon fiber wrapped Type-I vessels; and how much additional cost savings are projected or available to offset other station costs. The material permeation tests will contribute value beyond this project.

### **Question 2: Accomplishments and progress toward overall project and U.S. Department of Energy (DOE) goals**

This project was rated **3.5** for its accomplishments and progress.

- The manufacturing cost analysis was very good and seemed complete.
- This project has clear accomplishments towards the objectives of the project.
- This project appears to have made consistent and continuous progress over the past three years. The project is on track to initiate scaled prototype testing. This is a textbook example of taxpayer dollars well spent.
- This project has made good progress so far on the development of the system. The project needs to move quickly to demonstrate the system's proof of concept with inert gas and then hydrogen.
- The fabrication complexity and the cost of the layered vessel should be better understood. This project needs to establish details regarding a step-by-step manufacturing process for layered vessel design. More clarity is needed on the mock-up vessel design that will be used for the demonstration program, and the expected cost of the new vessels should be benchmarked against the cost of commercially available steel and composite ASME storage vessels.
- The biggest cost is vessel heads. It is unclear what is being done to address this in lieu of discarding 30/70 and if there is any room for further cost reduction. The project should consider if the manway can be eliminated in favor of cameras or other probe-type inspection techniques. The project should also consider how manufacturing techniques can be improved to reduce the pre-stress part of the process. This project has excellent designs for experiments with hydrogen permeation tests.

### **Question 3: Collaboration and coordination with other institutions**

This project was rated **3.7** for its collaboration and coordination.

- The collaboration and coordination requirements were met.
- This is a great assembly of contributing expertise partners. It is good to see Oak Ridge National Laboratory did not try to do this solo.
- There seems to be a good coordination with the project partners, and the approach to develop an ASME code case is very good.
- All collaborators appear to play a valuable role, but it is not completely clear what the contribution from the Department of Transportation (DOT) was besides funding, as the qualification approach to the storage vessel was not explained.
- This project has included professional organizations that regulate standards (ASME, DOT), academia (University of Michigan), and businesses representing a range of sizes.
- This project does not include collaboration with existing ASME vessel manufacturers.

### **Question 4: Relevance/potential impact on advancing progress toward DOE research, development, and demonstration (RD&D) goals**

This project was rated **3.7** for its relevance/potential impact.

- This project is key to reducing the cost of stationary hydrogen storage, and it is projected to surpass the DOE objectives.

- The research and development activity involving innovative high-pressure ASME storage vessels is required to achieve long-term DOE cost targets in the area of storage.
- The hydrogen storage on the forecourt is a key cost to reduce in order to achieve the DOE goals outlined in the roadmap. This project focuses on one of these key barriers.
- The reviewer is looking forward to the outcomes of 2013 and 2014 activities, as the results show clear progress towards the targets. The potential of this product is clear, even if it was only that the lessons learned became available to manufacturing companies.
- The total weight of the storage system, the cost and practicality of shipping the complete vessel system, and the cost of site work if the components are shipped to the site for integration all provide some reservations.
- The project has made a very good effort at meeting cost goals. The opportunity to further reduce costs is important, as other station elements are cost-challenged. The impact on station footprints may be good but needs further reviewer comment and valuation. The project should focus on finding out what the impact is of the full cost, including installation, testing, maintenance, station model cost and the percentage of overall cost reduction, and the possible offset of other station costs. The project should also discuss the cost impact of using manways versus alternative vessel inspection techniques, the reliability of manway seals, and the inspection requirements. According to the oral presentation, approximately 25% additional cost was added to the header for a manway. The project needs to provide more detail on hydrogen interlayer collection and venting. It was unclear how the millimeter-sized holes were arranged, how this affects cost, and if there is an optimum arrangement. In terms of manufacturing cost mitigation for pre-stressing, it was unclear if and how volume and automation will reduce the cost.

### Question 5: Proposed future work

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

- The reviewer is looking forward to seeing the results from the demonstration of the mockup SCCV design.
- This is a good plan for work for the future. This project should make sure there are no thermal effects that may interfere with the layered concept as a result of differential thermal stresses.
- The completion of the engineering design of mockup SCCV is necessary to move the vessel concept to the demonstration phase. A go/no-go decision point needs to be considered before any technology validation is conducted.
- This project has a clear path towards technology demonstration and transfer. It would be good if a location and demonstration project partner could be lined up before the next DOE Hydrogen and Fuel Cells Program Annual Merit Review (AMR); otherwise, the project should be expected to be delayed in 2014/2015.
- This project needs to address installation in more detail, from the code case to installation costs to benefits/problems. This project needs to comment on cycle life and lifetime costs and create a detailed manufacturing plan.
- The only limitation preventing a rating of four here is the lack of concrete plans for the prototype testing phase. For example, it was unclear if a site and primary contractors have been selected. There was a general lack of specifics on future safety analysis, which is key to the successful implementation of the vessels.

### Project strengths:

- This is a simple concept for storage that has great potential to reduce the cost.
- The cost of hydrogen storage appears to be quite competitive with conventional storage technologies.
- This is a practical focus on low-cost and common materials for reinforced high-pressure storage, coupon diffusion testing, and scale-up of the test plan.
- The project involves a novel approach to hydrogen storage, and the project team has followed a methodical approach throughout the project development.
- This project has excellent communication of the cost and potential for improvement. The low-cost enabling technology and careful consideration of cost and failure mechanisms up front are strengths.
- The use of common materials shortens the typical station storage equipment delays due to long lead times of more exotic materials and the availability of manufacturing equipment. Project strengths include the proposed underground storage instead of above-ground storage, as well as involvement of well-established

industry. This project should be testing and prototyping actual equipment and material resourcing, not only modeling and making assumptions.

**Project weaknesses:**

- This project needs to move to demonstration testing.
- This project should focus on a single vessel, including demonstrations.
- The cost and weight of shipping the complete storage system seem to be prohibitive.
- There is no narrative presented for installation costs, and an installation code case is not presented.
- There is a lack of consideration for variations of steel wall thickness in a given tank section (shell or end caps). More careful analysis of the safety hazards posed by small tank leaks is needed.
- With a wide range of storage volumes proposed, it is unclear if these vessels are planned to be shop- or field-fabricated, or a combination. The cost analysis should extend beyond the vessel design and should include the total cost from manufacturing, site installation, and ongoing operation and maintenance.

**Recommendations for additions/deletions to project scope:**

- There are no changes recommended for this project.
- This project should focus in the area of high-pressure (820 bar) storage.
- This project should consider an installation cost study and installation code case manufacturing plan detail.
- This project should consider a potential for variations in steel-wall thickness in a given tank section (shell or end caps). This project should include an analysis of flammability risks posed by small tank leaks. This project should also include identifying a test site for a prototype system and identifying contractors to move into a prototype development phase.
- This project should consider a smaller-size storage tank as well as a future economical option, as there is a limited variety of options in the market for smaller-capacity-size hydrogen stations. The lead time for typical FIBA Technologies tanks is significant and is limited by a minimum purchase order amount. These could also be used for renewable energy storage in the form of hydrogen. The project should consider smaller-size storage tanks in a “multiple tanks together in concrete” setup/demonstration. For the 2014 evaluation on the feasibility of material operations, this project could add a small layer of hydrogen-impermeable polymer on the outside, between the concrete and steel, to create a sufficient barrier to hydrogen, resulting in a manageable hydrogen vent stream. This could allow for increased use of lower-cost steels in more layers. For cost quotes, this project should consider requesting quotes for 1, 5, 10, and 100 steel vessel shell/head units. It is not clear if DOE targets for this project assume hundreds of units.

## Project # PD-092: Rapid High-Pressure LH<sub>2</sub> Refueling for Maximum Range and Dormancy

Salvador Aceves; Lawrence Livermore National Laboratory

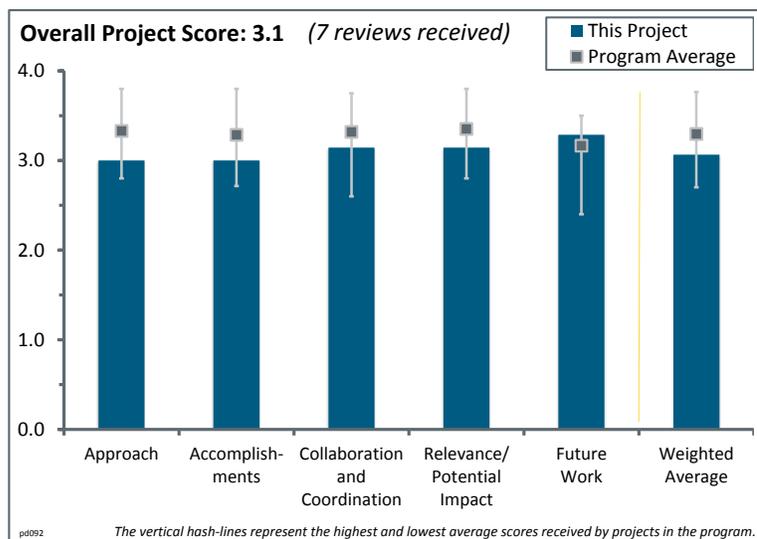
### Brief Summary of Project:

Hydrogen refueling is limited by onboard heating and power and capital at the station. A high-pressure liquid hydrogen (LH<sub>2</sub>) pump can resolve the refueling challenges, as liquefaction is accomplished upstream and onboard cooling is not required. The LH<sub>2</sub> pump provides rapid fueling at a high density and low power use, and it makes cryogenic refueling practical. This project verifies LH<sub>2</sub> pump performance up to 350 bar by determining LH<sub>2</sub> fill time, onboard density, refueling efficiency, and Dewar boil-off.

### Question 1: Approach to performing the work

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

- This project has a good approach to deliver cryogenic (cryo)-compressed hydrogen for refueling.
- This project demonstrates other methods of compression. The project partnerships include several industry partners. The design uses several simple mechanical advantages in cryogenics and thermal dynamics, allowing the total system to reach its performance targets. At the end of the project, a higher pressure is still required to address the technology gaps identified by the DOE Hydrogen and Fuel Cells Program (the Program).
- The team is doing nice work, and the application is justifiable. It is recommended that the project bring in other vehicle manufacturers to bolster the commercial relevance of the team's efforts.
- Although the presentation was not on target, the research approach likely is, and it is the role of the reviewers to differentiate the two in this case. Whether they are ready or not, Dr. Aceves has the responsibility to present an unbiased comparison of cryo-compressed hydrogen technology so that U.S. researchers may understand the benefits that researchers abroad have been pursuing for years. In order to do this, it is recommended that the project make the following changes for future presentations: (1) Immediately present a figure showing a plot of cryo-hydrogen fueling technology cost versus hydrogen density (add in the cost of liquefaction as a secondary point of reference). No other technology comes close on density. Questions remain about how the capital and operating costs compare and the eventual cost floor for the technology. (2) The project should break the system cost down by component to understand where the money needs to be spent and (hopefully) why the project is investing in the high-pressure pump. (3) After the project knows where the potential for improvement is, the researchers should make a pitch for what they are specifically doing and how this is distinctly different from other prior work, such as BMW's. (4) The project should then showcase the progress/accomplishments.
- The approach is unclear. This may be owing to the project title and the lack of a brief description of the envisioned processes.
- The concept is to fuel vehicles with high-pressure LH<sub>2</sub> to enable reliable, fast, low-cost refueling of hydrogen fuel cell electric vehicles (FCEVs). The Linde LH<sub>2</sub> pump technology being investigated appears to be state of the art and designed to minimize hydrogen boil-off. This is a good approach to charging high-pressure LH<sub>2</sub>. The question is whether charging LH<sub>2</sub> is the best approach to fueling FCEVs. On a well-to-wheels (WTW) basis, liquefying the hydrogen consumes a lot of energy. This energy use results in a relatively low WTW energy efficiency and emits a lot of CO<sub>2</sub>, unless the energy is sourced from an



electricity grid with low carbon emissions. A low-carbon-emission grid in the United States is, at best, a long way off. This approach to hydrogen refueling also results in a variable amount of hydrogen in the tank at the end of refueling, depending on the temperature, pressure, and amount of hydrogen in the tank at the start of refueling. Vehicle owners may not accept this situation. The approach to the testing the Linde LH<sub>2</sub> pump appears to be appropriate. The Linde LH<sub>2</sub> pump system appears to have the potential of a 1%–3% hydrogen boil-off loss from the pump and additional boil-off from the LH<sub>2</sub> storage tank. A 3% loss of hydrogen at the refueling station, after liquefaction, has a significant detrimental impact on WTW energy efficiency and cost. When the presenter was asked about this, it was suggested that the refueling station would also have high-pressure gas delivery. The boil-off would be captured and compressed for high-pressure gas delivery. This solution would solve this problem but would require both delivery systems at the refueling station and a hydrogen fuel cell vehicle fleet that would want both types of refueling. This is a lot to ask.

- The cost viability is ignored and should be included. This is a good technical plan, but the presentation does not tell why this is important and what is being done, other than what industry could already do. The building of a refueling system is important for demonstrating the technology, but the work does not show what is being done differently and what obstacles are identified and being worked on to be overcome.

### Question 2: Accomplishments and progress toward overall project and U.S. Department of Energy (DOE) goals

This project was rated **3.0** for its accomplishments and progress.

- This project is doing well and has much potential to satisfy DOE's objectives.
- The accomplishments and progress of the pump are very good, but it is unclear when there will be actual H70 data available.
- This project has made good progress on using both Linde and BMW technologies to address an issue important to DOE's hydrogen delivery technology team goals.
- The site for the installation has been prepared, and a section of hose has been successfully tested and approved for use. This seems like a very modest level of accomplishment after 1.5 years.
- Waiting on construction should not be a limitation; it is an opportunity to complete significant planning, modeling, and independent subcomponent validation. Careful planning could increase the number of minor accomplishments during the laborious construction phase.
- Thermal dynamic models indicate the mechanics will allow the cryogenic pump to meet the performance metrics. In March 2013, BMW started construction of the demonstration facility, presumably with DOE funds. Commissioning of the station will be completed shortly before testing the actual conditions. This is an excellent approach to proving the theoretical approach and ensuring project completion while also ensuring the safety of operation at industry partner locations.
- Since the past year's scope was primarily about building the infrastructure for the future work, excellent progress was made in building the fueling station. The tests are evaluating a simple piece of equipment (the pump) and not really an improved pump design. There was no cost-effectiveness evaluation.

### Question 3: Collaboration and coordination with other institutions

This project was rated **3.1** for its collaboration and coordination.

- These partners are quite knowledgeable in this area.
- This area deserves more attention; otherwise, the project represents government funding to help one foreign vehicle manufacturer, which ultimately will not work.
- This project has done good work with their partners, but there is no indication of which partners are addressing issues to make a better system.
- Although two industry heavyweights and a composite company have been included, no connection with academia was made. The United States is disastrously low on graduates trained to handle and design components for cryogenic hydrogen. This is an opportunity to begin fixing that problem.

- Working with BMW to construct refueling facilities that use cryogenic hydrogen to validate this ability is an interesting approach (i.e., 80 grams per liter density). This will provide reliability data that currently do not exist. Operators will be able to gain many data points for use when optimizing future stations.
- There is excellent collaboration with Linde, who developed this LH<sub>2</sub> pump, but this is the only collaborator. The project lists Spencer Composites as a collaborator, but it is not clear what the company's role in this project is.

**Question 4: Relevance/potential impact on advancing progress toward DOE research, development, and demonstration (RD&D) goals**

This project was rated **3.1** for its relevance/potential impact.

- This project is in alignment with the project goals.
- Past modeling efforts indicate the facility will meet the projected targets. Facilities construction and demonstration will validate the concepts and allow future concepts to be economical and be fully tested with the baseline station requirements.
- The “good” rating was awarded for the promise of the technology, not for the presentation. The problems with the presentation can be summed up by relevance. The prior research completed by BMW and others clearly shows the relevance. However, the progress on this work has not independently contributed anything that differentiates this work from the prior work, aside from pressure-testing a stainless flexline at cryogenic temperatures.
- Without identifying the technical barriers that this station will be used to address and overcome, it is difficult to see what new technology will be developed.
- It is not totally convincing that LH<sub>2</sub> dispensing is a practical solution for FCEVs, but it is much too early to make that decision.
- With the exception of BMW, it is not clear if anyone is seriously thinking of having LH<sub>2</sub> on board. However, an inexpensive and robust cryo-pump is relevant. It would reduce pressurization costs by at least partially pressurizing the hydrogen as a liquid prior to vaporization. Vaporization on board in the vehicle fuel tank may be a challenge because of the material properties of the various building materials.
- The concept behind this project is to fuel FCEVs with high-pressure LH<sub>2</sub> to enable reliable, fast, and low-cost refueling. Charging LH<sub>2</sub> to the vehicle does result in lower-cost refueling stations. The question is whether charging LH<sub>2</sub> is the best approach to fueling FCEVs. On a WTW basis, it takes a lot of energy to liquefy the hydrogen. This also adds substantially to the cost of the hydrogen (about \$1/kg). The energy use results in a relatively low WTW energy efficiency and emits a lot of CO<sub>2</sub>, unless the energy is sourced from an electricity grid with low carbon emissions. A low-carbon-emission grid in the United States is at best a long way off. Most car manufacturers developing FCEVs intend to commercialize using 700 bar gas storage on the vehicle. This approach is less costly, more energy-efficient, and lower in carbon emissions than a cryo-compressed LH<sub>2</sub> system on a WTW basis—although it has much lower volumetric efficiency for storage on the vehicle. This approach to hydrogen refueling also results in a variable amount of hydrogen in the fuel tank at the end of refueling, depending on the temperature, pressure, and the amount of hydrogen in the tank at the start of refueling. Vehicle owners may not accept this situation.

**Question 5: Proposed future work**

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

- This is a good plan to demonstrate technology at the lab.
- It is outstanding as long as the fuel is to be transferred into the vehicle as a gas.
- Funding should be continued and, if possible, increased to maximize the testing program.
- This is a good solid work plan, but more emphasis is needed on overcoming the identified technical obstacles, and a cost model is critical for the program direction.
- No clear justification was made for the need to make new density measurements or a complete performance characterization of the pump. If the entire point of the project was to extend this system for operation at higher pressures, it is unclear why the project waited to construct the high-pressure vessel.

- The design will allow for future technologies to be integrated simply. Running the system provides answers to reliability. High-pressure cryogenic dispensing will allow longer vehicle ranges as a result. However, boil-off losses for cryogenic storage are still quite expensive. It is unclear how the future work reduces boil-off losses.
- The work plan calls for constructing and assembling a complete system to test charging LH<sub>2</sub> using the Linde pump in a vehicle-type cryogenic vessel. Temperatures, pressures, flow rates, and power will be measured. This will first be done at 350 bar and then with a system designed to be capable of 875 bar. This is a good plan, but the experimental set-up may not be able to accurately measure the boil-off of hydrogen, which is a key issue relative to the success of this approach for fueling FCEVs.

#### Project strengths:

- The pump design is a strength of this project.
- This project provides added value to longer-range vehicle performance.
- This project uses some commercial, near-developed technologies to apply to the Program.
- The partnerships and the speed and efficiency with which the project is being conducted are strengths of this project.
- This is a solid extension of the prior research completed overseas. Given the difficulty and scale of the project, it is appropriately located.
- The Linde LH<sub>2</sub> pump technology being investigated appears to be state of the art and designed to minimize hydrogen boil-off. There is excellent collaboration with Linde, who have developed this LH<sub>2</sub> pump, and Spencer Composites, who are expert at building cryogenic pressure vessels.
- This project will demonstrate the capability of cryogenic refueling and address specific technology gaps and issues identified by the Program. The facility design will allow for future advancements in cryogenic refueling technologies. System components are designed and built with a higher rating than what is currently available to allow for higher densities during future component refueling demonstrations.

#### Project weaknesses:

- The project too closely replicates the work of foreign manufacturers of FCEVs.
- The facilities could have been constructed with future operator training classrooms available.
- It is unclear if this project is in sync with the industry's plans for refueling. If it is not, a re-scope may be warranted.
- There is a lack of identification of future technical obstacles that will need to be addressed. There is also no cost model.
- There is no demonstrated use under the conditions needed by the Program. It is unclear if the seals on the pumps will survive the 850 bar conditions.
- This project's weaknesses include communicating the project's relevance, planning ahead for efficiency, and identifying/pairing collaborators in academia with the appropriate sub-projects.
- The concept behind this project is to fuel FCEVs with high-pressure LH<sub>2</sub> to enable reliable, fast, and low-cost refueling. Charging LH<sub>2</sub> to the vehicle does result in lower-cost refueling stations. The question is whether charging LH<sub>2</sub> is the best approach to fueling FCEVs. On a WTW basis, liquefying the hydrogen consumes a lot of energy. This also adds substantially to the cost of the hydrogen (about \$1/kg). This energy use results in a relatively low WTW energy efficiency and emits a lot of CO<sub>2</sub>, unless the energy is sourced from an electricity grid with low carbon emissions. A low-carbon-emission grid in the United States is, at best, a long way off. Most car manufacturers developing FCEVs intend to commercialize using 700 bar gas storage on the vehicle. This approach is less costly, more energy-efficient, and lower in carbon emissions than a cryo-compressed LH<sub>2</sub> system on a WTW basis—although it has much lower volumetric efficiency for storage on the vehicle. This approach to hydrogen refueling also results in a variable amount of hydrogen in the fuel tank at the end of refueling, depending on the temperature, pressure, and amount of hydrogen in the tank at the start of refueling. Vehicle owners may not accept this situation. The Linde LH<sub>2</sub> pump system appears to have the potential of 1%–3% hydrogen boil-off loss and additional boil-off from the LH<sub>2</sub> storage tank. A 3% loss of hydrogen at the refueling station, after liquefaction, has a significant detrimental impact on WTW energy efficiency and cost. The experimental set-up may not be able to accurately measure boil-off of hydrogen, which is a key issue relative to the success of this approach to

fueling FCEVs. When the presenter was asked about this, it was suggested that the refueling station would also have high-pressure gas delivery. The boil-off would be captured and compressed for high-pressure gas delivery. This solution would solve this problem, but it would require both delivery systems at the refueling station and an FCEV fleet that would take both types of fuel. This is a lot to ask. The site for the installation has been prepared. A section of hose has been successfully tested and approved for use. This seems like a very modest level of accomplishment after 1.5 years.

### **Recommendations for additions/deletions to project scope:**

- There are no recommendations at this time.
- This project should add specific technology gaps and a cost model.
- The project should add a variety of other FCEV manufacturers.
- This project should test at scale at the laboratory when the shakedown is complete.
- This project needs to resolve the fueling process questions and test the pump for H70 systems.
- A sensitivity study could have been conducted using simple, first-order models while construction was under way. This analysis would have directed the future project scope and helped with reviewer confidence. As it stands now, there is not enough information to make an accurate recommendation for additions or deletions to the project scope. One accomplishment mentioned was the pressure validation of stainless flexible tubing. It was not made clear why this line must be flexible instead of a relatively easy solid line. One issue with flex tubing is flow-induced vibration due to vortex shedding around the corrugated tube sections. This vortex shedding can cause fatigue and premature failure (the National Aeronautics and Space Administration has studied this for filling shuttle tanks). This test did not consider flow-induced vibration or fatigue testing of the tube under pressure. This problem should be considered in future analysis, given the criticality of this component.

## Project # PD-094: Economical Production of Hydrogen through Development of Novel, High-Efficiency Electrocatalysts for Alkaline Membrane Electrolysis

Katherine Ayers; Proton OnSite

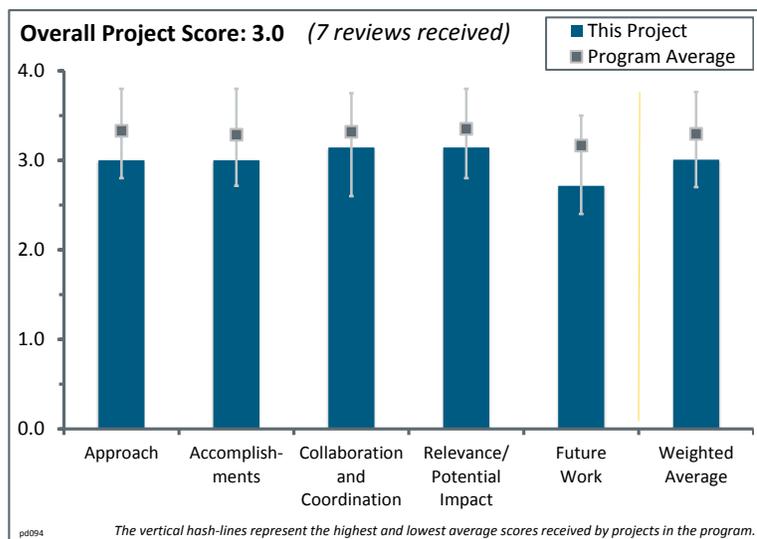
### Brief Summary of Project:

The objectives of this project are to demonstrate high activity of reduced noble metal content pyrochlore catalysts for oxygen evolution, optimize catalyst composition and microstructure, form and characterize new anion exchange membranes and demonstrate acceptable conductivity for electrolysis, process promising membrane and catalyst materials into membrane electrode assemblies (MEAs), scale up to a relevant stack active area and height, and operate in a relevant environment.

### Question 1: Approach to performing the work

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

- The reduction in noble metal catalysts for electrolysis is a good approach, and the focus on materials cost reduction is very good. A Hydrogen Analysis (H2A) would have been very helpful to see if the materials cost savings outweighed the performance losses and the additional cost of including a gas diffusion layer (GDL) and other components.
- This is a very solid overall approach to the program, especially since much time is spent motivating the role of pH and the catalysis challenge. Few groups can make this link as logically, given Proton OnSite's experience. This is very well motivated. It would be good see a little more fundamental effort on understanding the low surface area.
- Alkaline membrane electrolysis is a promising approach to developing lower-cost electrolyzers since non-precious metal catalysts can potentially be used. This project is taking an excellent approach in developing electrocatalysts for the alkaline environment and integrating them into alkaline membrane cells, leveraging Proton OnSite's experience in membrane-based electrolyzer assemblies.
- The approach is valid. Development of the catalyst along with the membrane is a concern (there is little work shown here, though), but the interfaces between the catalyst and the ionomer are not in the scope. It is assumed that no work on the catalyst layer is required in moving from polymer electrolyte membrane (PEM) to alkaline exchange membrane (AEM), yet the nature of the catalyst has changed. Some focus on porosity, etc., would be helpful in Phase II.
- The approach has followed the routine proof-of-concept route through Phase I, which is good. Phase II needs to be reconsidered. The key drivers for product acceptability through manufacturing and commercial deployment should be considered at this point, and the Phase II approach should be adjusted based on addressing the critical tasks first. For example, if the noble metal choice and level will never be commercially viable, there is no sense in trying to optimize the existing catalyst.
- The approach to the project is fairly broad, particularly for such a limited funding level. The inclusion of catalyst studies, membrane studies, and system studies are relatively independent and do not allow for prioritization of the areas of highest concern. A pyrochlore class of catalysts should be compared to other catalysts, such as platinum and silver, to properly address performance improvements. For most electrolysis applications, the catalytic over-potential is more important than the capital cost of the catalyst.
- The approach of an alkaline electrolyzer with an AEM has the potential to reduce electrolyzer costs. The main issue with AEM electrolyzers is membrane durability. Membrane durability (without carbonate recirculation, which decreases performance) should be the main focus. Durability tests need to be longer (at



least 1,000s of hours and probably at least 10,000 hours for commercial electrolyzer products, but Proton OnSite should have durability targets). It is not clear what is new in the catalyst development work, as the catalysts described were reported in the early 1980s. It is not clear what advantages these catalysts have over the nickel-based catalysts used in alkaline electrolyzers or other known non-platinum group metal (PGM) catalysts that can be used in alkaline electrolysis. It is not clear what barrier or need the catalyst development work is addressing.

### Question 2: Accomplishments and progress toward overall project and U.S. Department of Energy (DOE) goals

This project was rated **3.0** for its accomplishments and progress.

- For the scale of the project and the time spent, this project appears to be very productive. This is a very well-managed set of activities, some rather scientific and some engineering, yet they are well integrated into one program.
- Progress has been good thus far, and timeliness has been demonstrated. Whether the end product of this proof-of-concept stage is viable is a question that needs answering. The world's supply of iridium is not so great that this approach makes sense for the future. If this is so, then the project should stop now and use the models developed to find better, more viable catalyst choices.
- The initial electrolyzer results are encouraging. The membrane durability shown is with carbonate recirculation, which will decrease conductivity and performance and may add additional costs in hydrogen cleanup. Durability without CO<sub>2</sub> should be shown. The surface areas of catalysts are low and need to be increased. The D-band orbital theory model is questionable. Activity mostly follows surface area trends. Comparing the activity of catalysts with orders-of-magnitude difference in surface area leads to considerable uncertainty. Variations in area-specific activity for materials with the same metal-adsorbate repulsion ( $V^2$ ) is as large as the variation between materials with  $V^2=4.45$  and  $V^2 = 5.13$ .
- The researchers have developed active electrocatalysts and were successful in integrating them into MEAs. This is directly in line with their objectives. However, so far the catalysts are all precious-metal based, which limits the potential for cost reduction in using alkaline membrane cells versus the more conventional acidic membranes. However, the results on the precious-metal based catalysts still represent an important stepping stone. The researchers showed that their MEAs are better than existing AEM electrolyzers. It was unclear, however, if this improvement was due to better MEA fabrication or better catalysis. While it is clear that the catalysts are active for water oxidation, no comparisons were made to known state-of-the-art materials using standard three-electrode electrochemical techniques such as rotating disk electrodes. Comparisons along these lines would have been helpful to assess the progress on catalyst development, which is a major component of this project. Regarding the theory component of this project, it was not made evident if and how it was helpful in catalyst development.
- The down-selected pyrochlore would appear to be Pb<sub>2</sub>Ru<sub>2</sub>O<sub>7</sub>. This should be a stated accomplishment. The benefit here is to reduce the cost of hydrogen production, but that value is not clearly stated here.
- The results reported are impossible to fully attribute to a Small Business Innovation Research (SBIR) Phase I award and the low level of funding being reviewed. The results show the high potential promise of a system based on anion exchange with carbonate as the conducting ion.
- Ruthenium and iridium are not inexpensive catalysts. It seems that their use would negate some of the cost savings of not using platinum. The addition of a GDL would also negate some of the cost savings. The overall objective was to determine if there was some cost benefit to going to an alkaline system, yet there was no cost analysis to show that this was the case. Using the carbonate form of the membrane was very clever. The loading was high for the anode. On slide 15, the project claims good stability with carbonate recirculation, but there are not enough data presented to support this. It is not clear if the current was held constant. These systems need to run for thousands of hours, so 130 hours is not enough to say it is stable. However, for Phase I, a 130-hour test is about all that can be done given the time constraints. This shows a step in the right direction and reason to be optimistic, but it is not enough to justify saying it is "good."

### Question 3: Collaboration and coordination with other institutions

This project was rated **3.1** for its collaboration and coordination.

- Collaboration with the Illinois Institute of Technology (IIT) seemed to work very well. Proton OnSite did a good job leveraging the DOE Advanced Research Projects Agency – Energy project.
- The collaboration between Proton OnSite and IIT is working extremely well; it is clear that they are working closely and synergistically with one another.
- Proton OnSite has brought in other parties to add value to the program and augment their skill sets. For a program of this size, the level of collaboration is outstanding.
- For a small award, there is a limit to the extent of collaboration possible. IIT is a reasonable partner for catalyst development.
- Collaborations between Proton OnSite and IIT appear to be working well. This project may benefit from collaboration with AEM fuel cell projects at Los Alamos National Laboratory and the National Renewable Energy Laboratory being funded by the Fuel Cell Technologies Office.
- The extent of collaboration with IIT on membranes was not clear. If the membrane is one of the key limiting features, then IIT should be quite actively involved in resolution.
- Pyrochlore synthesis is at IIT. Some characterization with regard to structure would suggest an involvement of someone at Oak Ridge National Laboratory, for example. Phase I should involve optimization of the structure and interfaces to improve efficiency and demonstrate durability.

### Question 4: Relevance/potential impact on advancing progress toward DOE research, development, and demonstration (RD&D) goals

This project was rated **3.1** for its relevance/potential impact.

- As AEM electrolyzers have promise in lowering stack costs, this project is highly relevant with significant potential impact.
- The project seems adequate at this stage, although many choices are yet to be made.
- Focusing on capital cost is not as large of a driving factor as focusing on increased efficiency. The system has shown the potential to address both, but only capital cost was called out in the overview slide.
- The motivation makes the overall relevance of the program very clear. Still, there is some question about what will really be required to displace the PEM technology at Proton OnSite, including additional research and development and engineering efforts. For this to be a completely successful project, that investment would be more than offset by market growth. It seems somewhat unlikely that will happen over the next five to ten years. Nevertheless, as a piece of DOE's portfolio, this is very relevant work.
- The approach to reduce the capital costs is very relevant. For the smaller electrolyzers, which may be used in the near term, capital cost is a larger portion than electricity cost, so this has some advantages. The lower operating current, compared to PEM electrolyzers, will require a larger stack size increasing the amount of materials required. PEM electrolyzers are operating at two to three times the current density. So even if the cost of titanium is eliminated and a less expensive membrane, compared to Nafion, is used, the overall stack cost may not be decreased substantially. The AEM system will likely have a larger footprint than a PEM system; however, it is becoming evident that the stack is one of the smaller components in a hydrogen generator.

### Question 5: Proposed future work

This project was rated **2.7** for its proposed future work.

- This project is focused on the right things. It would be good to see a more fundamental look at the low surface area of some candidate catalysts, slide 10.
- The future work seems appropriate. An H<sub>2</sub>A cost analysis should have been done in Phase I as a justification to move to Phase II, and long-term tests need to be done. This project should plan on using water and moving away from the carbonate stream in Phase II, which is needed for this project to be successful.

- The proposed future work is in line with improving AEM electrolyzer performance; however, it would have been good to see more attention paid to the integration of non-precious metal catalysts, since avoiding precious metals is a primary motivating factor for alkaline membrane electrolysis.
- The proposed future work addresses electrolyte stability issues, electrolyte performance issues, and a system trade-off study, which this reviewer considers more important than catalyst development work for AEM electrolyzer systems.
- The Phase II plans are vague. It would be good to know more about tuning the ionomer and membrane. There is little evidence of real collaboration with Tokuyama here.
- This is an area that should be aggressively addressed with straightforward techno-economic rigor. The key limiting features should be identified and addressed first and aggressively. Optimization seems premature. Noble metal pyrochlores are not likely to be a real solution, for example.
- Out of the four future work items presented on slide 18, three are of high value (investigating AEM properties, performing trade study, and product cost analysis). Further work into catalyst development is of low concern/priority, but for the work done in this area, proper comparisons should be made (platinum, iridium, ruthenium, and silver on anodes; platinum and others on cathodes).

### Project strengths:

- The demonstration of real electrolyzers is good.
- The approaches are methodical, which should allow for a positive outcome.
- This project is well motivated, is well managed, has good collaboration, and is very productive.
- This has the potential to reduce the capital cost of electrolyzers. It has the potential to use a non-precious metal catalyst.
- This project explores new, potentially interesting approaches to hydrogen production that allow for cheaper materials to be employed.
- This is an excellent team of researchers, combining catalyst development efforts with integration into MEAs and devices. This project has had early success with the development of high-performance AEM electrolyzers.

### Project weaknesses:

- There are no significant weaknesses.
- This project has a strong focus on catalyst development.
- The plans for optimization seem premature. Some techno-economic stage-gating of a simplistic type should be employed to help direct Phase II work.
- Pyrochlore characterization is limited. There is no discussion of the electrode/electrolyte interface (perhaps in Phase II). There is no real collaboration with the membrane/ionomer supplier.
- Establishing working devices based on precious metal catalysts is an important stepping stone; however, it would have been good to see more results on non-precious metal systems. While the MEAs performed well, it was not made clear how the inherent activity of the electrocatalysts developed in this project compare to state-of-the-art, known water oxidation catalysts. It was not made clear how the modeling component of this project has helped in the development of catalysts.
- There should be an H2A analysis on the hydrogen cost of this new technology. The replacements for platinum are either expensive (iridium or ruthenium) or toxic (lead). Durability tests in a relative environment need to be done. The researchers are eliminating some costly materials from their system, but they are adding components (GDLs); increasing the materials required since the stacks will need to be bigger to produce the same amount of hydrogen compared to a PEM, due to the lower operating current; and increasing the complexity (need to monitor and control carbonization), so the cost benefits may not be realized. The project should have reported on the catalyst loading per electrode area.

### Recommendations for additions/deletions to project scope:

- It is difficult to comment without seeing the Phase II proposal.
- There should be a focus on why certain materials exhibit low surface area.

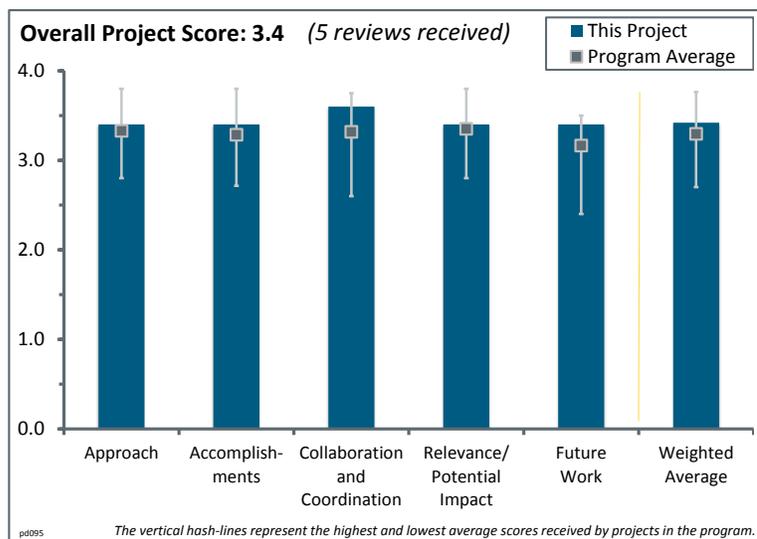
- This project should reduce the catalyst development work and focus on the membrane performance and durability issues.
- This project should remove the catalyst development and focus on the other three areas highlighted in the future work.
- This project should do an H<sub>2</sub>A analysis. The researchers need to do the cell- and short-stack testing in a relevant environment to better understand carbonization mitigation.

## Project # PD-095: Probing Oxygen-Tolerant CBS Hydrogenase for Hydrogen Production

Pin-Ching Maness; National Renewable Energy Laboratory

### Brief Summary of Project:

Photolytic microbes such as algae and cyanobacteria co-produce oxygen with hydrogen. The oxygen inhibits the activity of hydrogenase, the enzyme responsible for hydrogen production. The objective of this project is to develop a robust oxygen-tolerant cyanobacterial system for light-driven hydrogen production from water while increasing system durability. The long-term goal is for the system to be oxygen-tolerant for eight hours (during daylight hours). The first task of this project probes hydrogenase maturation machinery in the oxygen-tolerant Casa Bonita Strain (CBS) of *Rubrivivax gelatinosus*. The second task transfers the oxygen-tolerant CBS hydrogenase and its maturation genes into a *Synechocystis* host that has had the native genes for hydrogen production removed.



### Question 1: Approach to performing the work

This project was rated 3.4 for its approach.

- This project has successfully utilized classic approaches, such as quantitative real-time polymerase chain reaction (RT-PCR) and cloning, which are challenging and yet have been repeated successfully in the principal investigator's (PI's) laboratory. The methodologies are well designed and integrated exceptionally well with the research being conducted by other labs and collaborators.
- This project appears to be well focused on the "oxygen accumulation" barrier (barrier AN) of the Fuel Cell Technology Office's 2012 Multi-Year Research, Development, and Demonstration Plan (MYRDDP). The approach appears to be effective as a new set of maturation genes has been discovered and has been incorporated into gene expression studies.
- The approach to identifying robust hydrogenase activity in CBS and moving it into cyanobacteria is sound.
- This is a good approach, especially the use of a better promoter. There is still no good analysis that links all the laboratory results to a production model that provides some guidance to reviewers on how laboratory accomplishments will lead to a more economic system. This project uses good science, but there are many different approaches at different levels of development, and there is no clear path to having them get integrated and result in a stable mutant.
- NiFe hydrogenase is a logical gene candidate that expresses in the production host because of a long half-life (>21 hours) in air. The pursuit of maturation proteins is also a very logical target for heterologous gene expression. However, the rationale was not explained clearly, and it is unclear why the growth assay is a good proxy for HypE1 and E2 hydrogenase activities.

### Question 2: Accomplishments and progress toward overall project and U.S. Department of Energy (DOE) goals

This project was rated 3.4 for its accomplishments and progress.

- These are good accomplishments in terms of meeting the milestones for individual CBS improvements.

- This is a very impressive set of experiments, results, and publications. The PI's group appears to have tested all assumptions and results. Thus, the work is accomplishing tasks, is generating novel scientific findings, and is on task to accomplish future goals.
- Task 1 milestones appear to have been completed on schedule while adding the newly discovered set of maturation genes to the study. A milestone of Task 2 has been completed ahead of schedule while achieving an order-of-magnitude improvement above the milestone's target.
- The RT-PCR gene expression study of the hydrogenase operon (hypE1 and E2) milestone for January 2013 was completed on time. Gene integration and expression in the production host milestone was completed on time. Identification of a strong promoter (psbA) that will improve gene expression milestones was completed on time.
- The presenters have successfully transferred the Hyp1 genes. They have also discovered a second hydrogenase system (Hyp2), which is being evaluated. The evaluation of the stronger promoter has been completed. The presenter referred to milestones due in May 2013 (the current month) as being "on track." If the milestones were to be completed by the end of the month, it is a concern that they are, in fact, behind schedule. It would have been good to have a clearer outline of the milestones due in May 2013, detailing their actual status.

### Question 3: Collaboration and coordination with other institutions

This project was rated **3.6** for its collaboration and coordination.

- The project was able to leverage low-cost (no-cost) expertise and services (genome sequencing and annotation) from partners to achieve better understanding of the system.
- The collaborations with others in the field indirectly and directly are smart. The PI seems to have a "big picture" concept of what needs to be done in the laboratory to coordinate well with other labs and achieve the larger goal of the MYRDDP.
- The collaboration with Michigan State University (MSU) and Pacific Biosciences is well defined and productive. The collaboration with the J. Craig Venter Institute (JCVI) is not well defined in terms of how the projects are different enough to warrant individual funding.
- The project appears to have strong collaborations with JCVI (Task 2), MSU, and Pacific Biosciences (Task 1). Research has resulted in multiple publications and presentations (including a joint international symposium) run over the past year by National Renewable Energy Laboratory and JCVI team members.
- This project has good collaboration, but it still appears that all of the laboratories are working in parallel, not in combined research and development efforts. Each laboratory is working towards its own objectives, but no single laboratory is integrating all the work.

### Question 4: Relevance/potential impact on advancing progress toward DOE research, development, and demonstration (RD&D) goals

This project was rated **3.4** for its relevance/potential impact.

- If successful, this work will result in a photosynthetic hydrogen production system, which should be very valuable to the renewable energy community.
- Successful acquisition of a cyanobacterium with an oxygen-tolerant hydrogenase would be a significant step towards achieving MYRDDP targets.
- The potential impact of identifying and characterizing mechanisms related to growth profiles and hydrogenase production is critical to understanding how to control hydrogen production while maintaining viable and productive organisms. This fundamental and basic research can be far-reaching.
- This is still one of the biggest barriers for photolytic microbial hydrogen production. However, these approaches all need to be integrated into a single mutant to validate that this approach will work for a complete production strategy.
- The project has made progress towards improved hydrogenase activity for hydrogen production. But the R&D appears to be very early in terms of technology readiness levels; it is unclear at this point whether this project principally supports reaching the \$10/gasoline gallon equivalent cost target for biological hydrogen production.

### Question 5: Proposed future work

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

- The proposed work is a logical extension of ongoing efforts.
- The proposed future work is rational and well integrated with previous work and the work of collaborators.
- The presenters have a clearly defined pathway to move forward and produce results that will support DOE missions.
- The plans build on accomplishments, but the project should spend the time to assemble a mutant with all the hydrogenase improvements to validate that the process will work as planned and that it can be modeled.
- The continued work on CBS hydrogenase is novel and should bring new contributions to the field. The *in vitro* hydrogenase activity assays will be key for further optimization of oxygen tolerance.

#### Project strengths:

- This is a good team of researchers and facilities.
- This project has strong collaborations with external groups and a multi-pathway approach to the work.
- The addition of private partnerships should help facilitate progress towards commercial goals and cost targets.

#### Project weaknesses:

- There is possible redundancy with the JCVI group.
- There are parallel paths to improving oxygen tolerance and increasing hydrogen yield, but nothing has been integrated.
- This project has not tested the redundancies the researchers found. These redundancies would seem to have impacts on fitness due to energy inputs, and it would be an easy test.

#### Recommendations for additions/deletions to project scope:

- This project should ensure the fitness phenotype is addressed.
- Gene expression is one factor that can lead to low enzyme activity, but so can inefficiencies in protein folding. It is suggested that a near-term experimental objective should include comparing the heterologously expressed protein in *Synechocystis* with the native protein isolated from *Rubrivivax* (if it is possible to scale up) in a circular dichroism assay to see if protein folding might be a limitation. Alternatively, the detection of protein aggregates, inclusion bodies, or truncated proteins on western blots using antibodies raised against different regions of the enzyme can help the project direct further optimization efforts.

## 2013 — Hydrogen Storage

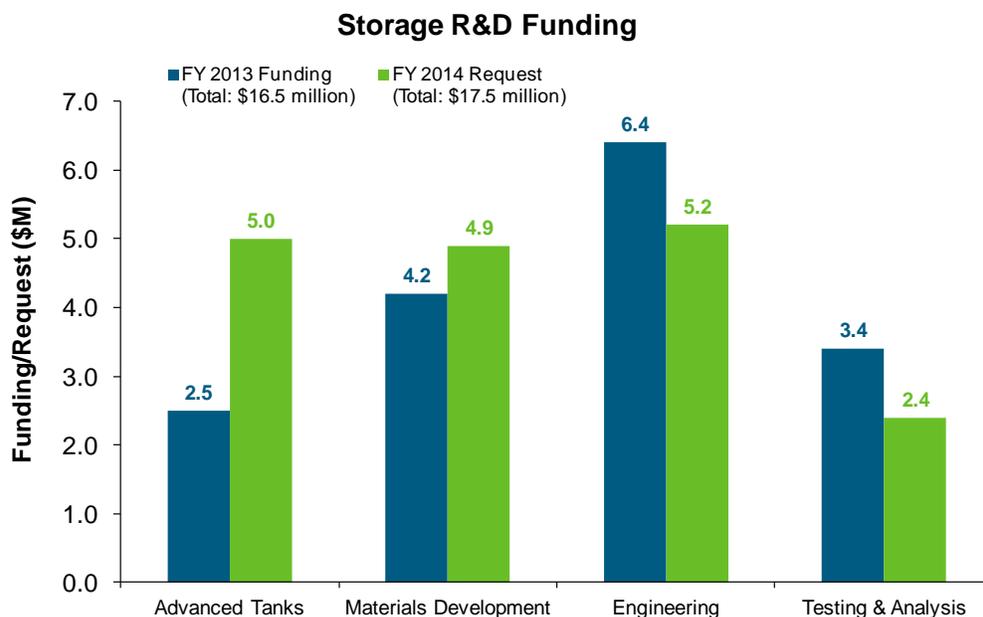
### Summary of Annual Merit Review of the Hydrogen Storage Program

#### Summary of Reviewer Comments on the Hydrogen Storage Program:

In fiscal year (FY) 2013, the Hydrogen Storage program portfolio focused on system engineering for onboard transportation applications, with continued efforts ongoing for materials-based research and development (R&D) and physical storage options for near-term deployments. Reviewers commended the program's use of valuable results from the Hydrogen Storage Engineering Center of Excellence (HSECoE) to help direct and focus materials development. Reviewers felt that the program's efforts to expand the research portfolio to include non-automotive applications, such as material handling equipment, portable power, and stationary applications, were good. Reviewers remarked that the program was underfunded, though they also stated that the current portfolio does a good job of covering key areas. With additional funds, reviewers noted the potential benefits of more materials discovery research efforts. Overall, reviewers commented that the program is very well managed and should continue to focus on meeting all onboard automotive targets and encouraging the development of hydrogen storage for non-automotive applications.

#### Hydrogen Storage Funding by Technology:

The chart below illustrates the appropriated funding planned in FY 2013 and the FY 2014 request for each major activity. The program received \$16.5 million in funding in FY 2013, and it has a budget request of \$17.5 million for FY 2014. The HSECoE continues to be a major activity for the program with additional efforts aimed at lowering the cost of compressed hydrogen storage. Work on hydrogen storage materials development is also an important part of the portfolio that will continue to be an area of focus, especially as more information regarding material-level property requirements is derived from the system engineering efforts. Additionally, there is a planned increased emphasis on early market storage applications in FY 2014.



#### Majority of Reviewer Comments and Recommendations:

The Hydrogen Storage portfolio was represented by 27 oral and 11 poster presentations in FY 2013. A total of 28 projects—via 24 oral and 4 poster presentations—were reviewed. In general, the reviewers' scores for the storage projects were good, with scores of 3.6, 3.1, and 2.2 for the highest, average, and lowest scores, respectively.

**Advanced Tanks:** Four projects on advanced tanks were reviewed, with a high score of 3.4, a low score of 2.7, and an average score of 3.1. Overall, reviewers felt that the work being done is addressing key areas and that significant progress is being made. Reviewers felt that the projects are well organized and that efforts to improve carbon fiber precursor materials and composite-overwrap properties were appropriate because the carbon fiber composite is the largest contributor to the overall tank costs. Reviewers thought that strong progress was made in the projects but noted that some projects could be aided through additional collaboration. Reviewers also suggested inclusion of clear cost assessments for the projects.

**Materials Development:** Eleven materials-based hydrogen storage projects were reviewed, with a high score of 3.4, a low score of 2.2, and an average score of 2.8. Generally, reviewers commended the materials development projects for integrating computational and experimental efforts. The reviewers appreciated the wide range of material types being investigated, including metal hydrides, adsorbents, chemical hydrogen storage materials, liquid carriers, and nano-confined liquids, and found continued investigation of all material classes to be relevant to the program. However, they also commented that many of the materials currently under investigation would not be able to meet the full set of U.S. Department of Energy (DOE) targets for automotive onboard storage of hydrogen. The reviewers also commented that negative results are of value to the community, including when materials and synthesis approaches are not successful, because capturing that information for future reference is valuable. Materials projects will continue in FY 2014, subject to appropriations, with an emphasis on a stronger link and feedback route between the experimental and theoretical efforts and more emphasis placed on meeting projected material-level property requirements to meet the system-level targets.

**Engineering:** Ten projects were reviewed on hydrogen storage engineering, with a high score of 3.6, a low score of 3.0, and an average score of 3.3. Reviewers stated that the HSECoE made significant progress in FY 2014 and featured strong coordination and clear collaboration among the partners. They also commented on the importance of systems engineering efforts, especially in determining the material-level properties required to achieve the Hydrogen and Fuel Cells Program storage targets. The reviewers commented favorably on the development and use of integrated models on projecting system performance. In general, the reviewers considered the projects of individual HSECoE partners to be well thought out and feature expert personnel who execute clear plans. The reviewers considered the sorbent system efforts to be making good progress and to be well designed. Similarly for the chemical hydrogen systems, the reviewers favorably commented on the progress of reactor design, gas cleanup, and balance of plant work. However, for both system types, the reviewers were concerned with the applicability of the efforts to the broad class of materials because none of the surrogate materials being tested are able to satisfy the full set of DOE onboard storage targets. Overall, reviewers thought the HSECoE and its partners were making good progress in evaluating materials-based storage systems and making decisions to meet DOE performance targets.

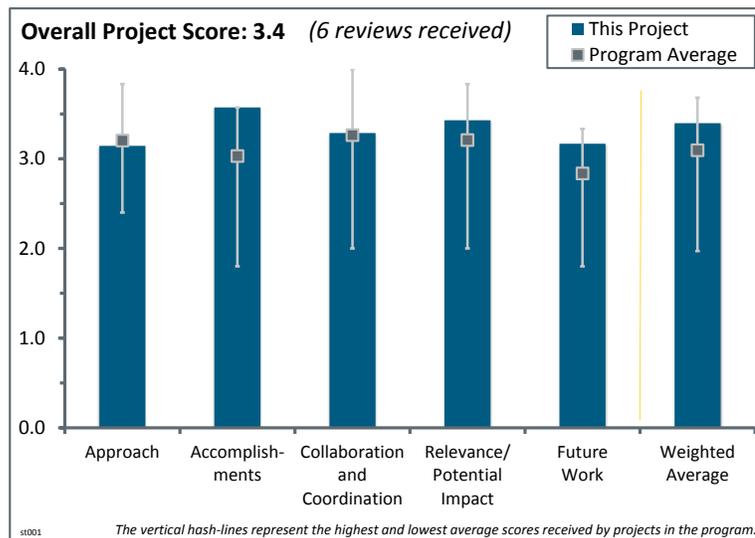
**Testing and Analysis:** Three projects related to testing and analysis were reviewed, with a high score of 3.6, a low score of 3.3, and an average score of 3.4. Reviewers stated that these projects are critical to the program because these analyses help develop targets and guide research to maximize impact. Reviewers felt projects in this area used a robust and comprehensive approach, and that significant progress has been made in cost reduction through carbon fiber and compressed tank cost estimates. Reviewers commended the excellent collaboration and cooperation displayed in each project to ensure coordinated assumptions and efforts in the community. Reviewers thought that validation of models and analysis was worthwhile and suggested prioritizing carbon fiber analysis over metal hydride work in the future. Reviewers thought the Best Practice manual was extremely useful for the community and very well done, and that good progress has been made on thermal and mechanical properties. Overall, reviewers noted that a strong team performed thorough analyses and emphasized the importance of these projects in improving the quality of research in the program and providing clear insight to guide future research.

## Project # ST-001: System Level Analysis of Hydrogen Storage Options

Rajesh Ahluwalia; Argonne National Laboratory

### Brief Summary of Project:

This project performs independent analysis to evaluate the onboard and off-board performance of materials and systems for hydrogen storage. Results are provided to material developers for assessment against performance targets and to help them focus on areas requiring improvement. Inputs are provided for independent analysis of the costs of onboard systems. Interface issues and opportunities and data needs for technology development are identified. The project develops and validates physical, thermodynamic, and kinetic models of processes in physical and material-based systems to address performance targets including capacities, rates, and efficiencies.



### Question 1: Approach to performing the work

This project was rated **3.1** for its approach.

- The project employs a multifaceted approach, which is well suited to the variety of technologies being addressed.
- The approach taken for both of the tasks reviewed appears to be reasonable, and the work appears to be well integrated.
- The work is well coordinated with the efforts of the Hydrogen Storage Engineering Center of Excellence (HSECoE), although there are some redundancies. The U.S. Department of Energy (DOE) needs to decide going forward who should take the lead on systems modeling—Argonne National Laboratory (ANL) or the HSECoE. The principal investigator (PI), however, is a natural fit for these tasks. The focus is not necessarily to achieve the overall U.S. DRIVE Partnership targets, but rather to understand the systems engineering trade-offs/trends required to package materials into a system. This provides guidance to material developers on what materials characteristics to consider.
- This project features a very nice and comprehensive approach that looks at very different systems both for near-term (compressed gas storage) and long-term (metal hydrides) usage for automobile applications (as well as some stationary applications). Simulations on the stress profile ought to be verified by experiments. So far none have been conducted; however, they are important and must be done in this or a follow-up project. Because mobile applications are currently a long-term option for usage of metal hydrides, some suggestions ought to be made about possibilities for using the gained knowledge in the meantime. Perhaps there are possible spin-offs?
- It is not clear which approach was chosen to address the barrier “life cycle assessment.” The project takes a good approach to combine different fiber qualities. It would be desirable to have a matrix or an overview to show the correlations between barrier, approach, and accomplishment.
- Barriers identified are realistic targets for improvement and the approach directly addresses them. However, the scope of the presentation is extensive to the point of perhaps being too broad. It is hard to take in comparison of these different technologies given that they are really at different readiness levels. The ranking reflects an inability to get a complete view of the “big” picture.
- The approach of the project to conduct technical modeling of various storage systems is fine, but validation of the assumptions or results is lacking. It would be useful to include further background regarding the sources of certain assumptions and comparison of model results with physical testing or values. For

example, the tank and system weight projections could be compared to actual systems. Also, it would benefit the industry to have an explanation of the reasons for changes in the model projections from previous years.

### **Question 2: Accomplishments and progress toward overall project and U.S. Department of Energy (DOE) goals**

This project was rated **3.6** for its accomplishments and progress.

- The progress appears to be excellent.
- The project's progress includes an improved assessment of the compressed tank carbon fiber (CF) utilization. The effort in reverse engineering the metal hydride material target values was also a valued accomplishment.
- Progress is excellent relative to the HSECoE targets, which are lower than the overall DOE targets. The systems modeled will not achieve DOE targets but are in line with the HSECoE targets. The modeling highlights how much improvement in particular metrics are required to achieve DOE targets.
- The project features a very good, broad approach, considering physical and chemical hydrogen storage and different types of materials. Researchers have achieved very good results concerning cost reduction and needs for materials.
- Researchers have shown some possible combinations of how to reduce the amount of high-quality CF. However, there is no direct correlation to the DOE targets.
- The project has done thorough work in the areas of focus to date. The integration approach for the resin end cap could be more clearly spelled out. Sensitivities to fiber winding model assumptions should be examined. The project should also examine whether the candidate list of metal hydride materials changes if the fueling time assumption is relaxed somewhat.
- Good progress was shown for both the physical storage and the metal hydride tasks, but no or very little progress was described for the sorbent and off-board regeneration tasks. Also, the summary of work on slide 5 states that a comparison of hydrogen storage in metal hydrides for this project would be made with results and methodology from the HSECoE; however, it would have been good if some of those comparisons were discussed in more detail in the presentation.

### **Question 3: Collaboration and coordination with other institutions**

This project was rated **3.3** for its collaboration and coordination.

- The collaboration and cooperation seem to be very reasonable.
- It seems that all relevant partners are included.
- The project supports and coordinates well with industry, engineering centers, universities, and national laboratories.
- This project's work complements the HSECoE effort and has the appropriate mix of industry, academia, and national laboratories.
- It is clear collaboration is occurring between the right parties, but it is hard to discern if it is the best collaboration possible.
- Collaboration with the HSECoE for the metal hydride task and with Pacific Northwest National Laboratory, Ford Motor Company, and Lincoln for the compressed hydrogen task was good, but the collaborations on the unreported tasks were difficult to evaluate at this time.
- ANL has a good level of collaboration with others in hydrogen storage research. ANL should be encouraged to coordinate its assumptions and effort with the HSECoE to avoid duplication of work. In particular, the metal hydride target material properties were already evaluated by the HSECoE. It would have been useful to compare the results and provide a consensus table of target values for the metal hydride material.

#### Question 4: Relevance/potential impact on advancing progress toward DOE research, development, and demonstration (RD&D) goals

This project was rated **3.4** for its relevance/potential impact.

- The project's contributions to the two completed tasks are well aligned with the current Fuel Cell Technologies Office objectives.
- The project provides needed analysis input to develop targets for other Hydrogen Storage program projects.
- This project shows very high relevance and potential impact by looking at near-term progress (compressed gas) as well as long-term potential (metal hydrides).
- Because CF costs are the main part of the total system cost, the results of this project are very important. However, the proposed future work on metal hydrides should have a lower priority compared to CF.
- The achievements, if incorporated into products by industry, will advance the capability of the systems.
- The project has relevance as an independent system analysis of various hydrogen storage concepts. The effort is very similar to the HSECoE effort, but it does not include the physical confirmation of the modeling that is included in the HSECoE analysis. The potential impact could be further improved by highlighting areas of uncertainty in the models that should be validated or emphasizing the key research needs to further advance the hydrogen storage system research.

#### Question 5: Proposed future work

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

- The future work plan looks good, especially in the efforts to conduct validation with physical confirmation testing and complete reverse engineering for various material-based hydrogen storage systems.
- Validation of the models and results is exactly what is needed and is planned.
- The proposed validation of CF simulation is very important. The metal hydride effort should have a lower priority.
- Additional material targets are needed. Validation of CF designs may require more than coupon testing—possibly standards-based qualification testing.
- The PI should provide a trade-off analysis of how to accommodate for buffer hydrogen volume (required for system start-up) to determine whether a separate buffer tank be included in the system or if extra volume should be added to the existing sorbent vessel. A cost and volume trade-off analysis would be beneficial at the next review.
- The proposed future work logically derives from the work just reported. However, at some point the storage capabilities of each particular technology will face comparison and there will be a need to select the technologies that most realistically meet market requirements. This focus is not addressed here, nor was it indicated in the project scope.
- The researcher should not continue the metal hydride task for higher temperature metal hydrides, especially for automotive applications. Even for non-automotive applications, the researcher should spend more effort on the sorbent and the chemical hydride regeneration tasks.

#### Project strengths:

- A strength of this project is its broad approach.
- The work on physical storage is straightforward and seems to be making good progress.
- This project featured excellent coordination with industry and academic partners to provide realistic system performance and data.
- This is a broad-based project that is providing important data to other projects within the Hydrogen Storage program.
- The PI and ANL have extensive background in hydrogen storage and capability in modeling.
- A strength of this project is its focus on the main cost driver (CF) to reduce the amount of high-quality CF.
- The PI has a good background and experience and expertise in this area. The work appears to be thorough and sound. The PI has demonstrated a good ability to partner with other PIs during his analyses.

**Project weaknesses:**

- Experimental verification is required.
- The PI has made numerous presentations but should strive for more journal publications.
- The project could improve by providing validation of results and confirmation/progress in the assumptions.
- While the work on metal hydrides, sorbents, and off-board regeneration is clearly making progress, the presenter did not spend enough time comparing the capabilities of the different technologies.

**Recommendations for additions/deletions to project scope:**

- The skill set and model should be adapted to model compressed natural gas sorbent-based systems.
- The project team should clearly articulate which work package is for automotive and which is for non-automotive applications.
- The project should include recommendations for future improvements to hydrogen storage systems by conducting sensitivity analysis with the models.
- The project team should separate the metal hydrides and sorbent efforts from the physical storage. Then it could consider allowing another project element (presenter) to address cost effectiveness.
- The work on the metal hydride tanks is an important task because—even if targets have not been met so far—metal hydrides are the only storage option that, in the long term, offers a possibility to overcome present restrictions concerning weight, volume, and cost. Nevertheless, at present for automobile applications, they offer only a long-term perspective. Therefore, it is required that the scientists also give some ideas about possible short-term applications that could allow for a return of investment for the taxpayer in the medium term.

## Project # ST-004: Hydrogen Storage Engineering Center of Excellence

Don Anton; Savannah River National Laboratory

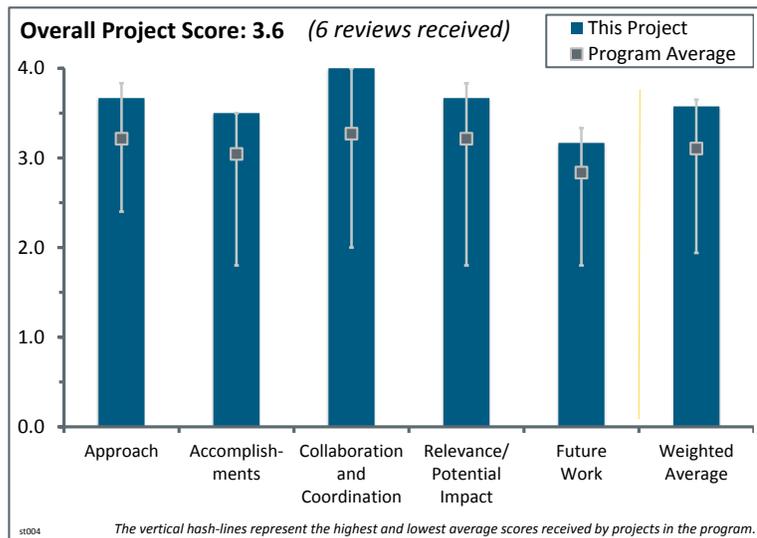
### Brief Summary of Project:

This project uses systems engineering concepts to design innovative, material-based hydrogen storage system architectures and to build and evaluate subscale prototype systems to assess those architectures to improve both component design and predictive capability. The project will develop and validate models for measuring fuel cycle efficiency. Data from these models will be compiled to define required materials properties to meet technical performance and cost targets.

### Question 1: Approach to performing the work

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

- This project has an outstanding and comprehensive approach that includes several different storage alternatives and compares them in one project. It is very good.
- The Hydrogen Storage Engineering Center of Excellence (HSECoE, the Center) approach has proven much more effective than having individual partners attempt these tasks. The task of designing novel systems based on hydrogen storage systems requires knowledge that was previously unavailable. The tasks require the guidance of industry end users to determine system requirements, the resources and expertise of national laboratories, and the materials synthesis expertise and knowledge of academia. The HSECoE targets are generally lower than the overall U.S. Department of Energy (DOE) targets. These targets were set based on the knowledge that storage materials available today cannot yield systems that would achieve the targets. The targets set are challenging and are intended to provide an understanding of what further characteristics in storage materials must be considered to ensure efficient system design.
- This is a comprehensively well-organized project that is focused on the critical technical barriers to achieving a broadly implemented hydrogen-fuel-cell-based passenger vehicle market in the United States. The project matrix structure presented in slide 6 of the Savannah River National Laboratory (SRNL) presentation illustrates the well-integrated nature of this highly effective collaboration in a clear and concise manner. The spider charts provide a fully transparent map of progress over time. In this regard, the modified spider charts, showing year-to-year and/or phase-to-phase progress, are a valuable addition to the presentation format.
- The principal investigator (PI) has created a credible organization with well-defined teams and division of responsibilities. The scope of work for Phases I, II, and III is clearly laid out, as are the Phase II go/no-go milestones. The Center has made a no-go decision on metal hydride systems and is pursuing adsorbent and chemical hydride system options in Phase II. Although a Phase III go/no-go determination was to be made by March 31, 2013, the PI did not discuss what was decided and how the decision was made.
- The Center has several approach variants to two general hydrogen storage options—chemical hydrides and cryo-adsorbents. The sub-projects have analytically and experimentally studied the storage materials, the system designs, and some of the balance of plant (BOP) components. The Center has done well in developing and leading this approach.
- A sensible and comprehensive technical approach comprising modeling, system concept development and testing, and component integration has been adopted for the Phase II effort. Surrogate adsorbent metal-organic-framework-5 (MOF-5) and chemical hydrogen storage materials (ammonia borane [AB] and alane) have been selected for engineering prototype development. It seems reasonable that engineering



development based on MOF-5 will be extendable to future adsorbent systems. Also, given the lack of an ideal chemical hydrogen storage material, the development of prototypes based on both endothermic and exothermic systems is appropriate and prudent. However, the numerous problems faced by the AB system (not the least being the lack of a cost-effective regeneration pathway and the complexity of the overall system design) seem to make the adoption of that material highly problematic. The approach should include a more tightly focused effort on engineering development with the alane system.

### **Question 2: Accomplishments and progress toward overall project and U.S. Department of Energy (DOE) goals**

This project was rated **3.5** for its accomplishments and progress.

- The accomplishments and progress in the different technologies are amazing and convincing. They are very good.
- Tremendous progress has been made in the last year. In particular, for the sorbent systems, many of the results are now available regarding the relationship between materials, packing, heat, and gas flow. These were the Center's original goals.
- Progress has been made in all aspects of the project during the past year. All three storage types (compressed gas, chemical hydrogen storage, and sorbent) have been brought to a higher level of detail and performance. Unmet gravimetric and volumetric storage targets, as well as cost targets, still prevail. In truth, the spider charts reflect only incremental advances toward targets in most cases. Considering the level and quality of the experimentation and analysis going into the project as a whole, this incrementalism suggests that perhaps the project as a whole is nearing the limits of what is possible. The continued expansion/validation of analysis and modeling capability on the website is resulting in the establishment of a valuable resource to the DOE Hydrogen and Fuel Cells Program that must be maintained to accommodate future advances in the state of the art for hydrogen storage and in-vehicle fuel treatment. Performance analyses show that, at present, there exists the possibility of getting close to a vehicle with a 300-mile range with what they expect to have by the end of Phase III.
- Good progress has been made in 2012/2013, especially in two areas: (1) chemical hydrogen reactor development, reactant delivery, and BOP gas purification; and (2) media system engineering, including a down-select of workable solutions for optimized heat exchange and thermal conductivity. The technical effort obviously has been tailored to transition to Phase III implementation. The selection of MOF-5, as well as AB and alane as surrogate material systems, allowed solid progress to be made on the development of a framework for adsorbent and chemical hydrogen storage systems. However, it will be essential for the Center to take a much more critical look at the overall efficacy of AB and its derivatives in a practical vehicular storage system. The evolution of the chemical hydrogen storage AB prototype engineering system design to ever-increasing complexity is a disconcerting trend.
- The HSECoE has done a good job in moving chemical and adsorbent hydrogen storage systems forward. For the overall Center cost of approximately \$500,000/month over 5 years, the progress appears to have been somewhat slow. There are some valuable accomplishments, but it is not completely certain that all of the remaining barriers will be sufficiently addressed for the chemical or adsorbent storage approaches to be fully competitive for light-duty fuel cell electric vehicles by the end of the project. The reduction in operating pressure and the move to an aluminum Type I tank for the MOF-5 material was very helpful in reducing system cost. The addition of usable models on the website can be valuable in opening the opportunity for others to contribute to improved hydrogen storage systems. Hopefully the site will be able to be maintained following the end of the Center
- The Center has done good work in developing engineering methods of handling and dealing with AB as a hydrogen carrier. AB in BmimCl has been abandoned in favor of AB slurry using the SafeHydrogen approach of using silicon oil. The Pacific Northwest National Laboratory (PNNL) results seem to indicate that 45 wt.% AB (7 wt.% hydrogen) and spent AB slurry are stable after sonication, but the kinetics are very slow at 120°C in that more than 100 minutes that are needed to release >1.5 hydrogen equivalents. Los Alamos National Laboratory has developed an auger reactor for slurry dehydrogenation, but 280°C is needed for 100% conversion in 6.8 minutes. It is not clear if this holdup time is excessive and how it impacts start-up, shutdown, and transient response. United Technologies Research Center (UTRC) has developed a gas-liquid separator that meets the volume but not the weight target. UTRC has also

successfully tested ammonia and borazine filters. PNNL has tested a volume displacement tank for storing AB in silicon oil. All in all, good progress has been made in developing the system components. Further work is needed to increase the solid loading and improve the hydrogen purification system. The problem all along has been that the off-board efficiency of AB regeneration is unacceptably low (<30%) and the cost is prohibitively high (>\$50/kg). It is difficult to see how the AB system can pass the Phase III go/no-go decision.

- The Center has done good work in developing engineering data and components for cryogenic hydrogen storage in adsorbents. The Ford Motor Company/University of Michigan/BASF team has collected useful data on the effect of MOF-5 densification on hydrogen uptake and permeability but has not been successful in identifying a “compact” structure that meets all of the requirements. The Center has confirmed that Type IV tanks are not suitable for service below the polymer glass transition temperature. The Center has selected Type I rather than Type III tanks for cost savings and manufacturability at the expense of additional weight. The effort possibly could have been avoided if a proper literature review was made. Perhaps better planning could have also been done before embarking on the cryo burst test facility and exhausting the funds. It appears that the Jet Propulsion Laboratory effort to find alternate cryo-insulation materials has not been successful because the Center is using multilayer vacuum insulation (MLVI) with Dacron spacers. The Center continues parallel development of modular adsorption tank insert (MATI) and internal flow (HEX) options for heat exchange. In summary, the Center has done well in addressing the material behavior and component design issues and in developing models for system performance. However, the projected well-to-plant efficiency for hydrogen storage at 80 K is very low and the fuel cost will be high. It will be interesting to see how these factor into the Center’s go/no-go decision for hydrogen storage in cryo sorbents.

### Question 3: Collaboration and coordination with other institutions

This project was rated **4.0** for its collaboration and coordination.

- This is the best balanced center that the Hydrogen Storage program has had. It has the right level of collaboration from industry, academia, and laboratories. Guidance from the U.S. DRIVE Hydrogen Storage Tech Team, e.g., from Ford Motor Company on sorbents and General Motors on chemical hydrogen storage materials, has helped to provide realistic goals and targets and critical automotive feedback for the Center. The laboratories provide the capability to build, analyze, and test these systems that the original equipment manufacturers do not have resources to conduct. Materials development and characterization is being conducted by the academic partners.
- The project has a strong team of partners from national laboratories, academia, and industry. The PI appears to have done well in coordinating the contributions of the team members. There was little evidence of collaborations from people and institutions outside the team.
- It is amazing how well these different and excellent people and research groups collaborate and how well such a big project is coordinated by the PI. He succeeded to form an excellent working team of outstanding researchers doing a great job. The project is internationally well recognized and has an enormous impact both nationally and internationally. Very good job!
- This project is replete with examples of closely coordinated interfacing of partners. All of the presentations reflected an attitude that the project has been very effectively led by SRNL. The project is well directed/supervised by SRNL at a very reasonable per annum management cost (\$300,000 per year).
- This is a complex project comprising multiple technology thrusts with a large number of technical obstacles and challenges. Success depends strongly on close collaboration and careful oversight of complementary and synergistic activities. The PI and his management team have done an excellent job of coordinating the work and ensuring that the numerous cooperating partners are communicating effectively and are all contributing in a significant way to the overall effort. The robust communication channels that are operative in the Center have enhanced the synergy among partners and have created a means of effectively communicating to all collaborators the technical challenges that must be met to successfully deploy a working prototype system that meets DOE targets.
- The Center continues to coordinate all of the collaborators very well.

**Question 4: Relevance/potential impact on advancing progress toward DOE research, development, and demonstration (RD&D) goals**

This project was rated **3.7** for its relevance/potential impact.

- Hydrogen storage is the major hurdle for the implementation of a future hydrogen-based society. The relevance and potential impact of this outstanding and very well managed project for the Hydrogen and Fuel Cells Program, the United States, and the world is enormous.
- The project is addressing all of the critical aspects of the technology required to provide a fully functional hydrogen storage and in-vehicle fuel delivery system for a passenger vehicle (see slide 2 of the Anton presentation). The entire HSECoE project is really a materials-to-wheels activity that is showing steady progress toward the DOE Hydrogen and Fuel Cells Program goals and targets. All aspects of the HSECoE effort align with DOE RD&D objectives.
- The project directly supports the DOE hydrogen storage objectives, and the project team is doing a commendable job of addressing the daunting challenges to developing a practical engineering prototype that meets the DOE goals. The lack of material systems that satisfies all DOE targets is especially problematic because the project has been forced to create and implement prototype engineering solutions based on surrogate materials whose properties may or may not be representative of optimized storage media that may emerge in future work.
- It is very important for the Phase III experiments and their iterations to show whether storage materials or systems can meet the DOE storage goals. To date, the analysis and testing appear to be lagging in some areas to where the technical status of all of the project elements may not be sufficiently understood to determine the likelihood of achieving DOE goals.
- Understanding the systems implications of hydrogen storage serves a dual function: it promotes understanding of 1) what improvements are needed in the materials to allow for more efficient systems, and 2) the physical limitations of systems. This will help both materials developers and vehicle packaging experts to better understand the limits and capabilities of hydrogen storage systems.
- The objective of this project is to design innovative material-based hydrogen system architectures to meet DOE performance and cost targets. Even at the start, it was recognized that a storage system could not be engineered to overcome the limitations of the materials that are currently available. The hope is that the analysis and characterization methods and components developed in this project will be useful and relevant when new promising materials are discovered by others.

**Question 5: Proposed future work**

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

- The proposed future work is recommended and necessary, and it should be done as planned.
- This keynote presentation on the progress of the HSECoE contained a clear, concise overview of the future plans and future expectations for the Center. A no-cost extension to March 2015 is planned in order to allow completion of all essential testing. This seems reasonable and should be viewed as such by DOE's EERE.
- The Phase III plans look very aggressive, but all of the elements of the plans are important. It is difficult to see how a significant portion of the Center's plans can be accomplished by the end of the first quarter of fiscal year 2015.
- The PI presented Gantt charts and "Specific, Measureable, Attainable, Relevant, and Timely" (SMART) milestones for Phase III work. He considers the Phase III demonstration as critical to model validation. DOE and the HSECoE need to discuss whether this should be the main purpose of the final phase of this project.
- The focus on gas cleanup techniques should be deemphasized in favor of materials that do not produce side products that are this undesirable. Gas cleanup is very specific to the hydrogen storage material. Because these materials are not suitable for the ultimate goals, the PI should provide justification that future materials may have some of the same undesirable side products in order to justify further work on cleanup. Cleanup systems are difficult to tune so that they work in all automotive working conditions.

- Based on this overview presentation and the supplemental charts that were supplied, it was not completely convincing that a carefully developed plan that addresses critical technical problems has been proposed for the Phase III effort. A clear and unambiguous statement of obstacles, specific technical challenges, and risks (especially in the AB work) was not provided. It is difficult to fully discern what the project team believes are the most critical technical problems that must be addressed. At this stage of the project, a straightforward and compelling statement of the remaining problems, areas of technical risk, and mitigation strategies is needed in order to provide DOE and the reviewers with confidence that a Phase III effort will result in solid progress toward a system (or systems) that satisfies DOE goals.

#### Project strengths:

- This project has excellent management and collaborations and a well-defined approach. The Center Director should be commended for forming and managing a great team.
- This project features brilliant management and a brilliant consortium. The stronger focus on what really matters in the end—i.e., the cost—is very good.
- This project benefits greatly from a well-conceived and effectively implemented project management structure as well as the fact that it is superbly well staffed at all partnering institutions. The overview presentation covered the operational and performance aspects of the project in sufficient detail to give a clear picture of where the technology stands and what needs to be done to achieve a successful outcome.
- A highly qualified technical and management team is conducting work on this project. The team has expertise and background in all areas that impact the successful development of a practical storage system. The HSCoE has done a good job of down-selecting candidate material systems and engineering solutions that should provide a solid basis for final prototype system development.

#### Project weaknesses:

- There are no glaring weaknesses that need to be corrected. One observation is that, considering the overall budget, the HSECoE has not produced any landmark innovations. The activities are developmental rather than being research oriented. The Center builds on system concepts that existed before it was formed.
- This project grows stronger by the year. The intensity of the efforts of all participants is obvious. If in the end the final outcome is not overwhelming, it will not be for lack of dedicated/productive effort by the HSECoE participants. The principal weakness of the project from day one has been the fact that the original DOE/EERE hydrogen system storage capacity targets were never achievable in the first place. Back-of-the-envelope calculations (calculations any educated scientist could do) will show that (1) the currently chosen storage options are very near the limit of what is possible and (2) the “current” 2017 system target for capacity (gravimetric and volumetric combined) is not achievable at the presently stated values.
- Because of its exothermicity, researchers should look into measuring the spatial stability control to demonstrate the ability to confine the reaction within a specific linear region of the AB slurry reactor.
- The signature problem that may ultimately limit overall project success is that no single material that meets all of the DOE targets has been identified. Consequently, engineering systems based on sub-optimal materials are being developed. It is becoming increasingly apparent that the AB system has some severe limitations; a more concentrated effort on the alane system is needed. It is unfortunate that the presentation did not include the critical work that was most relevant to understanding the progress made on the alane system engineering development.

#### Recommendations for additions/deletions to project scope:

- This is a very successful and well run project that should not end in 2014. It should be extended because hydrogen storage will remain an important task in the future and further improvements are still required in costs, operation conditions, and density. This consortium has acquired a huge know-how in hydrogen storage technologies that is not found elsewhere. In the case of those technologies that cannot meet the gravimetric targets so far, the consortium should think about other possible applications (portable or stationary) or spin-offs of their research work. In the case of the metal hydrides, the project team should

also consider how much the costs can be reduced if, for example, used structural materials are recycled as hydrogen storage materials, because recycling is becoming a more important aspect in many industries.

- As knowledge accumulates between the interactions of the materials and system design, the HSECoE should begin to provide more sensitivity analysis to understand where improvements can be achieved and how much is required in particular metrics to achieve not just the Center's targets, but the ultimate targets; that is, how much better do heat transfer, hydrogen diffusivity, material packing, and material density need to be to reach the ultimate targets. Priorities should be assigned to which areas could be improved and which are beyond physical limits, etc.
- DOE and the Center should carefully discuss the scope of Phase III activities. Given that the system's architecture depends on the storage material and that a suitable material does not currently exist, building a complete prototype with controls may not be useful in the long run. Perhaps the resources will be better spent looking at alternate approaches.
- If the DOE Hydrogen and Fuel Cells Program (the Program) is going to keep funding research on hydrogen storage, it should consider a "reinvention" of the HSECoE into a new entity that keeps the core HSECoE capabilities intact and enables continued progress toward large-scale implementation by providing validating analyses of new developments from future hydrogen storage research. Some type of DOE-sponsored project should exist for the entire Program through Technology Readiness Level 7 on slide 45 of the SRNL presentation. A great deal of research and development continuity will be lost if DOE does not stay involved. Also, if DOE steps away from this project too soon, it probably will never get the credit it deserves for a successful commercial outcome. It would have been a bit easier to evaluate this project as a whole if the reviewers knew the outcome of the go/no-go decisions that are presently under consideration by DOE.
- A clear and detailed statement of the specific technical challenges and plans for addressing those challenges should be included in the plans for the Phase III effort. Specific attention should be paid to the evolving complexity of the AB-based system and whether those complications could be ameliorated in an alane-based hydrogen storage/delivery system.

## Project # ST-005: Systems Engineering of Chemical Hydrogen, Pressure Vessel, and Balance of Plant for Onboard Hydrogen Storage

Jamie Holladay; Pacific Northwest National Laboratory

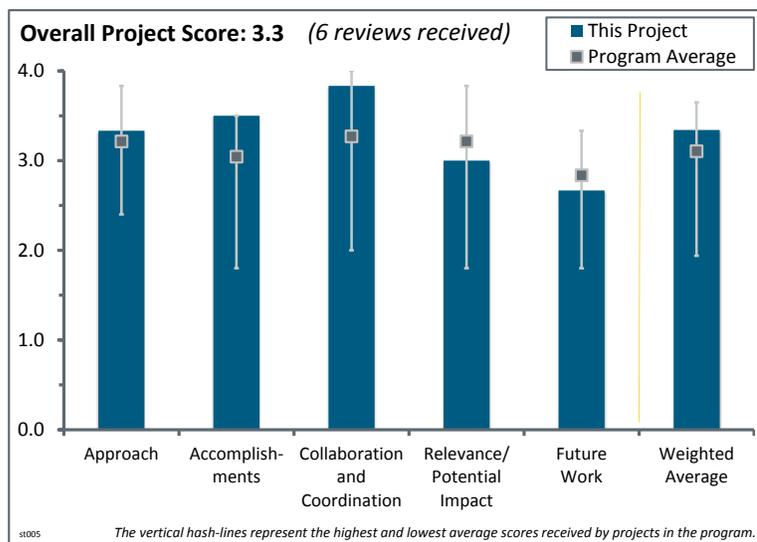
### Brief Summary of Project:

The objectives of this project are to address most of the engineering challenges for materials-based hydrogen storage for endothermic and exothermic chemical hydrogen and cryo-adsorbents and to provide feedback and recommendations on materials requirements. The project will demonstrate chemical hydrogen storage systems for light-duty vehicles and identify and develop solutions to overcome component materials deficiencies that affect performance in light-duty vehicles.

### Question 1: Approach to performing the work

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

- The work is well organized and of extremely high quality. All milestones have been met, and several non-milestone achievements have been accomplished.
- Researchers investigated alane and ammonia borane (AB) materials systems and considered Type I and Type III cryo-adsorbent tanks and the use of friction stir welding as a joining technique. Their approach also included development of system models and experimental validation of these models, as well as component validation, prototype demonstration, and cost estimations. This approach is very good!
- The approach is generally effective and contributes to overcoming some barriers. Researchers demonstrated a clear pathway for meeting gravimetric and volumetric targets, but other targets are not being addressed (such as well-to-power plant efficiency).
- The approach is good. It is focused on the challenges of slurry flow management and settling behaviors. The design of the reactor, heat exchanger, exchange tank, and pump components are critical to chemical hydrogen storage system success. The project is focused on pressure vessel design and validation for adsorbent storage.
- The team worked with known materials to design systems for solid/slurry-based storage materials. This is a very challenging medium to work with and essentially a nonstarter for automotive use. Demanding automotive conditions, such as temperature, humidity, noise, vibration, harshness, etc., make moving anything other than gas or low-viscosity liquids very challenging. The complexities of and amount of hydrogen cleanup required by these systems start to approach those of onboard reformers, which the DOE Hydrogen and Fuel Cells Program (the Program) down-selected several years ago. Future work should shift emphasis to liquid materials that both simplify material movement and post-process H<sub>2</sub> cleanup. Volume exchange tank work should consider heat transfer issues that can cause hydrogen release on the fuel side.
- Modeling of reaction rates for alane shows good results. No clear justification was given for using polymer slurries as proxies for AB. It is unclear whether particle size distributions, particle shapes, and bulk densities were equivalent. Slurries appear to require periodic agitation. This is likely a non-starter for fuel applications.



**Question 2: Accomplishments and progress toward overall project and U.S. Department of Energy (DOE) goals**

This project was rated **3.5** for its accomplishments and progress.

- The accomplishments are impressive. The range of projects and technical challenges is unusually broad, and the combination of modeling and experimental work is particularly noteworthy.
- Milestones have been met or exceeded or the potential to do so has been shown.
- The volume exchange tank work was well done. This approach is also valuable for other fuel cell systems, including small and mid-sized portable units using other chemical hydrogen storage material approaches.
- A tremendous amount of work was accomplished in pushing these systems to their maximum. Of particular note is the work on membranes, which showed impressive results in durability. The team should, however, consider heat exchange between spent/unspent fuel that could cause premature hydrogen evolution on the fuel side. Perhaps a double-walled membrane could be considered. The extra volume and weight of such a solution should be accounted for in the overall system calculations.
- Researchers have made nice progress toward meeting the objectives and overcoming one or more barriers. They demonstrated a flow reactor with AB and  $\text{AlH}_3$  at 45% loading, but higher loadings are needed if targets are to be met. The kinetics look decent for both AB and alane, but improvements are likely with other slurry media. Some important differences between  $\text{AlH}_3$  and AB were identified:  $\text{AlH}_3$  has no gas cleanup issues and flows well (hydrided and dehydrided), but it requires an extra mass of approximately 30 kg. Fully hydrogenated AB showed some issues with clogging, which should be addressed. The use of pleated membrane for a partitioned tank seems to work well, which may enable conformable tanks. The balance of plant and costing of an optimized design for the cryo-adsorbed tank look good. The team achieved costing for 135 cryo-adsorbed tank configurations. Most milestones were met or exceeded.
- Publication of a “tankinator” model for tank modeling allows for design optimization without extensive trial-and-error experimentation. Waterfall charts showing system improvements should be accompanied by credible strategies for achieving targeted improvements or some idea of how likely improvements are. The basis for the improvements should be explained and justified by preliminary experimental accomplishments.

**Question 3: Collaboration and coordination with other institutions**

This project was rated **3.8** for its collaboration and coordination.

- The Hydrogen Storage Engineering Center of Excellence (HSECoE, the Center) is an excellent collaboration of industry, academia, laboratories, etc. This model should be emulated by other technical teams.
- This project features close, appropriate collaboration with other institutions within the Center; partners are full participants and are well coordinated.
- The breadth and diversity of this project demand close coordination with other institutions and partners. Management of these interactions and relationships is effective and results in the whole operation being significantly more than the sum of its constituent parts.
- There is good collaboration within the Center but limited work with outside investigators.

**Question 4: Relevance/potential impact on advancing progress toward DOE research, development, and demonstration (RD&D) goals**

This project was rated **3.0** for its relevance/potential impact.

- This is a key project that underpins the central activities of the HSECoE, and it is of general value to the wider hydrogen storage community.
- This project’s relevance is limited because a significant part of the work is being carried out on materials that are not viable.
- The project partially supports the Program and DOE RD&D objectives. The impact of the cryo-adsorbed tank could be high. However, engineering efforts on the chemical hydrogen storage systems seem

premature. This project has revealed some interesting new issues (such as clogging with AB and the need for gas cleanup), but many of these issues could have been anticipated from materials studies. The real issues with chemical hydrogen storage materials remain with the regeneration efficiency, and it is unclear how much value further engineering studies can provide until this key issue is addressed.

- The bill of materials and cost estimation portions are relevant. Future work should shift emphasis on liquid materials that both simplify material movement and post-process H<sub>2</sub> cleanup. The volume exchange tank work should consider heat transfer issues that can cause hydrogen release on the fuel side. It is unlikely original equipment manufacturers will use complicated chemical hydrogen storage systems unless the systems can be dramatically simplified and the recycling energy issues of the materials can be resolved.
- Meeting the next DOE performance goals will be difficult for both chemical hydrogen storage materials and adsorption approaches.

### Question 5: Proposed future work

This project was rated **2.7** for its proposed future work.

- Future plans are sensible and build on progress made to date. Comments from last year's DOE Hydrogen and Fuel Cells Program Annual Merit Review have been carefully considered and addressed.
- Proposed future work includes cost and experimental validation of pressure vessel cooling and heat loss with tank design.
- It would be nice to see an increased focus on the sorbent tanks and cryo vessels—these have a larger chance of success for vehicular use. Understanding heat exchange issues for sorbent-based materials is key to designing high-capacity systems and the knowledge is mostly transferrable to new sorbent materials as they become available.
- Plans may lead to improvements, but they should be more focused on overcoming all barriers. Plans to design sub-scale prototypes for AB and alane are unlikely to make significant progress in overcoming barriers. Plans for a cryo-adsorbed prototype seem worthwhile and, although unlikely to meet all targets, the system design/engineering will be a valuable contribution. This type of tank may be an appropriate near-term solution over compressed gas.
- Given the recent work on well-to-wheels efficiency of chemical hydrogen storage materials, the Program should consider stopping work on these systems until a more efficient material is found. The Center should consider combining the cost model with other models developed in the Program.

### Project strengths:

- This project's strengths include providing a system bill of materials, bladder concepts, and cryo-sorbent tanks.
- The work on the cryo-adsorbed tank is progressing nicely. This may prove to be a useful alternative to 700 bar compressed gas.
- This project features excellent organization and coordination, partnerships with strong groups and companies, and an interactive consortium.
- The approach of making engineering and design information available to the portable and stationary applications can be very valuable. The volume exchange tank and general slurry behavior are examples.

### Project weaknesses:

- The project team did a good job, but perhaps they are going down a rabbit hole on slurry pumping for AB- and alane-type materials.
- The fact that the Center is working on proxy materials limits the usefulness of these results.
- The project objective is to demonstrate a hydrogen storage system that meets DOE 2017 targets for light-duty vehicles using chemical hydrogen storage, but efficiency remains a key barrier and is not being addressed.
- A lot relies on the need to have a well-behaved slurry that is higher than 50% wt.% AB, as well as a reliable and stable exothermic auger reactor. It is unclear whether the failure modes (or full failure mode and effects analysis) have been studied for the auger reactor and the ability to control the reaction region

location and length. Perhaps an intrinsic stability design can be included for the exothermic reaction scheme.

- There are no weaknesses evident from the material presented.

### **Recommendations for additions/deletions to project scope:**

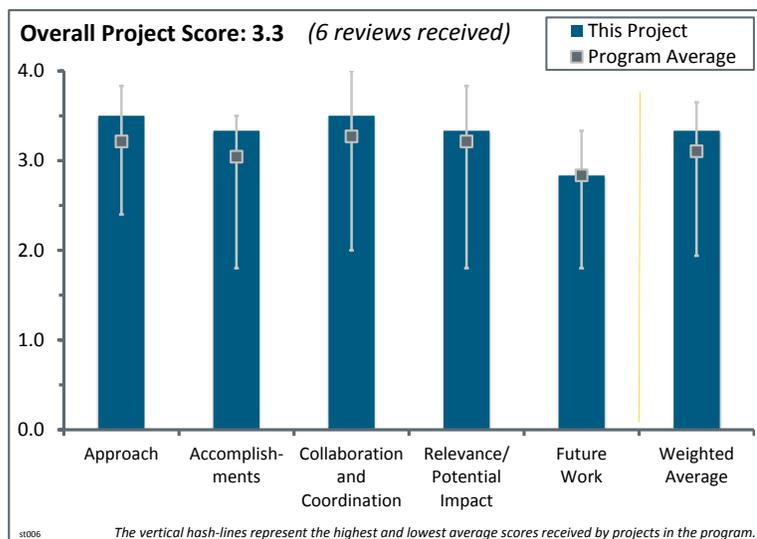
- The project team should reduce its work on slurries and increase its work on sorbent and cryo tanks.

## Project # ST-006: Advancement of Systems Designs and Key Engineering Technologies for Materials Based Hydrogen Storage

Bart van Hassel; United Technologies Research Center

### Brief Summary of Project:

The objective of this project is to design materials-based vehicular hydrogen storage systems that will allow for a driving range of greater than 300 miles. The project leverages in-house expertise in various engineering disciplines and prior experience with metal hydride system prototyping to advance materials-based hydrogen storage for automotive applications. The project has focused efforts over the past year on gas/liquid separation of liquid chemical hydrogen storage materials, hydrogen quality, integrated power plant storage system modeling, and risk assessment.



### Question 1: Approach to performing the work

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

- The approach is well planned and executed. Coordination with partners is effective and productive.
- This project is part of the Hydrogen Storage Engineering Center of Excellence (HSECoE, the Center) and has been involved in a number of different critical tasks. The researchers' focus on identifying and sizing end-of-the-line purification systems is a good illustration of the positive attributes to which they contribute. United Technologies Research Center (UTRC) provides sound and solid work.
- UTRC's effort within the HSECoE embraces many barriers, but with particular emphasis on system weight and volume, durability/operability, and thermal energy management. The UTRC work is sharply focused on lingering system performance issues that must be addressed and mitigated, including gas-liquid separation, hydrogen purification (e.g., ammonia [NH<sub>3</sub>] removal), particulate removal, risk abatement, and other issues.
- This is a well-formulated approach that addresses several important problems inherent in the successful implementation of a hydrogen storage/delivery system based on chemical hydrogen storage materials. The development of an efficient gas-liquid separator (GLS) for separating hydrogen gas from the spent liquid chemical hydrogen storage material and the development of an NH<sub>3</sub>/particulate filter for purifying the hydrogen gas stream are especially critical to the ultimate deployment of a fully operational prototype system based on ammonia borane (AB). The design concepts and engineering implementation have been developed in a sensible and straightforward way.
- The approach is well formulated in that it is designed to develop and refine solutions for mitigating impurities (NH<sub>3</sub>, borazine, and particulates), as well as understand the relative upstream flammability risk in using an AB slurry.
- No clear justification was given for using polymer slurries as proxies for AB. It is unclear if particle size distributions, particle shapes, and bulk densities were equivalent. Demisting is a common unit operation. It is not clear that a computational fluid dynamics model needed to be developed to accomplish effective gas liquid separation. Safety assessments need to include thermal runaway experiments. These are standard tests using methods, such as accelerating rate calorimetry, that are available at contract laboratories. These tests are generally mandatory for work with solids capable of exothermic reactions.

**Question 2: Accomplishments and progress toward overall project and U.S. Department of Energy (DOE) goals**

This project was rated **3.3** for its accomplishments and progress.

- The project achieved several targets.
- UTRC appears to have made excellent progress on every system performance issue it addressed in the past year. Results in the area of gas-liquid separation and NH<sub>3</sub> scrubbing are impressive and are essential to the success of the project as a whole. It appears that some impressive publications emanated from work done to date (as indicated in the extra slides).
- The filter developed here is a very valuable accomplishment. NH<sub>3</sub> filtering is valuable to AB systems and can also be valuable to other portable and small stationary fuel cell systems using other chemical hydrogen storage materials. The GLS design and model were well done, but it may be better to consider a cyclone separator. On the particulates slide (slide 19), the particle sizer looks like it had an upper measuring limit of 0.5 μ, which is 1/20th the <10 μ SAE International specification. If so, measurement ability should be extended up to 10 μ.
- Most milestones have been achieved. The carryover issue in the GLS remains to be solved. The NH<sub>3</sub> filtration work is impressive.
- Solid progress has been made on the development of a GLS test facility and GLS model development. In particular, careful attention was paid to characterizing the effects of a distribution in droplet sizes at the outlet of the GLS and to developing plans for integrating the GLS with the chemical hydrogen storage material thermolysis reactor. The onboard NH<sub>3</sub> sorbent filter simulation and experimental validation data are encouraging. However, removal of borazine contamination in the gas stream still remains an outstanding issue. Risk assessment comparisons on the flammability of solid AB versus liquid AB are providing useful information that will undoubtedly impact the ultimate selection of the most appropriate storage medium. Overall, the technical accomplishments in 2012–2013 are impressive in all areas of the project and should facilitate a smooth transition to successful development of a working subsystem in the Phase III effort.
- The researchers provided the NH<sub>3</sub> filter to Los Alamos National Laboratory for some testing with NH<sub>3</sub>/borazine mixtures. It is unclear whether borazine decreases the efficiency of the NH<sub>3</sub> filter. One could imagine the borazine forming a weak complex with the MnCl<sub>2</sub> if NH<sub>3</sub> forms a strong complex. For the liquid separator, it seems like the vapor pressure of the carrier fluid is the key property defining the size of the GLS. If the Center were to use a liquid carrier with half the vapor pressure, it would be nice to know whether the size of the separator decreases by half. An analysis of liquid separator versus vapor pressure of a carrier solvent could be useful to target liquids with the appropriate viscosity and vapor pressure. There are questions about (1) whether there is any physical insight into how borazine might partition in the gas and the liquid droplets formed from the carrier fluid; (2) if borazine could form droplets on its own at a given temperature, e.g., below the boiling point of 55°C, and whether the droplets can be separated from the gas; (3) whether borazine could be preferentially soluble in the liquid droplets and thus be removed from the hydrogen gas; and (4) whether one could measure the enthalpy of dissolving borazine in different carrier fluids to see if this is a favorable physical reaction. If borazine is trapped in the liquid separator, it could be added to the spent fuel for regeneration. It is unclear what fluid is used for the alane carrier and what its vapor pressure and reactor size are.
- It will be interesting to learn how well the beta testing on the beta version of the graphical user interface model turns out. It will be a challenge but a critical output of the HSECoE to provide models that can be used by other researchers to help them test new ideas.

**Question 3: Collaboration and coordination with other institutions**

This project was rated **3.5** for its collaboration and coordination.

- This project's collaboration and coordination are very strong.
- The collaboration is well organized and effectively managed.

- The specifics of the UTRC collaborations within the HSECoE are clearly specified throughout the presentation slides. Coordinated efforts with Oak Ridge National Laboratory, Sandia National Laboratories, and BASF/Ford are highlighted.
- Collaborations with multiple HSECoE partners are listed for all of the tasks on the project. However, with a few exceptions, the specific contributions of the HSECoE partners are not specifically noted or acknowledged. Consequently, it is difficult to discern what contributions (if any) were made by the collaborating organizations.
- It was unclear from the presentation who did what. Nevertheless, the results from this project are critical to chemical hydrogen storage materials. The overall project looks like it was well coordinated and that all sub-elements received the right attention and effort.
- There was no mention of collaboration in the presentation.

#### Question 4: Relevance/potential impact on advancing progress toward DOE research, development, and demonstration (RD&D) goals

This project was rated **3.3** for its relevance/potential impact.

- UTRC appears to do what is asked of it to help the HSECoE, and does it very well.
- At the present stage of the HSECoE project, everything UTRC is engaged in is pivotal to a successful outcome during Phase III. The project's relevancy is very high.
- The project provides important engineering support to several key areas of HSECoE activity.
- The GLS and NH<sub>3</sub> filter are critical elements of slurry AB hydrogen storage systems. (The GLS is also critical to AlH<sub>3</sub> slurry systems.)
- This project is an integral component of the overall HSECoE effort. In addition to supporting storage system modeling and integration activities in the Center, UTRC is developing important balance-of-plant technologies, including a gas-liquid separator for liquid chemical hydrogen media and sorbent filters for removing NH<sub>3</sub> and particulates from hydrogen gas liberated by thermolysis of AB. These activities directly support the HSECoE goals for storage system prototype development and are closely aligned with DOE's RD&D objectives.
- The relevance is limited because a significant part of the work is being carried out on materials that are not viable.

#### Question 5: Proposed future work

This project was rated **2.8** for its proposed future work.

- Plans are aligned with long-term project objectives and with other HSECoE partners.
- A well-thought-out plan with associated workflow and schedule information is provided. However, it would have been helpful if specific, technical obstacles and plans for overcoming those obstacles had been included in the proposed future work plan.
- The plan forward considers all of the necessary elements, but it does not plan for the likely contingency for iteration on the Phase III components, system, model, or controls.
- Technologies developed for model materials may not be applicable to commercially viable materials.
- The UTRC future plans were covered on slide 20 of the presentation in a very general way. Much is left to surmise about the details of what will be done in the coming year. Even though it is obvious that UTRC is on an appropriate and effective path in its work, it would be reassuring to see a list of the specifics and an explicit statement of the expected outcomes.
- It would be useful for UTRC to provide some feedback to the HSECoE on an optimum vapor pressure for a carrier fluid. It is unclear how small the researchers could make the separator if the vapor pressure was reduced by 50%, or even 90%. There must be a size that is as small as it can get. Also, it is unclear if borazine can form droplets that can be trapped in a liquid separator. Besides vapor pressure and temperature, it is unclear what leads to droplet formation. Maybe UTRC could help reduce borazine with the liquid separator. The vapor pressure of borazine versus temperature has been published.

### Project strengths:

- The research and development, planning and execution, close coordination with other HSECoE projects, and project leadership at UTRC are excellent. These factors greatly strengthen the project in terms of achieving objectives and mitigating barriers. The presentation was very well delivered—clear, crisp, and concise. The additional slides for reviewers were appreciated. It shows that UTRC is taking the reviewers' comments seriously.
- This project addresses several important technical problems that impact the successful development of an AB-based hydrogen storage/delivery system. The project team is well qualified, with expertise and background in all aspects of modeling/simulation and the system engineering needed to achieve the goals of the project. This work is an important component of the overall HSECoE effort.

### Project weaknesses:

- It is unlikely that AB will meet the overall DOE hydrogen storage targets. Consequently, it is not entirely clear whether the work that has been conducted in this project will translate effectively to a system based on an alternate chemical hydrogen storage medium having improved material properties.
- The need for auxiliary equipment (demister, NH<sub>3</sub> adsorber, etc.) makes a marginal chemical hydrogen storage system even less desirable.
- It is not obvious that the project made extensive inquiries with manufacturers of gas-liquid separations equipment.
- The UTRC project shows no discernible weaknesses in approach/relevance, collaboration, or productivity.

### Recommendations for additions/deletions to project scope:

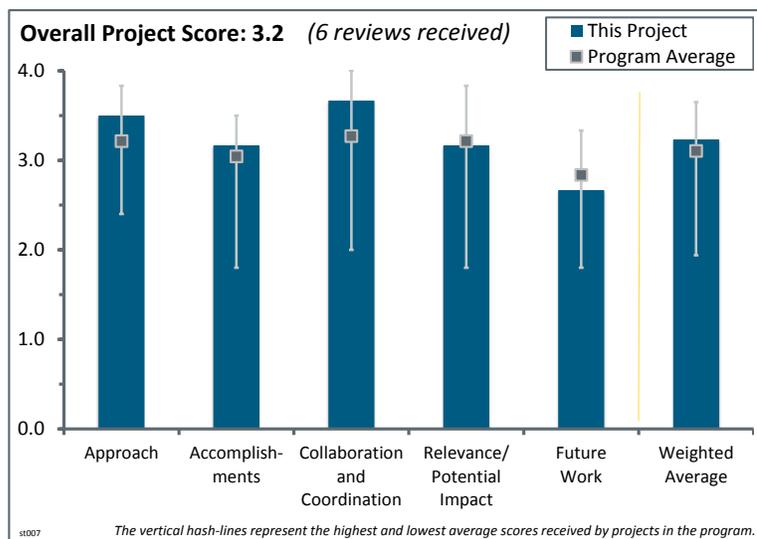
- More detail on future plans would be a helpful addition for reviewers.
- Insofar as AB is unlikely to be the storage medium that will be used in a practical storage/delivery system, the principal investigator and his team should consider how this work can be extended to address a storage system employing a different material (e.g., alane) with potentially superior storage/delivery properties.
- For the GLS, the project team should look into a miniature cyclone separator with tangential flow input. The axial flow GLS with swirl vanes is not a very efficient use of volume, and it is heavy. There should be cyclone versions available in the configuration and size needed, and if not, it is relatively simple to design, build, test, and iterate upon. It should significantly reduce volume and weight. The presence of swirl vanes in the axial flow GLS reagglomerates the input droplets on the blade surfaces then redistributes them downstream in a new droplet size distribution. The Weber and Reynolds numbers strongly affect this, and the shedding velocity profile and length scale in the vaned environment is difficult to model. In addition, using nitrogen to model hydrogen may strongly change the density-ratio-driven droplet breakup. The flow in a cyclone separator is much more controllable, predictable, and able to be modeled. For an absorbed system (MOF-5 assumed), there does not seem to be a plan to improve on the particle size diagnostic.

## Project # ST-007: Chemical Hydrogen Rate Modeling, Validation, and System Demonstration

Troy Semelsberger; Los Alamos National Laboratory

### Brief Summary of Project:

The objectives of this project are to: (1) provide a validated modeling framework; (2) provide an internally consistent operating envelope for materials comparison with regard to mass, volume, cost, and performance; (3) provide component scaling as a function of chemical hydrogen storage media and application; (4) provide the materials operating envelope required to meet the U.S. Department of Energy (DOE) 2017 targets; (5) identify and advance engineering solutions to address material-based non-idealities; and (6) identify, advance, and validate primary system-level components.



### Question 1: Approach to performing the work

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

- The reactor designs and expanded scope of materials studies provide an excellent approach to the evaluation of the practical performance of this class of hydrogen storage materials.
- The project is charged with providing a modeling framework and systems validation for several key activities relating to chemical hydrogen storage material technology within the Hydrogen Storage Engineering Center of Excellence (HSECoE). This requires close control and integration of a broad and diverse set of subtasks and milestones. These are managed efficiently and effectively, creating an impressive operation for which the whole significantly exceeds the sum of the individual parts.
- The Los Alamos National Laboratory (LANL) approach embraces a well-conceived blend of technical tasks that address pivotal aspects of the hydrogen storage system, including component design/development/testing, system integration, performance modeling, and comprehensive system validation. The output of the LANL project factors into much of what goes on throughout the HSECoE as a whole. The LANL effort is properly focused and well directed; it addresses all of the critical barrier issues head on and it is difficult to identify any substantive ways to improve the overall approach.
- The general approach seems effective and there is a clear path to overcoming some barriers. It is nice to see alane slurry is being considered along with ammonia borane (AB). The project team may also want to consider  $\text{LiAlH}_4$  because the regeneration is simpler. There is no clear path to improving well-to-power plant efficiency.
- The team is doing a reasonable job of addressing onboard issues, but optimization of an onboard system without considering the implications for the forecourt will likely lead to suboptimal solutions.
- The approach is adequate but it leaves room for improvement. The 50% alane slurry would never meet expectations. It is not clear why it was investigated.

**Question 2: Accomplishments and progress toward overall project and U.S. Department of Energy (DOE) goals**

This project was rated **3.2** for its accomplishments and progress.

- The reactor designs and expanded scope of materials studies provide an excellent approach to the evaluation of the practical performance of this class of hydrogen storage materials.
- The number of accomplishments laid out in the LANL presentation is close to overwhelming. Progress has been made on many fronts; gaps in performance versus targets have been reduced in several key areas; and the prospects for demonstration of a functional hydrogen storage system by the end of Phase III have been substantially improved. The accomplishments summarized on slide 31 of the LANL presentation for alane and AB represent important advances toward storage capacity targets. Especially impressive are the advances in reactor performance for both types of chemical hydrogen storage material.
- Accomplishments have been good, with evidence of significant progress toward the stated objectives. Particularly important outcomes include the optimization of chemical hydrogen storage material reactor conditions, the quantification of all gaseous products from AB fluid fuels, and the development of a regenerable borazine scrubber.
- The team has made significant progress toward the objectives and overcoming one or more barriers. It has made nice progress with demonstrating flow reactors for AB, alane, and methoxypropyl amine borane (MPAB), as well as characterizing reaction rates and impurity gases. These results are a nice confirmation of the viability of these flow systems. Identification of CAN-210-15 as a high-borazine absorber is an important step forward for the viability of any boron-based hydrogen storage system. MPAB (3.9%) results show promise because it remains a liquid after desorption—no slugging or fouling and only minor trace impurities. Slurry alane and AB results with an auger reactor also look promising, but higher loadings are needed to truly test slugging/fouling.
- The team achieved good results on system modeling. At the same time, the 50% alane slurry would never meet expectations and the materials with the higher alane content are hard to handle. It is unclear why alane was even evaluated.
- Although borazine and ammonia can be successfully scrubbed, logistics associated with their collection, recovery, and regeneration will make recovery difficult and expensive. It is hard to imagine going to higher (70%) loading slurries from 20%, where settling can be a problem already.

**Question 3: Collaboration and coordination with other institutions**

This project was rated **3.7** for its collaboration and coordination.

- There is clear collaboration with other institutions within the HSECoE; the partners are full participants and are well coordinated.
- It is clear that the LANL team is well connected with and integrated into the aggregate HSECoE. Interactions with DOE management and with other organizations that serve or assist the DOE Hydrogen Storage program were also highlighted. Much of what LANL does drives the research and modeling efforts in other parts of the HSECoE project.
- This project demands close collaboration and interaction with several other institutions, including the United Technologies Research Center, Pacific Northwest National Laboratory, and the National Renewable Energy Laboratory. The interactions are close and mutually supportive.
- This project features good team work; the team could benefit from participation of some additional chemistry partners, especially those manufacturing AB and related materials.
- There is excellent collaboration and coordination among team members and with the HSECoE, but there is no wider range collaboration.
- The project team needs to include fuel providers and well-to-wheels (WTW) modelers to look into forecourt implications.

#### Question 4: Relevance/potential impact on advancing progress toward DOE research, development, and demonstration (RD&D) goals

This project was rated **3.2** for its relevance/potential impact.

- The project is very relevant to the Hydrogen and Fuel Cells Program (Program) goals and objectives.
- This is a central, multidisciplinary project of high importance to the HSECoE's overall objectives.
- The LANL work scope contributes in a major way to the definition and refinement of the storage system operating envelope. This work includes identification and testing of engineering solutions to system component deficiencies, together with component function modeling and validation. As presented, the LANL effort is critical to the Phase III objectives and goals of the HSECoE. The tasks involving reactor functionality, fuel purification, and overall system optimization are producing pivotal results on the path to a target-meeting system. In short, the relevancy of the LANL project is at a very high level.
- The project partially supports the Program and DOE RD&D objectives. This project supports and advances progress toward meeting the Program's goals, but further optimization and new engineering concepts are not going to result in a system that meets all of the targets. The spider charts clearly indicate that the key challenge with AB and alane is well-to-power plant efficiency. The impact of this project is likely to remain low until new regeneration routes can be identified with improved efficiencies.
- This project addresses problems associated with the development of viable hydrogen storage systems based on chemical hydrogen storage materials. During the past year, the scope of the project has been greatly expanded to cover a much wider variety of chemical hydrogen storage materials, and thus it is now of much greater overall relevance to DOE objectives. However, like many of the chemical hydrogen storage material projects in the Hydrogen Storage program, its relevance is limited because the key problem of re-hydrogenation is largely ignored.
- Because these materials do not meet goals associated with fuel cost and WTW energy efficiency, specific work on hydrogen generation may or may not have relevance. Slurry pumping is likely a nonstarter for forecourt operations.

#### Question 5: Proposed future work

This project was rated **2.7** for its proposed future work.

- The proposed future work builds on the achievements presented and is logical and sensible in terms of scope and objectives.
- Plans build on past progress and generally address overcoming barriers. The future work plan seems reasonable. Clearly higher loadings are needed for AB and alane. It may be worth considering other slurry media, such as those that undergo reversible (de)hydrogenation reactions. This will likely complicate the regeneration efforts, but it would be worth demonstrating.
- Future work is just a continuation of the current effort. Given that 2014 is the planned completion date, this section could have been more extensive.
- Continued work on marginal materials is of questionable value.
- This project is in its last year. Rather than gather further information on AB slurries that will not meet DOE targets, future plans should focus on obtaining at least some preliminary results on the liquid material.
- The proposed future work was presented in a somewhat sketchy manner. It appears to go forward in a logical way from the progress to date to the final stages of system testing (i.e., refinement of reactor experiments together with further research and development to mitigate the remaining barriers to a proof-of-concept demonstration). Like most of the other HSECoE presentations, the LANL presentation focused more on the accomplishments (of which there were many). The future plans for the remainder of the project deserved more emphasis and a bit more detailing.

#### Project strengths:

- This project features solid modeling work, good collaborations, and interesting results to date.
- This project is well coordinated with HSECoE. It has made steady progress with slurries and borazine scrubbers.

- The project team consists of an outstanding group of experts that has consistently obtained high-quality, well-analyzed results.
- This project clearly benefits from strong, intuitive leadership at LANL; excellent research planning and execution by people who are now at the cutting edge of hydrogen storage science and technology; and close coordination/collaboration within the HSECoE as a whole.
- Strengths of this project include dynamic interactions between capable partners, a good overview of strategic objectives, and objective down-selection and refocusing of resources.

### **Project weaknesses:**

- The project remains too focused on AB.
- The choice of materials is an area of weakness. The collaborations still have room for improvement.
- The project is unlikely to make much of an impact on the well-to-power plant efficiency target, which is the key outstanding issue.
- More direct chemical input would be helpful (e.g., in choice of appropriate ionic liquids).
- This project has no weaknesses, but all should keep in mind that the projected Phase III spider charts are a picture of what might be if everything goes as well as is credibly possible. The researchers are hoping for an outcome that is still far from guaranteed.

### **Recommendations for additions/deletions to project scope:**

- The project is functioning just fine as is. The project team should keep up the great work.
- It is worth trying MPAB or other liquid hydrogen carriers as a slurry agent for alane or AB. Other slurry media should be considered for alane. Silicon oil is a reasonable first choice, but other liquids show much better kinetics. It may be worth investigating  $\text{LiAlH}_4$  slurries because  $\text{LiAlH}_4$  is much simpler to regenerate.
- The work on AB should be curtailed and the more generally relevant work on the representative liquid material should be expanded.
- Given the recent energy efficiency results and all of the difficulties associated with contaminants, flow assurance, etc., the Program should consider dropping the chemical hydrogen storage material work until more promising materials can be found.

## Project # ST-008: System Design, Analysis, Modeling, and Media Engineering Properties for Hydrogen Energy Storage

Matthew Thornton; National Renewable Energy Laboratory

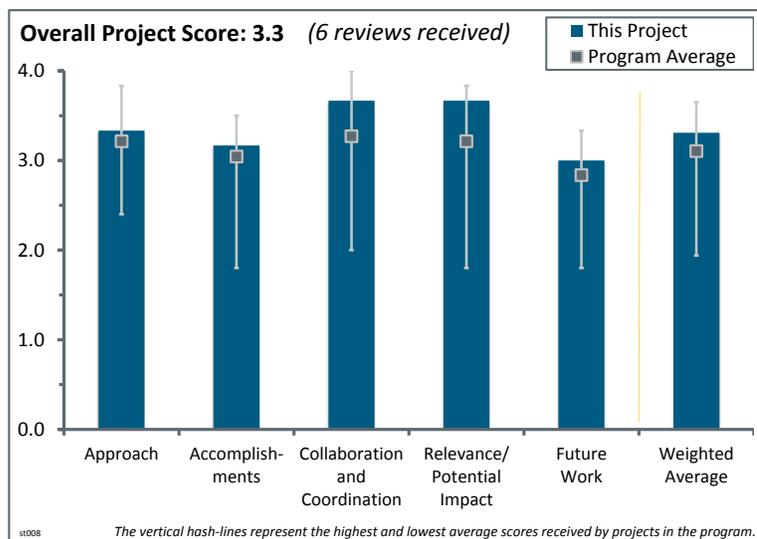
### Brief Summary of Project:

The objectives of this project are to: (1) develop and apply a model for evaluating hydrogen storage requirements, performance, and cost trade-offs at the vehicle system level; (2) provide high-level evaluation of the performance of materials-based systems; and (3) perform hydrogen storage system energy analysis to evaluate well-to-power-plant efficiency, energy requirements, hydrogen cost, and greenhouse gas emissions.

### Question 1: Approach to performing the work

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

- This project features a good approach to addressing vehicle performance and energy analysis.
- The analysis approach is sound—using different drive cycles to run vehicle simulations provides a realistic assessment of fuel economy, range, onboard efficiency, and vehicle performance.
- As part of the Hydrogen Storage Engineering Center of Excellence (HSECoE, the Center), this project has a focus on developing cost/operating models for high-priority systems under consideration by the HSECoE. The National Renewable Energy Laboratory (NREL) led the Adsorption Center of Excellence (CoE) and is a logical location to provide the data needed to model a metal-organic-framework-5 (MOF-5)-based adsorption system. Because NREL has led the effort to validate the experimental techniques in other laboratories, data on MOF-5 should be reliable.
- The NREL effort is focused on seven technical barriers, all of which are pivotal to the success of the overall HSECoE project. The vehicle model is comprehensive and well validated. It is widely used within the HSECoE to evaluate candidate storage system designs on a common vehicle platform with consistent assumptions. In the presentation, NREL did a thorough job of documenting its approach—this was arguably the best “approach” documentation presented among the HSECoE projects reviewed at the Hydrogen and Fuel Cells Annual Merit Review and is a model others should follow in the future.
- The project is structured with two fairly separate approaches: modeling and simulation of hydrogen storage systems and an experimental component to determine materials properties for MOF-5-based adsorbents. The vehicle simulation work provides a common framework to evaluate various hydrogen storage technology options in a self-consistent manner. Some of the well-to-wheels (WTW) analysis appears to be a bit far afield for the work of the HSECoE because the Center does not consider off-board requirements.
- Having valid vehicle systems models is critical to designing appropriate storage models. The system selected is for a mild hybrid fuel cell vehicle. This is likely the appropriate powertrain configuration to select if limited to one choice. It would be nice to have at least a sensitivity analysis completed with a powertrain on the other end of the spectrum (e.g., range extender) to see what storage systems could be relaxed/modified, etc. Such a study would help original equipment manufacturers (OEMs) determine the best powertrain configurations for these storage systems.



**Question 2: Accomplishments and progress toward overall project and U.S. Department of Energy (DOE) goals**

This project was rated **3.2** for its accomplishments and progress.

- Based on the WTW analysis, these chemical storage systems have the highest costs and lowest efficiency numbers compared to compressed and cryo-compressed hydrogen storage systems. These are very important pieces of information and should have an impact on other projects that are dealing with chemical storage systems. The off-board regeneration should have a higher priority compared to work on chemical systems itself.
- Reasonable progress has been made since last year. Simulated vehicle performance results for AB slurry, alane slurry, and MOF-5 sorbent systems support the HSECoE's down-selection process for Phase III storage system designs and refinements. The project is developing a technique that removes helium calibration for standard isotherm measurements with a cryostat.
- Slides 13 and 14 of the NREL presentation tell most of the story. The results are very credible and very believable. No one should be surprised that compressed gas comes out on top. The increase in "system mass" from Phase I to Phase II may be a sign of the trend to expect by the end of Phase III. As the storage concepts are refined, the number, size, weight, and cost all tend to go up. The results leave the impression that progress toward goals from the end of Phase I to the end of Phase II has been incremental at best. Some breakthroughs are needed across the HSECoE in Phase III.
- The model does a good job of providing guidance to the system developers; however, it seems that the majority of the work was gathered from other contributors—the Greenhouse Gases, Regulated Emissions, and Energy Use in Transportation (GREET) model; Autonomie; OEMs; etc. It seems like most of the work was coordinating with existing models. This is not a criticism—the principal investigator (PI) leveraged existing models and eliminated redundancies. It is just hard to give the project a 4 for work that was not necessarily all original.
- The modeling and simulation results are good, but the material property input to the Center appears to be lagging—it is unclear how much more materials information is needed, but the experimental apparatus gives unreliable results at temperatures below about 40 K. The vehicle simulation results show that there is not a large difference in the gravimetric and volumetric densities or fuel economy for all 13 system variations that were analyzed. None met the DOE targets based on the current technology embodied in the HSECoE system designs. Breakthroughs in materials properties or some innovative systems concepts appear to be needed to enable the DOE targets to be achieved. The project team should also provide a better description of the materials properties work and how the information can be used by the Center.
- In these multilayered "analysis projects," it is difficult to tell who is doing what analysis, but it is obvious that they are all working together, which may be more important than assigning specific credit. It is beneficial to see that the modeling work shows that the fuel cell vehicle drive performance with the various storage systems appears to satisfy the various drive cycle demands. One part of the HSECoE analysis that really stuck out was the system volumetric size in liters required to carry 5.6 kg of usable hydrogen. It was not directly listed but one could derive the system volume, in liters, for the various storage systems under investigation on slide 14 from the gravimetric density (grams H<sub>2</sub>/kg system) and volumetric density (g H<sub>2</sub>/liter system). For example, the system volume of 700 bar compressed gas can be derived from the volumetric density, which is 25 g H<sub>2</sub>/liter of system at 700 bar. For a 5.6 kg system, the system volume is about [5,600 g H<sub>2</sub>]/[25 g H<sub>2</sub>/liter], which results in a 224 liter system. For the HexCell at 17.5 g H<sub>2</sub>/liter and the modular adsorption tank insert (MATI) at 20.7 g H<sub>2</sub>/liter, this comes to 320 and 270 liters, respectively. From a volumetric standard, this seems to be an eye opener. It would be fair to point this out and then focus on the positives of the sorbents, such as, perhaps, greater safety and lower pressure. (It is unclear what the operating temperature and pressure are for the sorbents.) The PI suggested that "they were close" on the volumetric targets. It seems the sorbents are not so close to the 40 g H<sub>2</sub>/liter DOE target for 2017. It is unclear if a 300-liter system would fit into a "mid-size class family sedan." If the above approach to estimating the system volume is incorrect, then it would be valuable to include the system volume in the table of results to prevent others from making the same mistakes. It was a little difficult to follow the materials testing results because they were specifically used to validate the models. It was unclear if it was gravimetric density at sub-liquid nitrogen temperatures. The researchers are trying to do some tricky measurements at temperatures below 77 K. It is interesting that this has not been done previously

elsewhere, and if not, the researchers should take more credit for pioneering work. It is unclear what the target storage temperatures are for the MATI and HexCell sorbents, whether the model suggests going to temperatures below 77 K will improve capacity that is worth the extra cost, and if there is an added cost to systems operating at temperatures below liquid nitrogen temperatures. This could be made more clear in future presentations. In the comments to the reviewers' slides, the PI suggests that materials development will be further reduced to provide more resources to modeling. It is unclear if the researchers got close enough to solving the problems with the sub-liquid nitrogen temperature measurements to bring the effort to completion, for example, regarding the unknown pressure dependence and how/why it is affecting the measurements.

### Question 3: Collaboration and coordination with other institutions

This project was rated **3.7** for its collaboration and coordination.

- The collaboration and coordination are very strong.
- It seems that all relevant partners are involved.
- NREL has strong collaboration with other HSECoE partners. Such collaboration helps this project to produce results seamlessly and cost effectively.
- The collaboration is good across the HSECoE as well as with other teams involved with production and delivery of hydrogen by various pathways.
- The NREL project is clearly tightly coordinated with the other partners in the HSECoE. To be as effective as it is, the collaborative relationships must be very well established. This seems to be the case across the entire HSECoE.
- The collaboration is excellent because of the HSECoE. This is a model that all should follow. The project team demonstrated good coordination to leverage work from other teams such as the GREET model, H2A model, etc. The coordination with OEMs is critical for this type of task—the PI is working well with Ford Motor Company in particular to develop models.

### Question 4: Relevance/potential impact on advancing progress toward DOE research, development, and demonstration (RD&D) goals

This project was rated **3.7** for its relevance/potential impact.

- Vehicle performance predictions and WTW studies are very important for future economic decisions.
- These models are critical to providing boundary conditions for good storage system designs—they provide insight into the operating conditions required for automotive applications.
- The modeling effort gives a side-by-side comparison of the systems under investigation. It points to specific strengths and weaknesses of the different systems and confirms that nothing is perfect.
- NREL focuses on the impact of storage system design on vehicle performance. These analyses allow the Center to assess the performance of various designs for the hydrogen storage system to guide the engineering effort in the most beneficial directions.
- This project applies the vehicle performance model Hydrogen Storage Simulator to evaluate the key performance metrics for various hydrogen storage options in support of the HSECoE's design selections. The second (and smaller) part of this project focuses on measuring MOF-5 isotherms at <75 K.
- NREL's contribution to the HSECoE in the modeling/system analysis area in a sense drives everything that goes on in the rest of the project because it provides a snapshot of where things stand with respect to vehicle performance, energy efficiency, and cost at all stages of the research and development (R&D). This is particularly important as the project heads down the stretch toward completion because it helps to identify where the remaining R&D should be focused.

**Question 5: Proposed future work**

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

- The proposed future work is appropriate—the project is 70% complete. If possible, the PI should add sensitivity analysis for sorbent tanks for a range extender fuel cell powertrain.
- The proposed future work is basically a continuation of the current work (minus the energy analysis portion). It does not appear that any new high-impact results should be expected this year.
- It will be helpful to include the volumetric system size as well as the gravimetric system size in future presentations.
- The vehicle performance modeling and analysis must continue to the end of the HSECoE project. It will provide the bottom line to the collective work of all HSECoE participants. The media engineering aspect, while important in some respects, may not be as critical down the stretch as the modeling/analysis.
- It seems that two additional years is a very long time to complete the remaining 30% of project content.
- The future work plans will continue to focus on evaluating the impact of system changes in Phase III storage system designs. It is good that the energy analysis work is complete because the Center was not intended to study off-board issues. The analysis to date assumes a fixed amount of hydrogen contained in the storage system. It would be instructive to redo the analyses on a fixed-volume basis. Fuel cell electric vehicles (FCEVs) will have a fixed packaging volume for fitting the storage system on board the vehicle. Greater discrimination between the various storage concepts could result from a fixed-volume analysis.

**Project strengths:**

- This project features good coordination with other modeling efforts being pursued by DOE, OEMs, etc.
- NREL has extensive experience in vehicle performance analysis.
- The coordination with HSECoE team members is an area of strength.
- Based on \$100,000 per year of funding, NREL's productivity and level of accomplishment are huge. The NREL work is well focused and expertly directed. The presentation was easy to follow and appreciated.
- The vehicle simulation model is a major accomplishment of the NREL effort. It allows for comparison of various storage system concepts on a consistent basis.

**Project weaknesses:**

- This project has no obvious weaknesses. A great deal of meaningful work is being done at a very low cost to the overall HSECoE project.
- There is a lack of variation in powertrain configurations.
- The progress in MOF-5 isotherm measurement appears to be slow, perhaps due to limited funding.
- Getting across how the NREL experimental effort—low-temperature adsorption—helps to improve or validate the modeling is an area of weakness. The project team should provide a clearer picture of the advantages of the sorbents (and chemical storage) systems compared to 700 bar compressed gas.
- The summary page at the end of the presentation is exactly the same as the summary page used during the 2012 presentation. The summary slide should also summarize accomplishments.
- The information needed by the HSECoE on the adsorption properties of MOF-5 is not well described. There also appear to be experimental difficulties in obtaining this information at low temperature.

**Recommendations for additions/deletions to project scope:**

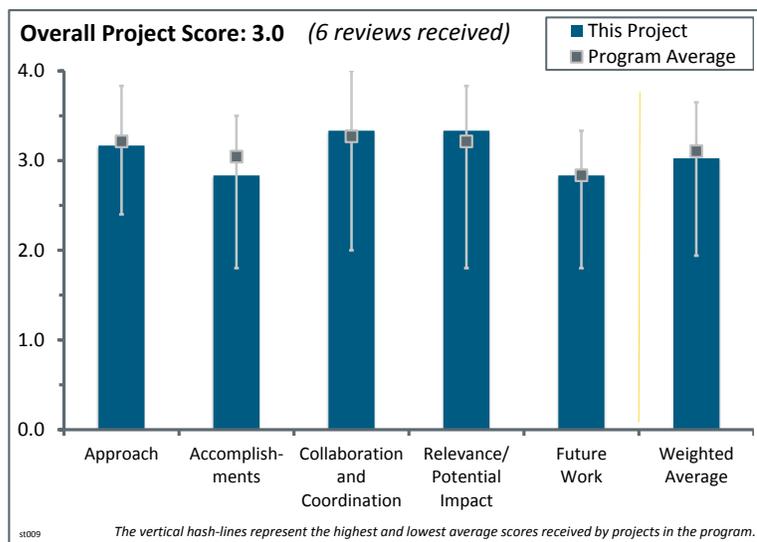
- The project team should keep up the good work.
- The project team should add range extender powertrain sensitivity analysis.
- The simulation work (vehicle performance and WTW) has no correlation to the material characterization. It is unclear if this project is the best platform to address this topic.
- It would be instructive to redo the analyses on a fixed volume basis. FCEVs will have a fixed packaging volume for fitting the storage system on board the vehicle. Greater discrimination between the various storage concepts could result from a fixed-volume analysis.

## Project # ST-009: Thermal Management of Onboard Cryogenic Hydrogen Storage Systems

Mei Cai; General Motors

### Brief Summary of Project:

Objectives of this project are to: (1) develop detailed simulation models for adsorbent systems; (2) develop detailed transport models to include adsorption and heat transfer to guide system models; (3) install and test a cryo-adsorbent apparatus containing metal-organic-framework-5 (MOF-5) powder; (4) experimentally validate flow-through cooling of an MOF-5 powder bed during charging; (5) utilize a desorption model to optimize a resistance heater design; and (6) experimentally validate a desorption model with a helical coil resistive heater in a cryo-adsorbent apparatus. The project will also determine the engineering properties of materials and assists in the development of an integrated modeling framework.



### Question 1: Approach to performing the work

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

- The overall approach is excellent, with very logical steps in experimental validation and feedback with the modeling. The critical barriers of refuel time, mass, and volume are being addressed well.
- A well-formulated approach incorporating modeling and simulation of thermal transport, thermal characterization in a fully instrumented cryo-adsorption test system, and development of an optimized resistive heater design has been employed in this project. The approach focuses on specific milestones established by the Hydrogen Storage Engineering Center of Excellence (HSECoE).
- This project is a continuing part of the HSECoE activities with General Motors' (GM's) specific focus during the current review period on the analyses and testing of adsorbent storage system using MOF-5 media. The objective and scope are fully supportive to establish the potential and determine limitations of this sorbent to meet several performance targets associated with adsorption and desorption rates, including using internal heaters and the thermal enhancement additive expanded natural graphite (ENG).
- The approach of simulation model development and experimental validation is appropriate and has been performed well. However, one iteration with one material is not sufficient for either validating or improving the models. It is unfortunate that there was not more focus on this earlier in the project because it should have been possible to achieve much more in the given time frame. A plan for transferring and continuing this effort appears to be in place, so it is important that the transfer and further efforts are monitored and given a high priority.
- The GM work is directed at four key barriers: capacity, energy efficiency, charging/discharging, and thermal management. The overall effort includes modeling together with experimental model validation and the investigation of essential engineering properties of MOF-5. The major emphasis appears to be on aspects of the fueling system related to recharging of the MOF-5 bed and GM seems to be the HSECoE partner most heavily focused on this critical aspect of the hydrogen storage system. The GM approach to its role in the HSECoE is generally effective; however, it is not clear that the approach for Phase III will close the remaining gaps. It seems like there is more to be accomplished than GM's resources for Phase III will support.
- The approach is adequate.

**Question 2: Accomplishments and progress toward overall project and U.S. Department of Energy (DOE) goals**

This project was rated **2.8** for its accomplishments and progress.

- GM has made significant technical accomplishment in line with its milestones and contributions to the HSECoE project. The development of an experimental test station and completing a first round of validation of modeling efforts with experimental data is extremely important and should continue to be refined. It would have been preferable to have arrived at this point earlier in the project.
- Good progress was made on understanding the thermal characteristics during adsorption and desorption from MOF-5 in different sample configurations. A useful analysis was performed on the refueling times that would be achieved from “stick-like” and “hockey puck” sample configurations with varying dimensional aspect ratios. This led to at least a notion of what kind of sample configuration might be needed in a prototype system. Researchers evaluated the performance of a helical coil resistance heater for efficient desorption of hydrogen from cryo-adsorbed MOF-5. This should be helpful in the development of an efficient prototype system by the HSECoE in Phase III.
- Progress is modest; only some expectations have been met. The presenter showed deficiencies in his understanding of the heat transfer events. Unlikely to use the modeling results in real-life applications.
- Conventional thermal modeling was done using two different-sized test vessels (e.g., 3 liters [L] and 200 L), while cryogenic experiments were performed on a 3-L bed containing MOF-5 powder. Thermal measurements were also performed on compacts of MOF-5. While these analyses and measurements are useful for developing prototype adsorbent hydrogen storage systems, the researchers have not been able to design a configuration capable of meeting desorption target performance levels within mass and volume constraints. The researchers also performed useful thermal conductivity tests on ENG-MOF compacts that yielded some improvements in behavior.
- GM reported significant progress toward meeting some performance targets, but there are still a few gaps. Modeling studies show generally consistent agreement with measurements, but it seems that the models may need to incorporate some yet unidentified factors to produce tighter fits to experimental data. The pellet size/shape optimization result is interesting and potentially very significant. The modeling results for the 200 L tank are in serious need of validation.
- The completion and use of the experimental setup is critical to this project. The results in desorption performance using model and experiment are very promising. It does not appear that the 4 L over the limit heat exchanger would seriously jeopardize the overall full-scale storage goals, and it may be improved upon with other geometries—perhaps an axial or radial heat exchanger asymmetry to optimize the time-dependent three-dimensional temperature profiles.

**Question 3: Collaboration and coordination with other institutions**

This project was rated **3.3** for its collaboration and coordination.

- Collaborations exist and are well coordinated.
- There is very good coordination and interaction among all of the partners. This is impressive.
- Good coordination was shown with Ford Motor Company and BASF partners on characterizing properties and behavior of the MOF-5 adsorbents. The cryogenic testing complemented the design and modeling efforts of other HSECoE partners.
- Collaborations with multiple industrial, academic, and national laboratory partners are evident. These collaborations have served to enhance and leverage the GM effort in this project. There is a significant effort at Savannah River National Laboratory on thermal management as well. It would have been helpful if the division of effort between that project and this one had been more clearly delineated.
- The collaboration relationships outlined in slide 19 of the GM presentation provide a clear picture of how GM connects and coordinates with other members of the HSECoE.
- Technology transfer by making the models and experimental equipment available to the HSECoE is critical for future work. It was not abundantly clear from the presentation how much interaction on modeling efforts and data sharing occurred within the HSECoE or externally.

#### Question 4: Relevance/potential impact on advancing progress toward DOE research, development, and demonstration (RD&D) goals

This project was rated **3.3** for its relevance/potential impact.

- This project is aligned with the DOE Hydrogen and Fuel Cell Program’s RD&D goals.
- The systems modeling and experimental work on cyrosorption materials is highly relevant and critical to DOE objectives.
- This project is critical in enabling one of the few realistic options for hydrogen storage in light-duty FCEVs.
- This project has reached the stage where it is making some significant contributions to meeting DOE storage system performance targets in the area of recharging and thermal management. System capacity and energy efficiency seem to be getting less emphasis, perhaps because they are covered at a higher level of effort by other HSECoE partners.
- Understanding heat transport issues and implementing effective thermal management approaches are vital for developing an adsorbent-based storage and delivery system that can operate with charging and discharging rates compatible with effective fuel cell operation. The project is an integral component of the overall HSECoE effort, and it directly supports the DOE RD&D objectives.
- Assessments of MOF powders and compacts with the ENG additives were valuable to the adsorption storage system development effort within HSECoE. This information provided some validation of design features to improve performance levels. However, thermal management issues still limit these storage devices from meeting critical mass and volume targets.

#### Question 5: Proposed future work

This project was rated **2.8** for its proposed future work.

- It is excellent that the test apparatus will be used for HSECoE Phase III efforts. Hopefully, it will be used with the other cryo-adsorbent architectures and at full scale. The plans are spot on.
- This project is nearly complete (85% as of March 2013). Plans are in place to complete the technical activity and fully document the results. It will be important for the PI and her team to ensure that the experimental and simulation results are communicated effectively to the rest of the HSECoE team. (GM will continue as a consultant to the HSECoE in Phase III.)
- The future work is not clearly defined; it is just a continuation of the existing research.
- GM will have a significantly reduced role during Phase III of the HSECoE program, and the former principal investigator (PI) from GM retired about a year ago. Hence, it is not clear whether GM will contribute much value in the future activities beyond a vague consultation role.
- The meaning of “prepare cryo-adsorbent test apparatus plus associated instrumentation for continued usage by the DOE HSECoE as needed in phase III” is unclear. It is unfortunate that GM will not continue with direct experimental and modeling work. It is critical that there is strong future advisory participation by GM in the HSECoE—not just at a bird’s-eye and management level, but also very much at a research and development level.
- The proposed future work (slide 17 of the GM presentation) is not very exciting to say the least. “Document, polish, and consult” seem to be the operative words. One gets the sense that GM will not be doing much more experimental validation, and perhaps parts of its effort will be phased out.

#### Project strengths:

- This project features good modeling work and a good project team.
- GM researchers have performed unique cryogenic testing of adsorbents in support of modeling efforts. The findings are valuable to the hydrogen storage community.
- The coordination among partners and the interrelation between experiments and models are strengths of this project.
- The measurement science and engineering appears to be very good work that is being expertly planned and executed.

- A well-qualified team is conducting the technical effort. The GM-led team provides a good connection between the HSECoE and a major automobile manufacturer. The project incorporates solid elements of simulation/modeling and experimental work to address a problem that is vital in the development of a practical hydrogen storage prototype system based on cryo-adsorption.
- An experimental apparatus was developed and used to test and validate the model simulations. This is very important and should be the focus of further work. It is important because MOF-5 is unlikely to be the ultimate storage material; therefore, the modeling will become increasingly important in the optimization of both materials and systems until the ultimate materials are developed, as well as a guide to the determination of the materials properties that need the most improvement.

### **Project weaknesses:**

- The project has no obvious weaknesses. The overarching problem is that MOF-5 will likely not be able to meet the DOE targets for hydrogen storage. An obvious question is whether the work conducted on this project will be fully transferable to another, more suitable, material if/when it is identified.
- Chances are low that MOF-5 will end up in real-life applications.
- Some key technical staff members are no longer working on this project, impacting both the GM modeling and testing contributions to HSECoE milestones. Questions remain whether GM will retain the cryogenic test facility and whether experienced laboratory staff will be available to support future testing.
- It is unclear how much coordination and collaboration have taken place on this project within the HSECoE and with international experts regarding incorporating existing experimental data into the task of validating the simulation models that have been developed. It is somewhat concerning that the MOF-5-centric approach may not challenge the modeling efforts extensively enough to make the simulation models sufficiently accurate for a wide range of physisorption materials.
- The modeling results appear to be approximations in some cases. The functional forms of the model curves do not always match the experimental curves. It is not clear how serious an issue this is. Thermal energy flow, in particular, is often hard to model. Perhaps the GM modeling results are the best one can hope to achieve at this time.

### **Recommendations for additions/deletions to project scope:**

- The remaining technical obstacles and challenges should be discussed in a straightforward but detailed way. There are questions about what the major risks are and what risk mitigation strategies are in place.
- Papers should be prepared and submitted for publication reporting on cryogenic testing of the prototype beds and MOF-5 adsorbent properties. Prior modeling and test results should be fully shared with other HSECoE partners.
- Time is running out, but it would be nice to test the current models against data of a promising adsorption material or two that is dissimilar to MOF-5 in as many physical properties as possible. This would help determine the robustness of the models and aid in their further improvement.
- The future plans slide invoked concern about the extent to which GM can effectively close gaps and demonstrate the achievement of “Specific, Measurable, Achievable, Relevant, and Timely” (SMART) milestones in the coming year.

## Project # ST-010: Ford/BASF-SE/UM Activities in Support of the Hydrogen Storage Engineering Center of Excellence

Mike Veenstra; Ford Motor Company

### Brief Summary of Project:

The objectives of this project fall under three tasks. Task 1 is to develop a dynamic vehicle parameter model that interfaces with diverse storage system concepts. Task 2 involves the development of robust cost projections for storage system concepts. Task 3 is to devise and develop system-focused strategies for processing and packing framework-based sorbent hydrogen storage media.

### Question 1: Approach to performing the work

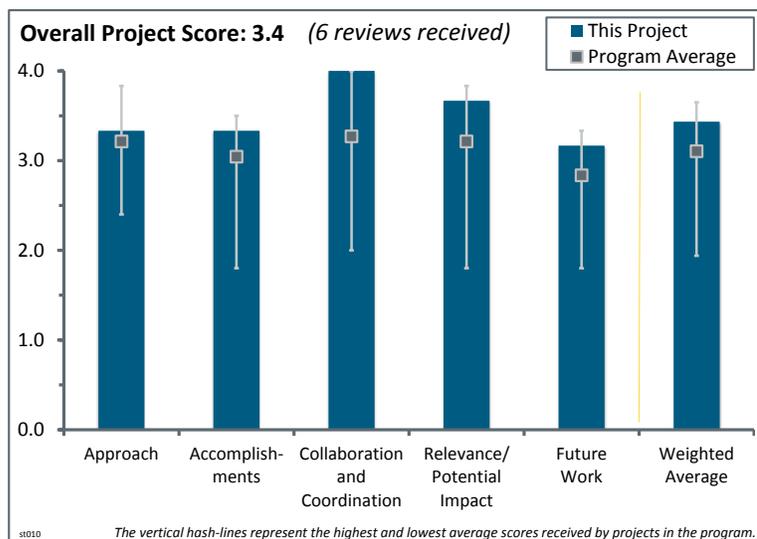
This project was rated **3.3** for its approach.

- The approach was very well balanced.
- The project is well organized, with clear roles and responsibilities for each team member.
- The approach has many well-considered features, including coordination of trade-off decisions, identification of strategic decision points, development of milestone criteria, spearheading of the go/no-go process, model development, failure modes analysis, and system ranking. The materials development and property measurement tasks are well thought out and sharply focused on critical technical barriers.
- The project team has adopted a well-reasoned approach for selecting suitable adsorption media, establishing design/performance trade-offs, and understanding and improving thermal conductivity in metal organic framework-5 (MOF-5) in different sample configurations. This information is important for developing and implementing an optimized prototype system.
- The approach was adequate.
- D. Siegel of the University of Michigan (UM) has the role of the system architect for the sorbent option. M. Veenstra of Ford Motor Company provides the original equipment manufacturer (OEM) perspective in developing fuel cell models, supporting cost studies, providing failure mode and effects analysis (FMEA) guidance, and ranking systems.

### Question 2: Accomplishments and progress toward overall project and U.S. Department of Energy (DOE) goals

This project was rated **3.3** for its accomplishments and progress.

- A large amount of very useful data has been collected; this is critical to the success of the overall Hydrogen Storage Engineering Center of Excellence (HSECoE, the Center) project.
- Numerous milestones were achieved or exceeded; several key system targets were met. Four high-importance system performance parameters were identified and addressed: fuel economy, driving range, vehicle acceleration, and cost. Ford performed a rational down-selection to MOF-5. Ford identified pathways for reducing the number and nature of potential failure modes. Ford achieved impressive results relevant to thermal conductivity issues; for example, the expanded natural graphite (ENG) additive improves thermal conductivity. In summary, it seems like every research and development (R&D) activity bore substantive fruit.



- Ford has done good work in performing FMEA for the sorbent option. The principal investigator (PI) presented new results on evaluating homogeneity of MOF-5 powder, pellets, and pellets with 5% ENG in terms of variations of density, particle size distribution, permeability, and thermal conductivity. The PI also discussed new data on the effects of humidity and air exposure and dust ignition safety. The data may not have value in the long term because it is specific to MOF-5, a material that does not meet storage targets, but the procedures and methods for FMEA should be useful for other promising sorbents. The PI presented old data on the impact of MOF-5 densification on hydrogen uptake, gravimetric and volumetric capacity, thermal conductivity, and permeability. The new data on kinetics and cycle testing should be useful.
- The accomplishments are very good. The only issue is that MOF-5 probably will not be the final material in a car. But it is required that programs such as the DOE Hydrogen and Fuel Cells Program also fund high-risk research, which this research should be considered.
- Although the quality of research is high, the results obtained are rather modest. It does not look like MOF-5 is going to end up in real applications. The presented results raise the question of whether MOFs are an appropriate hydrogen storage media for automotive applications at all.

### Question 3: Collaboration and coordination with other institutions

This project was rated **4.0** for its collaboration and coordination.

- This project features an impressive list of collaborations.
- This project is highly collaborative.
- Ford appears to be well connected with all Center partners where responsibilities overlap. It appears from the collection of HSECoE presentations that the overall coordination of effort is at a very high level and that all appropriate and necessary collaborations are going along smoothly. Ford comes across as a major player with significant responsibility in the HSECoE.
- Excellent collaborations with other Center partners are apparent and are reinforcing the solid technical progress that is being made in this project. The perspective and system context provided by the participation of a major automobile manufacturer in the activities of the Center are extremely valuable.
- The collaborations with UM and BASF seem to be very effective, although UM's contributions in fiscal year 2013 were not clearly identified.

### Question 4: Relevance/potential impact on advancing progress toward DOE research, development, and demonstration (RD&D) goals

This project was rated **3.7** for its relevance/potential impact.

- The project is relevant to the Hydrogen and Fuel Cells Program and DOE RD&D goals.
- The project objectives are clear, well defined, specifically oriented to address DOE systems level targets, and critical components of the HSECoE project.
- Ford is a major contributor to the HSECoE effort; its activities within the Center are focused on all hydrogen storage system barriers. It functions at both the executive and working levels of the project. Ford brings an automobile manufacturer's perspective to the project, provides leadership in a number of critical areas, and contributes effectively to key R&D and modeling tasks. The work done by Ford embraces all critical barriers to a successful outcome for the HSECoE. Much of the outcome of the Ford effort contributes to activities performed by other Center partners, or so it seems.
- This project is providing vehicle parameter modeling, system cost projections, and sorbent-media processing strategies that directly support the HSECoE mission. In addition, the participation of a major automobile manufacturer (Ford) in the planning and execution of the Center activities provides an important "real-world" perspective and validation of the overall HSECoE effort. The project directly supports the DOE RD&D goals for development and testing of a viable hydrogen storage system.
- The objective of this project is to design innovative material-based hydrogen system architectures to meet the DOE performance and cost targets. Even at the start, it was recognized that a storage system could not be engineered to overcome the limitations of the materials that are currently available. The hope is that the analysis and characterization methods and components developed in this project will be useful and relevant when new, promising materials are discovered by others.

- The risk analysis work is very important. In addition, Ford’s work on media compaction, air exposure safety assessment of MOF-5, and neutron imaging of MOF-5 (in collaboration with NIST) are all highly relevant areas of research for sorbent-based hydrogen storage systems.

### Question 5: Proposed future work

This project was rated **3.7** for its proposed future work.

- The proposed future work is very good and necessary.
- The future work is in line with the project’s proposed work. It is important that all of the data and knowledge generated from this project be made available to the HSECoE and the DOE Hydrogen and Fuel Cells Program for future work and that the expertise is not lost as the project comes to an end.
- The future work is clearly laid out. BASF’s work on scale-up to prepare kilogram quantities of MOF-5 is essential if the sorbent work continues in Phase III. The proposed work on thermal conductivity enhancement needs to be justified with a defensible conductivity target. The scope of work on failure modes could be curtailed because a noteworthy failure mechanism has not been identified. The proposed work on model development and validation is difficult to judge because of the involvement of other partners, including Savannah River National Laboratory, United Technologies Research Center, and the National Renewable Energy Laboratory.
- Phase III tasks are focused on engineering concept demonstrations, material property enhancements (e.g., thermal conductivity of a MOF-5 bed), enhancing system operational robustness, and system engineering validation. The goals for Phase III are presented in sufficient detail to give the reader a clear picture of what will be done and why. The future work proposed by Ford is well aligned with what was learned in Phase II and focuses on meeting the crucial “Specific, Measurable, Achievable, Relevant, and Timely” (SMART) milestones.
- The near-term plans follow directly from the Phase II effort and focus on important Phase III SMART milestones. The plans are clearly stated and address important system development issues. However, plans to achieve the specific milestone of “enhancing thermal conductivity beyond 10% ENG at operating temperatures” (slide 25) should be developed in greater detail (i.e., it is unclear what will actually be done to improve the thermal conductivity beyond the level achieved in 10% ENG samples).
- The proposed future work is somewhat poorly defined. This may be the result of rather modest success to date.

### Project strengths:

- This is a good proof-of-concept type of work.
- This project has strong collaboration with BASF, the material supplier. The facilities and experience at Ford and BASF are definite assets.
- The presentation included excellent slide formatting to illustrate main points and it was well presented by the PI. The viewer is left with the impression that the project team did a significant amount of good work and made major steps toward achieving system targets.
- A well-qualified team is making excellent progress on all experimental and modeling efforts. The involvement of a major auto manufacturer in the technical activities and management of the Center is extremely valuable.
- This project has accomplished a considerable amount and achieved a wide range of experimental measurements of engineering properties of MOF-5-based hydrogen storage materials. This information is critical for the validation and improvement of HSECoE modeling systems. In addition, extensive FMEA was done to identify the weak links in the application of these materials to real-world application. This provides valuable insight and an OEM perspective within the areas of material and system improvements that will be needed for successful commercialization of fuel cell vehicles using adsorbents for hydrogen storage.

### Project weaknesses:

- There were no detectable weaknesses one could attribute to this project.

- There are no real weaknesses in the project team or work. The team should continue to develop characterization methods using MOF-5 as the surrogate material.
- The material used to evaluate the concept has little chance to be used in real-life applications.
- An explicit and detailed statement concerning the technical obstacles, challenges, and risks that must be addressed in the Phase III effort is needed. Without that information, it is difficult to discern how development and engineering priorities were established.
- With the down-select, the focus of this work is now exclusively on MOF-5. At the same time, it is recognized that MOF-5 will not meet DOE targets. A viable physisorption storage material may ultimately not even be a MOF or related material. This means that the materials improvement methods, measurement techniques, and systems analysis tools being developed in this project must work for a wide range of materials to be discovered in the future. While studies have been performed within the HSECoE on activated carbons as well as MOF5, a concern is that it is not clear how representative the current MOF-5 analysis may be for a full range of adsorption materials. Without applying much of the same analysis to a significantly different physisorption material, it is hard to know: (1) how representative MOF-5 is for most adsorption materials in real-world systems, (2) how useful these analyses and models will be for other materials, and (3) what likely range of variations in all of the materials properties and performance being evaluated can be expected.

### **Recommendations for additions/deletions to project scope:**

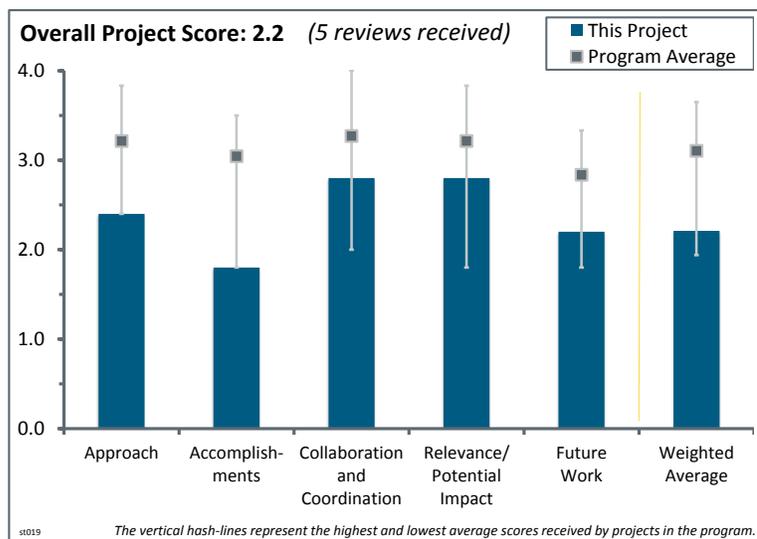
- Ford has a key role in the project and needs to remain a primary participant. This project has reached the point where the scope is honed to achieve a successful outcome. There is no need to change anything in Ford's future plan.
- There is no need to add or subtract tasks. DOE needs to make sure that the data and methods are properly documented and available to organizations outside of the HSECoE.
- The project team should look at density homogeneity within the single pellets with in-situ neutron tomography/radiography.
- It is highly unlikely that a system based on MOF-5 will meet the DOE targets for both gravimetric and volumetric capacity. It would be helpful if at least a pathway to identifying an optimum adsorbent system could be provided.
- A succinct set of similar experimental and modeling analysis should be performed on a promising physisorption material that is as different from MOF-5 in as many of its physical properties as possible. This would help to evaluate (1) how representative MOF-5 is for most adsorption materials in real-world systems, (2) how useful these analyses and models are for other materials, and (3) what likely range of variations in all of the materials properties and performance can be expected.

## Project # ST-019: Multiply Surface-Functionalized Nanoporous Carbon for Vehicular Hydrogen Storage

Peter Pfeifer; University of Missouri

### Brief Summary of Project:

The objectives of this project are to fabricate boron-doped nanoporous carbon for high-capacity reversible hydrogen storage and to characterize materials and demonstrate storage performance. The project aims to create high-surface-area material and subsequent monoliths with minimum pore space for high volumetric storage capacity. Materials will be doped with boron to increase binding energy for hydrogen. Material properties will be characterized, and hydrogen sorption kinetics and temperature evolution during charging/discharging of the material/monoliths will be determined.



### Question 1: Approach to performing the work

This project was rated **2.4** for its approach.

- The work examines several nanoporous carbon materials for their hydrogen sorption properties. The approach to the work is logical and step-wise. The investigators examine the processes to create high-surface-area monoliths of nanoporous carbon, then examine the doping of these monoliths with boron as well as characterize the hydrogen storage performance of these materials. The investigators present a predicted storage capacity as a function of boron doping wt.%. This predicted performance exceeds the U.S. Department of Energy (DOE) targeted milestones for sorption materials.
- The approach to focus on understanding the nature of the boron doping and its impact on enhanced hydrogen storage properties is important; however, a clear examination of the abilities of these materials to achieve DOE targets was not apparent in the results. This should be a focus of any future work.
- After many years of effort, it is disappointing to see that there are still unresolved questions regarding the most basic features of the materials, such as what the composition and local structure are.
- This project has two main objectives: (1) increase the binding energy by boron doping in the hope of operating way above cryogenic temperatures and preferably near room temperature and (2) increase the volumetric density by increasing the packing density of the activated carbon. The initial approach was plainly justified in the absence of relevant experimental results regarding these two aspects; however, the 2012 results clearly showed that boron doping does not provide a pathway for meeting the targets. The project should have been redirected in a more useful direction.
- The principal investigator (PI) does not adequately explain his approach to developing boron-doped hydrogen storage materials. In fact, not a single slide is specifically directed at the approach. While the concept is very interesting, it is based on some incorrect assumptions about the core possibilities associated with boron-doping levels in a carbon matrix (e.g., 20% brings one to boron-carbide). It is a step in the right direction that the PI is working with the National Renewable Energy Laboratory (NREL). However, a validation experiment on a single sample does not validate other past results; it validates the sample measured. The PI's later results need to be validated as well. It was very difficult to follow the talk as outlined by the PI.

**Question 2: Accomplishments and progress toward overall project and U.S. Department of Energy (DOE) goals**

This project was rated **1.8** for its accomplishments and progress.

- The investigators have prepared boron-doped nanoporous carbon materials with a volumetric capacity of 63 g/L and a gravimetric capacity of 12 wt.% (at 80 K). Likewise, the thermodynamic target window for enthalpy of adsorption is approximately 12 kJ/mol. The investigators show that boron-doping shifts this adsorption enthalpy to 10 kJ/mol. Both of these accomplishments are noteworthy. The foundational science is also addressed in this work. The full characterization of the boron-doped nanoporous carbons that the investigators completed using techniques such as x-ray photoelectron spectroscopy (XPS), thermogravimetric analysis (TGA), mass spectroscopy, and Fourier transform infrared spectroscopy (FTIR) clearly guided the choice of doping strategies (e.g., deposition temperature) and could possibly give useful insight into the optimal boron content.
- Doping modestly increased the binding energy, but clearly not enough to be a pathway for meeting the DOE targets. Moreover, the doping decreases the surface area of the adsorbent and thus decreases the hydrogen uptake. The results show a modest increase in uptake by unit surface area but do not show the cost of decreasing the surface area. There should have been a go/no go point for this approach. As for increasing the packing density of the adsorbent, this is also done at the cost of decreasing the gravimetric density by decreasing surface area and also by decreasing the gas phase density which is an equally significant portion of the total storage capacity. A sensitivity analysis should have been carried out to find an optimum combination.
- Progress has been made on gaining a fundamental understanding of the boron-doped materials and the reproducibility of synthesizing materials; however, little progress has been made to show that these materials will be able to achieve DOE hydrogen storage goals. If the fundamentals of the material are still not understood, it is unclear why researchers would scale up to monoliths. Such an effort seems premature, given the uncertainties in the materials properties.
- In fiscal year (FY) 2013, there did not seem to be any significant progress toward the go/no-go metrics. The accomplishments as presented are suspect. The PI admits the presence of boron oxide but then assumes his samples have none because the experiments were performed under anaerobic conditions. However, for these syntheses, even trace amounts of water or oxygen will create an oxide impurity. Yes, there is  $sp^2$  hybrid boron present in his samples, but the percentages are much less than assumed. The concentration variations of the monoliths were not explained adequately.

**Question 3: Collaboration and coordination with other institutions**

This project was rated **2.8** for its collaboration and coordination.

- The validation of measurements by NREL was an important milestone for this project.
- The PI did make an effort to work with NREL. This type of interaction should be encouraged further.
- The project lists many collaborators; except for NREL and the University of Missouri, the contributions of the others to 2012–2013 efforts are unclear.
- Although investigators list many other collaborating institutions on slide 18, the technical accomplishment slides (slides 7–13) and future work slides (slides 19–20) show primarily work done at the University of Missouri. The relationships with collaborating institutions could be further improved.

**Question 4: Relevance/potential impact on advancing progress toward DOE research, development, and demonstration (RD&D) goals**

This project was rated **2.8** for its relevance/potential impact.

- The project is relevant to the DOE storage objectives of increasing the volumetric capacity and the operating temperature of adsorption storage, among other properties.
- The project is unique in that the investigators have developed a method to “tune” the heat of adsorption using the variable of boron-doping content. This presents an exciting opportunity because the approaches

being developed in this research could be more generally applied to other nanocarbon materials to ultimately reach DOE-targeted adsorption temperatures.

- It seems unlikely that forming monoliths will improve capacity enough to significantly change the ability of the materials to achieve DOE goals.
- The presentation of data on slide 4 is disappointing. The PI made the effort to work with NREL, but then just changed the single data point. The other data in the chart were not validated, which makes the chart very misleading.

### Question 5: Proposed future work

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

- The planned future work takes logical steps to overcome barriers identified during the course of ongoing research. These barriers include boron free-radical formation, oxygenation of boron doping, and “tuning” the enthalpy of hydrogen adsorption at room temperature. The future work is lacking clear plans for interaction with the collaborators listed in slide 18.
- Enough capacity data should be collected on materials with different surface areas and boron-doping levels to project what values of each would be needed to meet DOE goals.
- The proposed work may offer a little improvement of the presented results, but the developed material will be far from meeting DOE goals. A more thorough measurement of the heat of adsorption measurement is definitely warranted; clear demonstration of the advantages and disadvantages of boron doping and pelletizing is also needed to direct future efforts. Cyclability, reversibility, and reproducibility should also be demonstrated.

### Project strengths:

- The project team has good knowledge of adsorption.
- The concept and verified increases in isosteric heats are an important step forward. The work with NREL is another strength.
- The validation of measurements proved the reliability of the project’s data collection. Analysis of the state of the boron in the material has provided useful insight into what needs to be done to improve the materials.
- The investigators do a really nice job of characterizing the new materials. The approaches used to arrive at boron-doped nanoporous carbon hydrogen sorption materials with the potential to meet the DOE targets can be used more widely for other nanocarbons.

### Project weaknesses:

- The project team is focused on improving one or two materials properties at the expense of the many others.
- It seems that most of the work is done at the University of Missouri; few results from interaction with collaborators were presented. This is a major weakness because this project relies on the fundamental characterization (offered by collaborators listed on slide 18) to guide the research to successful doping parameters (which in turn lead to useful thermodynamic properties).
- The interpretation of data: XPS, monolith, and densities is an area of weakness. There is boron oxide in the samples. Until the PI acknowledges and takes this data point into consideration, the interpretation of the data is incomplete.
- The presenter did not fully address the reviewer statement that not a lot of progress has been made in improving capacity; instead, the presenter pointed to efforts to validate measurements and improve reproducibility in production. So two years have passed without significant improvement in materials properties. While the data has been validated by measurements at NREL, the validity of methods to determine  $\Delta H$  (enthalpy change) should also be addressed. With isotherms measured at only two closely spaced temperatures, and depending on the method of determining absolute capacity, the margin of error may be quite large.

**Recommendations for additions/deletions to project scope:**

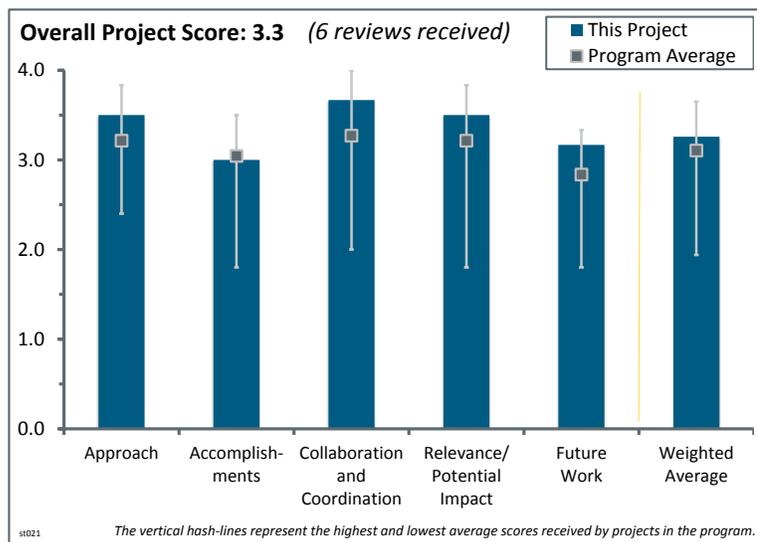
- This project should be discontinued.
- The researchers should add a go/no-go decision point after optimizing the doping of granular material. They should also measure reversibility and demonstrate cyclability and reproducibility. Using the current data, it should be possible to project how much capacity improvement can be achieved by compaction into monoliths. If the projections do not show that compaction provides a clear path to capacity goals, then the work on monoliths should stop.

## Project # ST-021: Weak Chemisorption Validation

Thomas Gennett; National Renewable Energy Laboratory

### Brief Summary of Project:

This project evaluates the spillover process for hydrogen storage on metal-doped carbon materials. The objectives of this project are to: (1) validate measurement methods, (2) identify and synthesize several candidate sorbents for spillover, (3) determine hydrogen sorption capacity enhancement from spillover, and (4) observe and characterize spillover hydrogen-substrate interactions with spectroscopic techniques. The project will validate observations for a narrow range of spillover material systems and will synthesize and distribute targeted materials for group analysis.



### Question 1: Approach to performing the work

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

- This project features an excellent approach designed to answer the question of whether or not there is significant spillover hydrogen storage at room temperature.
- The project team performed a very thorough analysis.
- The National Renewable Energy Laboratory (NREL) has demonstrated a good, disciplined approach to evaluate and demonstrate the “spillover” mechanism.
- The round-robin synthesis and measurement effort is an outstanding step toward the validation of hydrogen sorption capacity enhancement from spillover.
- The goal is to use a range of experimental methods to validate the role of spillover in physisorption systems that use metal-doped carbon. The experimental work is first rate and the researchers have developed a team to validate whether the effect is real. They have demonstrated that the effect is real with the determination of a carbon-hydrogen bond. There is no discussion of the weight percent enhancement. There is no discussion if all of the hydrogen comes back off and how often one can cycle the system. It is unclear if the spillover sites get blocked.
- The intent of this project was to clarify via cooperative and definitive experimental studies whether the widely touted hydrogen spillover mechanism could actually produce greatly enhanced hydrogen storage capacities of carbon adsorbents with properties conducive to meeting U.S. Department of Energy (DOE) hydrogen storage performance targets. The approach was to characterize shared samples with metal additives that reportedly exhibited at least 15% higher capacities at ambient temperature due to hydrogen spillover. Measurements were done in different laboratories and supplemented with spectroscopic techniques such as Fourier transform infrared spectroscopy (FTIR), neutron vibrational spectroscopy (NVS), and nuclear magnetic resonance spectroscopy (NMR).

### Question 2: Accomplishments and progress toward overall project and U.S. Department of Energy (DOE) goals

This project was rated **3.0** for its accomplishments and progress.

- The project has accomplished the specified goals and completed the necessary steps to confirm the existence of the “spillover” mechanism.

- Many techniques have been developed out of this project; using Diffuse Reflectance Infrared Fourier Transform Spectroscopy (DRIFTS) for the direct evidence of carbon-hydrogen interaction is a particularly great achievement.
- This project has definitely established that large amounts of hydrogen storage (e.g., 4 wt.%) do not occur at room temperature.
- The researchers have made excellent progress in reconciling the mechanism of metal mediated processes with different substrate matrices. The first direct spectroscopic evidence of a reversible room temperature sorption/desorption were apparently from a unique carbon-hydrogen interaction via DRIFTS, NMR, and neutron scattering spectroscopy techniques. Researchers validated results by using different groups to make the measurements. It is unclear what wt.% the researchers think they can get at what temperature. The project team demonstrated the need for more fundamental work in the area and showed the need for very careful experimental work. The team did not show what other metals might be practical or connect to other work in catalysis where the amount of hydrogen on iridium doped in a zeolite has been studied.
- Overall, this project has attained its goals. It would be preferred if this project would progress somewhat faster, but measuring such a small effect (as appears to be the case for spillover) is a non-trivial task.
- After nearly three years of effort by the various partners in this project, modest (i.e., circa 15%–30%) capacity increases can be attributed to hydrogen-spillover from metals such as platinum, palladium, and ruthenium on lower surface area carbons. Evidence for some hydrogen-carbon chemical bonding is indicated via FTIR and NMR; however, facile reversibility as required for practical storage applications was not found. While the spectroscopic techniques provided complementary information on the presence of hydrogen-carbon bonds, a comprehensive description of the spillover mechanism has yet to be presented.

### Question 3: Collaboration and coordination with other institutions

This project was rated **3.7** for its collaboration and coordination.

- A large number of collaborating groups are working together on this project—each bringing its own expertise—making it a great, coordinated effort.
- The team’s excellent collaboration helped demonstrate the effect. There were 4 groups focused on spillover and 11 groups on measurements. The project featured very good teamwork and is to be commended. Such a team approach is needed to determine if the effect is real or not.
- The collaboration on this project seems to be very good because they attempted to coordinate with many of the researchers in this field.
- Besides NREL, both domestic and international research groups with experience and expertise actively participated in producing test materials and conducting volumetric hydrogen capacity and spectroscopic measurements. However, subcontracting and other issues delayed the round-robin testing that ultimately reduced the time available to conduct the critically required experiments.
- It is curious that there was no collaboration with Ralph Yang at the University of Michigan.

### Question 4: Relevance/potential impact on advancing progress toward DOE research, development, and demonstration (RD&D) goals

This project was rated **3.5** for its relevance/potential impact.

- The evaluation of the spillover approach as a means to achieve DOE goals is very important for the overall objectives.
- This project provided a very important validation service to the DOE Hydrogen and Fuel Cells Program; it essentially “closes the book” on spillover.
- The project has significant relevance because it confirmed the “spillover” mechanism to the hydrogen storage research community. However, the initial impact or contribution of “spillover” to improving materials toward the desired storage goals at room temperature appears to be much less than previously predicted.
- The work shows the presence of a spillover effect. This is not unexpected based on the catalysis work, but it is nice to demonstrate that it is there. There did not appear to be any quantification of how much more hydrogen is stored and what the reversibility/cycling time is. It is unclear if all of the hydrogen comes back

off and for how many cycles this can be repeated. There is no discussion of the potential use of cheaper metals and what the next steps should be other than that more basic science studies are needed. Perhaps it can be made practical.

- It would certainly be important if the spillover phenomena could produce significant room temperature hydrogen storage. Sadly, this does not appear to be the case.
- The results generated during this project suggest that some positive impacts can be had from a hydrogen spillover process with selected metals. In particular, clear indication for the formation of carbon-hydrogen bonds has been demonstrated. However, the levels of storage enhancements are much too modest to be effective for meeting DOE performance targets.

### Question 5: Proposed future work

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

- The project has completed its goals and no significant future work remains.
- The proposed future work appears to be appropriate, especially in the determination of the ultimate spillover capacity possible once researchers completely establish/optimize the interactions and substrate chemistry.
- The ultimate spillover capacity needs to be determined under practical tank operating conditions; this is not included in the future work.
- The project is essentially complete. It would have been good to have seen a bit more on what is really needed to make this a useful storage system.
- The project is nearly over. The most important last order of business is to determine the ultimate spillover capacity possible.
- This project is nearly completed, with only one or two experimental tasks (e.g., NMR measurements under hydrogen pressure on perhaps one more sample) remaining at the time of the DOE Hydrogen and Fuel Cells Program Annual Merit Review. It would be most helpful if the principal investigator and his partners could prepare a comprehensive final report/paper fully describing their samples, detailed characterizations, observations, and whatever conclusions can be drawn either supporting or debunking the hydrogen spillover process. In particular, the challenges of performing reliable and robust measurements should be fully reported, including insights on technical difficulties and inconsistencies encountered during the study.

### Project strengths:

- This project features a strong team and experimental approaches.
- This project features a highly qualified team.
- A large number of collaborating groups are working together on this project—each bringing its own expertise—making it a great, coordinated effort.
- This project features excellent, high-quality experimental work. Other strengths include the excellent team approach to demonstrating the phenomenon and the very careful measurements.
- The project included various levels of supporters and skeptics to develop the assessment of the “spillover” mechanism.
- The involvement of diverse groups with qualified researchers to assess this contentious issue is appreciated. The intent of performing independent experiments on common samples with clearly specified handling and test protocols is clearly a very desirable aspect of this project.

### Project weaknesses:

- The real tank operating conditions need to be included under the evaluation of the spillover approach.
- The slowness of providing funding and samples for study probably limited the time to perform the actual experiments necessary. There are still unresolved issues with slow kinetics for hydrogen on the carbon substrate and oxygen/hydroxyl contaminations.
- There was no discussion of actual weight improvements. Other weaknesses include the lack of discussion about the following: the future for spillover; cheaper, lighter metals; how big the metal particle is; and what doping levels are needed to be an effective hydrogen material.

**Recommendations for additions/deletions to project scope:**

- It will be very important for this project to assess the potential of “spillover” before completion.
- This project is essentially complete. The researchers should finish the project and provide input on future directions for spillover studies.
- There are no recommendations because this project is nearly complete.

## Project # ST-024: Hydrogen Trapping through Designer Hydrogen Spillover Molecules with Reversible Temperature and Pressure-Induced Switching

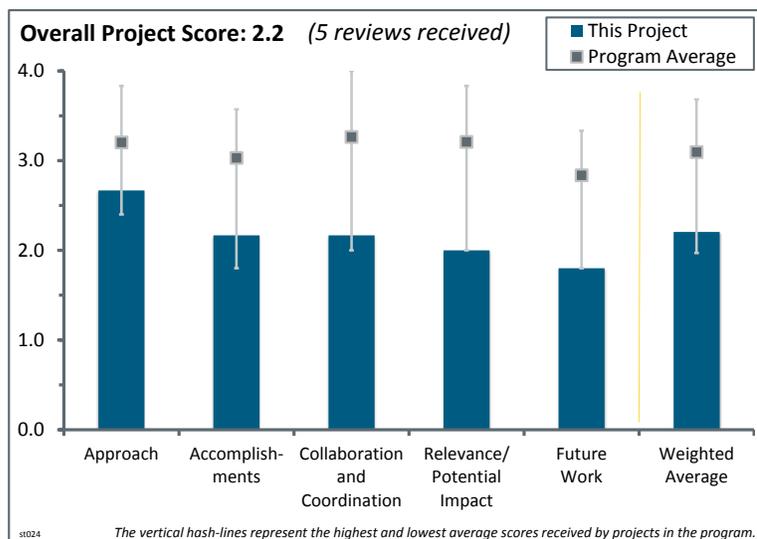
Angela Lueking; Pennsylvania State University

### Brief Summary of Project:

The primary objective of this project is to synthesize designer microporous metal-organic frameworks (MMOFs). The project focuses on synthesis and optimization of one catalyst-doped MMOF, addressing gravimetric capacity, delivery temperature, kinetics, and reproducibility. The goal of the research is to demonstrate the full potential for hydrogenating a MMOF.

### Question 1: Approach to performing the work

This project was rated **2.7** for its approach.



- The focus on attempting to show spillover in the best potential metal-organic framework (MOF) material was good.
- A rational approach is outlined and followed. Researchers have identified a particularly robust MOF that can be catalyzed and apparently remain crystalline. The efforts to identify and focus on one material have helped define the project.
- The primary objective of this project at Pennsylvania State University (PSU) is to discover and characterize specific carbon materials, namely MOF compounds, where hydrogen spillover processes from metal catalysts can give reversible hydrogen storage of several weight percent at ambient temperature. If this capacity can be verified, spillover effects may give a pathway to materials that would approach the U.S. Department of Energy (DOE) targets for passenger vehicles. A fiscal year (FY) 2013 milestone was to demonstrate at least a 3 wt.% reversible storage capacity near ambient temperature with acceptable kinetics. While the original approach was to synthesize promising MOFs then add metallic catalysts to confirm enhanced storage via volumetric and gravimetric experiments, extensive spectroscopic studies have been made to look for a hydrogen-carbon bond via spillover. Complementary first-principles calculations have been used to examine both thermodynamic and kinetic factors that either permit or inhibit the desired reversible reactions.
- The general approach is OK, but it needed to focus more on the practical hydrogen storage tank operation condition.
- When combined with the National Renewable Energy Laboratory (NREL) results, this study shows that spillover is not going to lead to even moderate uptake at room temperature and is rather difficult to measure.
- It is unclear why the project team thinks the chosen catalysts will perform better than those explored previously by other researchers.

### Question 2: Accomplishments and progress toward overall project and U.S. Department of Energy (DOE) goals

This project was rated **2.2** for its accomplishments and progress.

- The robust pre-bridge (PB) doping technique is very interesting and could have impact on other materials. However, the measurement must be focused on the high pressure. It would be a great achievement for the

hydrogen storage community if the principal investigator (PI) can demonstrate whether the spillover approach can or cannot achieve DOE goals based on the real measurement.

- If DFT calculations indicate that one can hydrogenate a substrate, it is unclear how that is evidence of reversibility. The hydrogenation is exothermic—the reverse is quite endothermic and not reversible.
- The project has shown a small increase in spillover hydrogen storage in MOFs, but only 1% hydrogen storage at room temperature. The project could not meet the go/no-go decision point criteria.
- Progress has been somewhat limited, mainly due to the difficulty in measuring spillover. To some degree, this is not the fault of the PIs.
- After investigating a series of MOFs with additives of microscopically dispersed platinum particles that would allow the hydrogen spillover process to take place where its laboratory tests did not reproducibly show enhanced capacities, PSU chose to concentrate on a single promising MOF-platinum combination. While initial low-pressure measurements suggested there could be substantial spillover effects, only limited enhancement (e.g., <1 wt.%) was seen at higher pressure where extremely slow reaction kinetics were also observed. Hence, PSU has failed to meet its go/no-go target. PSU continued to revisit and adapt its techniques for measuring hydrogen capacities in order to improve accuracy and reproducibility. PSU has decreased errors, but it did not verify past reports of room temperature capacities greater than ~1 wt.% nor did it achieve acceptable reproducibility. Raman and other spectroscopic data do suggest some hydrogenation does occur that may be associated with the spillover processes, although data interpretations are still rather controversial.
- Some improvements over native materials may be apparent, but given the 50% to 100% variability between batch and/or run, the magnitude for a typical bulk sample is uncertain. Additionally, reviewers were not told the timescale for these low-pressure uptakes; it is unclear if they are at equilibrium or for the 20-hour exposures. Surface diffusivities seem to be dominant and no clear connection between material stability and diffusion activation energy has been presented to see if these barriers can be reduced. MOF-nitrogen is not described or referenced, so most of the results to do with spectroscopy cannot be interpreted independently and reviewers must rely on the stated results. From slide 14, it is unclear if reviewers are to believe that this is a Cu-O<sub>2</sub> linkage at the metal. The difference between the MOF-nitrogen and PB-MOF-nitrogen shows a significant amount of reduced Cu-O<sub>2</sub> in the prepared sample that is further reduced and somehow partially reversible. There are no indicators of this being handling, sample-position, or sample batch dependent—this is something worth testing in this context. On slide 16, it seems that there has been some effect on 300 K, 70-bar hydrogen exposure: the lowest angle peak, broadened peaks, and the greatly reduced intensity with scattering angle indicates partial degradation—much the same as in the PB-MOF-nitrogen case, and further accentuated in the hot hydrogen plot. This might not be stable in the long term and needs to be tested.

### Question 3: Collaboration and coordination with other institutions

This project was rated **2.2** for its collaboration and coordination.

- The project features reasonable collaborative interactions.
- Some helpful collaboration was evident with projects outside of the DOE Office of Energy Efficiency and Renewable Energy (EERE).
- PSU continues to collaborate with the co-PI at Rutgers University (RU), who is synthesizing different MOFs with properties for potentially greater hydrogen capacities. There have been interactions with several other researchers on characterizing samples and looking to verify reproducibility of the capacity measurements. A strong theoretical relationship is evident with the University of Crete.
- The PI should coordinate more with NREL's team and utilize its expertise in this work, since the scopes of the projects are similar.
- It is not clear whether there were candid discussions between the collaborators about spillover and why the project has received a no-go decision in 2013.
- The presentation did not detail any significant collaborations besides obtaining MOFs from RU and independently funding modeling work at the University of Crete.

**Question 4: Relevance/potential impact on advancing progress toward DOE research, development, and demonstration (RD&D) goals**

This project was rated **2.0** for its relevance/potential impact.

- The project is relevant, but the potential impact is low due to the limited benefits of spillover.
- Even if the spillover concept works, the high cost and low density of the selected material will not likely meet the overall DOE objectives.
- There has not been convincing data supporting the “reversible” spillover mechanism in prior years and this presentation does not change that.
- Achieving significant hydrogen storage near room temperature would have a major impact. Alas, this does not appear to be possible via the spillover approach.
- Hydrogen spillover involving platinum-catalyzed MOFs to sufficiently enhance the storage capacities to meet the DOE targets does not appear to be a viable pathway. Not only is there minimal additional hydrogen storage, but the kinetics are atrocious. The results of the recent modeling are not really encouraging. There seems to be little potential for such hydrogen spillover processes to contribute to meeting practical hydrogen storage in any application.
- As identified by the PI, there is little hope for spillover being useful within the scope of EERE goals until fundamental spillover knowledge is gained. Even then, using relatively heavy MOFs as a spillover target will never meet the hydrogen loading levels needed to achieve DOE’s goals. Uptakes of catalyst-bridged species up to 0.04 wt.% at 1 bar and between 0.3 and 0.6 wt.% at 70 bar are practically meaningless compared to the DOE targets. For activated carbons, the final capacity has to be almost one hydrogen per two carbons, so it is unthinkable to achieve this with the weight penalties of metals in these hybrids. However, a bullet point indicates that 3.5 wt.% may be possible from a calculation (no details were given).

**Question 5: Proposed future work**

This project was rated **1.8** for its proposed future work.

- The project is essentially over. A no-cost extension to allow the students to finish has been requested.
- This question is not applicable. The project is ending.
- There are no direct, high-pressure measurements planned in the future work.
- Rather than performing DFT calculations, the project team should collaborate with an experienced theoretician who can pick the modeling methodology.
- The current work raises more questions than it solves. These should be addressed by peer review prior to embarking on a new series of materials properties that require further doping to potentially enhance diffusion rates.
- The plans shown on slide 21 for completing preparation and characterization of modified MOFs are reasonable if they can be accomplished within the current funding levels. This project will miss its revised go/no-go decision point of demonstrating 3 wt.% hydrogen capacity at “moderate” temperatures in FY 2013. Based on results obtained by the team to date, this goal is probably not achievable using currently investigated materials and treatments.

**Project strengths:**

- This is a valiant attempt to demonstrate room temperature H<sub>2</sub> storage in MOFs via the spillover approach.
- The isotherms for “spillover” type materials are better than the water-generating initially high uptakes of previous years.
- PSU undertook a committed effort to improve the accuracy of its methods for measuring storage capacities that included interactions with other organizations. It has revisited issues of doping materials and looked for more promising candidates to be studied. The use of various spectroscopic methods has been insightful and worthy of praise.

- This project provides the hydrogen storage community with some fundamental understanding of how the spillover concept works. The team also developed some robust doping techniques that can be used for other materials.

### **Project weaknesses:**

- The measurement is not focused on the high pressure. It would be a great achievement for the hydrogen storage community if the PI can demonstrate whether the spillover approach can or cannot achieve DOE's goals based on the real measurement.
- Reproducible and accurate measurements of hydrogen storage capacities remain a major challenge with small samples. Apparently, the processes and procedures used both to prepare the MOFs and to incorporate the catalysts remain difficult and still lead to irreproducible measurements. The very slow kinetics for the transfer of hydrogen during the spillover process remain a very serious issue, even if slightly greater capacities are demonstrated compared to undoped samples. The idealized conceptual mechanisms for hydrogen spillover are apparently greatly oversimplified and unrealistic. While first-principles calculations might be helpful using graphene surfaces for MOFs and other carbons, transference of these predictions can also be highly misleading. This phenomenon has been greatly oversold to the hydrogen energy community as a way to meet hydrogen storage performance targets.
- This project does not help to resolve uncertainty in the spillover field. It is clear from the NREL-led project (ST-021) that spillover is small and frequently difficult to reproduce for many systems. Worthy of consideration, however, is that according to the presentation of Gennett (ST-021), the opinion of a dozen or more researchers, apparently including this PI, is that it would be impractical for DOE to continue R&D on spillover at this time. It is unclear how the resources were spent, including for a co-PI who seemed to provide limited contributions to the project's goals. All of the units on the uptake graphs should be the same. Publications are limited—they are mostly from 2011, with one published in 2013 and one submitted.

### **Recommendations for additions/deletions to project scope:**

- The PSU/RU team has failed to meet its FY 2013 capacity target and should not receive additional funding from DOE. However, a no-cost extension of the contract would be desirable to complete publication of the results/analyses and to allow students to finish their theses. It seems unclear whether additional work on these systems is warranted due to the myriad issues with reproducibility, very bad kinetics, and minimal evidence for reversibility.

## Project # ST-028: Design of Novel Multi-Component Metal Hydride-Based Mixtures for Hydrogen Storage

Christopher Wolverton; Northwestern University

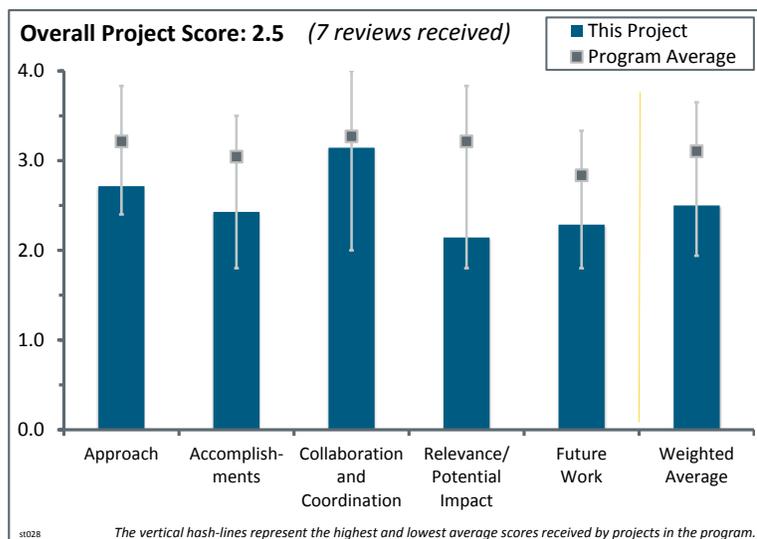
### Brief Summary of Project:

This project studies combinations of materials to form novel multicomponent reactions. The research includes hydrogen storage measurements for automotive applications, computational prediction of novel reactions, and kinetics/catalysis/synthesis experiments. Efforts in the past year were focused on two main reactions predicted to have high capacity and suitable thermodynamics for hydrogen storage applications:  $2\text{LiBH}_4 + 5\text{Mg}(\text{BH}_4)_2$  and  $\text{B}_{20}\text{H}_{16}$ .

### Question 1: Approach to performing the work

This project was rated **2.7** for its approach.

- The approach is excellent and involves complementary methods: experimental measurements, characterization, and computational modeling. The researchers compared pure chemicals, composites, and catalyzed systems, and they have a strong focus toward well-defined automotive applications.
- This project is sharply focused on critical barriers; it is difficult to improve the approach significantly. The project is well designed to address some of the key barriers. It is nice to see that the project is focused on a few of the most promising reactions obtained from computational screening. The computational efforts seem well integrated with the experiments.
- This joint project of Northwestern University (NWU); the University of California, Los Angeles (UCLA); and Ford Motor Company involves a combination of first-principles calculations (NWU and UCLA) of candidate hydrides and their structures along with predicted reaction pathways. The goal is to identify mixed component hydrides with potentially sufficiently large storage capacities that might meet U.S. Department of Energy (DOE) targets for passenger vehicles. Over the past couple of years, the emphasis has been on the role of defects that can underlie diffusion processes with implications for a better understanding of the kinetics. Experiments are being used to determine the as-prepared and decomposition phases in order to ascertain reaction pathways. Solid-state nuclear magnetic resonance (SSNMR) experiments were utilized to identify “amorphous” components in desorbed borohydrides to complement past characterizations. The team has also looked at catalysts to enhance the kinetics. The objectives generally comply with the DOE targets and goals.
- There were significant changes apparent in the project from the previous year, with more focus and outside expertise to assist in the experimental work. The project has obvious strengths in computational expertise but is still lacking on the experimental side. This is a surprise given the reputation of the experimental co-principal investigator (PI) and makes one wonder if the project team is involved at an engaging level of interest.
- The approach may have some impact on the understanding of the diffusion of species in complex metal hydrides. The team may not have the best makeup to take advantage of this because the diffusion modeling then calls for diffusion studies by nuclear magnetic resonance (NMR) and or quasi-elastic neutron scattering (or other appropriate techniques relevant to the diffusion time scales) to confirm the modeling results. The approach could be sharpened by not investing more resources in combing over systems looked at extensively by the Metal Hydride Center of Excellence unless it can be justified via new observations or modeling insights. The approach could be improved by reconciling the current project with information



from the literature. The approach included the addition of an SSNMR capability this year, and it was good to see the project respond to suggestions from various reviewers. The approach included the synthesis of the difficult  $B_{20}H_{16}$ ; it is unclear whether the theoretical modeling result truly justifies the effort because the synthetic thermal chemistry route appears to include  $B_{10}H_{14}$  as a required reagent that does not appear to be accounted for in the modeling result.

- This project needs more of a balance between experimental and computational work. Additional experimental work was added this year but it appeared too late in the overall project plan. There is no real link between theory and experiment in the project. The simulations are what are easy for the researchers to do, not what is relevant to the hydrogen storage problem. Their approach can only deal with diffusion in essentially idealized materials with possibly some defect sites. They cannot readily study the hydrogen release mechanism from the actual compounds because their solid-state DFT approach does not work well for this and they do not know what the various intermediates are. They have not looked at the costs of the materials. They propose to make  $B_{20}H_{16}$  (icosaborane-16) with Dr. Shore at The Ohio State University (OSU), yet the starting materials cost is approximately \$50/g, so 1 kg costs around \$50,000; although, one might be able to get close to 1 kg for \$10,000–\$15,000. The process to make  $B_{20}H_{16}$  might result in a yield of only 10%, thus the cost of the  $B_{20}H_{16}$  is likely on the order of \$100,000–\$500,000/kg. This is not practical in terms of cost for a hydrogen storage system and makes this work completely irrelevant. If instead the researchers started with pure boron as the product, the rehydrogenation cost would be around \$100,000 for 1 kg. This is not feasible because the material would have to be remade each time. There is a lack of understanding of cost and practical engineering issues with the proposed work. Since most of the computationally determined compounds have not been reversible or are unable to be synthesized, there is little practical value of the work. Production of BN and boron by-products can give a reasonably high weight percent, but the products cannot be readily regenerated so it is all useless effort. There is nothing relevant being proposed here at all. The team appears to be unaware of the work on  $(B_{12}H_{12})^{2-}$  complexes with  $NH_4^+$  in the literature for hydrogen storage purposes. One has to be careful of calculating the energetics on a per mole of hydrogen basis because this does not really show what is happening. There can be very high-energy steps that may make the overall thermodynamics irrelevant in terms of kinetic issues because these high-energy intermediates may need to be coupled with low-energy ones to get hydrogen released at a reasonable temperature. The team could not find such intermediates with its computational approach and has not accomplished it with its experimental team, either.

## Question 2: Accomplishments and progress toward overall project and U.S. Department of Energy (DOE) goals

This project was rated **2.4** for its accomplishments and progress.

- There has been progress toward meeting objectives and overcoming barriers. Three of the more promising reactions (determined from an earlier screening effort) were investigated. The predicted thermodynamics for  $B_{20}H_{16}$  look good. The study focused on kinetics, specifically mass transport. The synthesis of  $B_{20}H_{16}$  with OSU is showing limited progress with low yield. Hopefully,  $B_{20}H_{16}$  can be isolated/purified for further experimental studies. The NMR work on  $LiBH_4$  and  $Mg(BH_4)_2$  shows an indication of  $B_2H_6$  being present, as predicted computationally—that is a nice synergy between experiment and theory.
- Efforts to better model the hydrogen transport processes in prototype B-based hydrogen storage systems have continued over the past year and have suggested that  $B_{20}H_{16}$  might have properties amenable to improved storage behavior. The first-principles calculations of defect energies and diffusion parameters clearly show that kinetic barriers generally impede the performance of B-containing phases—even if thermodynamic properties are improved by using a combination of hydrides. NMR measurements suggest that most past speculations on decomposition reactions and products are inconsistent with experimental observations. Further investigations will be needed to unravel the actual mechanisms. Many challenges remain in the development of hydrides that can meet DOE's performance targets.
- The productivity of the theoretical modeling work appears to be good; the experimental aspects of the work seem to be lagging behind. The NMR effort appears to have come up to speed fairly quickly and is providing good feedback to the materials effort. There was little evidence of researchers reconciling data from the literature with their own results, which would be helpful to put their accomplishments into perspective.

- The research is focused on light element hydrides with high theoretical hydrogen capacity. A major part of the experimental measurement appears to investigate moderate temperatures, which is also very good. In some cases, some reversible hydrogen storage capacity is observed, and catalytic additives clearly have a positive effect. In particular, for the system  $2\text{LiBH}_4\text{-}5\text{Mg}(\text{BH}_4)_2$ , it may be only  $\text{Mg}/\text{MgH}_2$  that stores hydrogen reversibly under the chosen physical conditions.
- Very little experimental work was done on  $\text{B}_{20}\text{H}_{16}$ , which was identified as “extremely promising.” More experimental results should have been shown for this material.
- The researchers have done bits and pieces without looking at the overall system. The computational work is simple in terms of the diffusion studies, but more is needed. Their tools do not provide the proper chemical insight into the mechanism and the experimental component is not focused on determining/understanding the mechanism. Their computational energetic results provide minimal insight into the actual energetic or kinetics of the real processes. A global mechanism here is of little value. The cost issue has not been addressed.
- Regarding the  $\text{B}_{20}\text{H}_{16}$  project, the reason why the research team does not spend some time on the “reverse reaction” is unknown; perhaps the PI explained it at the 2012 DOE Hydrogen and Fuel Cells Annual Merit Review. It seems that if the reactions of interest are reversible, the research team could start on both ends and work toward a common middle ground. Perhaps it would be more direct to start with “20B” boron and hydrogen under pressure to make the more stable product  $\text{B}_{20}\text{H}_{16}$ . It could save significant time and effort in making the  $\text{B}_{20}\text{H}_{16}$ . The good news is the  $\text{B}_{20}\text{H}_{16}$  is stable, slightly hygroscopic, and apparently nonflammable. However, the bad news is that it is likely to be too stable. Melting occurs at  $196^\circ\text{C}$  without decomposition. It would appear that the kinetic barriers leading to hydrogen release are significantly higher than the diffusion barriers. It is great that the researchers have approached Dr. Shore and his group at OSU to make the material, but it is unclear if they also asked Dr. Shore his opinion on how this complex would decompose. It is good that the PI has observed a decrease in hydrogen release temperature by adding 10% product to the  $\text{Mg}(\text{NH}_2)_2\text{-LiH}$  mixture; however, it is unclear how “seeding” the  $\text{B}_{20}\text{H}_{16}$  with boron would make a significant difference in the decomposition. It is unclear if there is a scientific basis for this or if it is just hopeful thinking. It would be beneficial to have a mechanistic idea of when and how the product leads to decomposition in the hydrogen release temperature. It is possible that an impurity of any type could lower the melting point and the decomposition could be enhanced in the liquid state. However, it is unclear how general this observation is and how “profound” it really is. Decreasing the onset decomposition from  $200^\circ\text{C}$  to  $80^\circ\text{C}$  is asking a lot. For the  $\text{BH}_4$  project, the PI is commended for bringing in expertise in NMR spectroscopy. The researchers provide a good start toward interpreting the NMR results, but it is quite likely that the broad peak at 26 ppm is a complex mixture of products. It is unclear if there is some rationale that would explain why one species is so broad and the other species is narrower. The Yan paper in “Mater Trans” (Mat. Trans. [2011] 52:1443-1446) could not be readily obtained to discover if it was an experimental or computational paper. However, Dr. Chong and her co-workers at the University of Hawaii at Manoa collected both solid-state NMR and solution NMR for the decomposition products of magnesium borohydride decomposition. Based on the early literature of Hawthorn, Shore, and others, the researchers described a BH condensation decomposition pathway of  $\text{BH}_4$  followed by a multi-step reaction involving several  $\text{B}_x\text{H}_y$  ( $X = 1\text{--}12$ ) intermediates, and that the broad signal observed in the solid-state spectra is most likely due to a wide range of products, not just one or two species. It is unclear if there is some scientific explanation for a change in reaction mechanism for neat magnesium borohydride to the mixture proposed here. Without access to the Yan paper, it was difficult to know what the paper described. The researchers’ admitted surprise that they observed a B5 species prior to a B2 species, leading them to believe there are other explanations and a more complex reaction scheme. It is unclear how the calculated NMR shifts compare with the observed chemical shifts. It is unclear if the NWU researchers have shared the  $^{11}\text{B}$  NMR data with Dr. Shore and asked his opinion on the product assignments. It could be very helpful to obtain the mass spectrum of the decomposition products. This would be a more certain lock on product identity, whereas the NMR can only provide an ambiguous result.

### Question 3: Collaboration and coordination with other institutions

This project was rated **3.1** for its collaboration and coordination.

- Excellent interaction was indicated between the theoretical members of this team. The addition of the NMR measurement and borane synthesis researchers was a definite improvement.

- This project features well-coordinated collaboration with the California Institute of Technology (Caltech), Ford, and OSU.
- The project appears to be very well coordinated. The number of partners and collaborators is appropriate compared to the amount of funding available.
- The additions of Caltech and OSU were good additions to this project since last year.
- The teaming with Dr. Hwang at Caltech for NMR is great. He is one of the best at collecting solid-state spectra. The teaming with Dr. Shore is also great. The researchers need to talk to Dr. Shore more about the chemistry and NMR data collected by Dr. Hwang. The team members deserve a rating of “outstanding,” but less than outstanding for getting the new subcontractors more involved in analysis and interpretation.
- The team is lauded for incorporating the SSNMR capability and was thus responsive to reviewers’ comments from the previous year. Collaboration between experimental efforts and the modeling effort could be tightened up with better mechanisms for feedback. Collaboration from outside of the project could help this team better approach some of the observations it is making in the  $\text{LiBH}_4$  and  $\text{Mg}(\text{BH}_4)_2$  systems.
- The internal collaboration of the team members is good, but no details were provided on the roles of the external collaborations or even about what the UCLA or Ford groups are doing. The focus is on the computational work at NWU. Working with Dr. Shore at Ohio State is good.

#### **Question 4: Relevance/potential impact on advancing progress toward DOE research, development, and demonstration (RD&D) goals**

This project was rated **2.1** for its relevance/potential impact.

- Most project aspects align with the DOE Hydrogen and Fuel Cells Program and DOE RD&D objectives. Like many other projects, the potential impact is high, but the likelihood of success is probably pretty low. In these cases (when no high-capacity reversible hydride is discovered), the value comes from the publications and other documentation that will allow others to build on this work.
- The work conducted in this project is of high quality and relevant to the Program. There is a strong focus on thermodynamically stable compounds. However, the kinetic properties for composites are equally relevant and important. Therefore, the composites investigated in this project may be those that are not useful for reversible hydrogen storage because the decomposed reaction product is a very thermodynamically stable compound.
- This project partially supported the Program by identifying some new candidate materials by computational methods, but not enough experimental work was performed to validate the models and assumptions.
- Understanding transport within these complex materials is an important aspect of this work and can indirectly lead to approaches that address certain current barriers to hydrogen storage in complex metal hydrides. The project’s impact would be improved if there were some experimental feedback of diffusion rate measurements into the modeling effort. The impact could also be improved by better integration of theory effort with the experimental effort.
- There is a serious disconnect between the kinetics of diffusion and the kinetics of bond breaking. The defect and diffusion calculations may be useful for some chemical transformation, but if the  $\text{B}_{20}$  does not decompose at  $200^\circ\text{C}$ , this is a strong indication that bond breaking and bond making are the rate-limiting steps. It is not trivial to calculate the kinetic barriers. First, one needs to know the key intermediates, and it is not apparent that this group is identifying the key intermediates unless it gets more involvement from Dr. Shore.
- Some potentially attractive candidate reactions have been theoretically predicted and their thermodynamics and defect properties were at least partially verified by testing or other analyses, but none exhibit the highly desirable reversibility behavior at moderate conditions. The work on the  $\text{LiBH}_4\text{-Mg}(\text{BH}_4)_2$  phases appears to show much of the same behavior found and published by other research groups over the past couple of years. It seems that none of the hydride phases or compositions evaluated will be acceptable for most hydrogen storage applications.
- The cost of 1 kg of material of interest is at least \$100,000–\$500,000 per kilogram—this makes these materials somewhat impractical. In addition, the regeneration cost would most likely be the same if not more than that for the starting material. There is no discussion of the issues with solid-state materials. Also, there is no consideration of the regeneration costs or issues.

### Question 5: Proposed future work

This project was rated **2.3** for its proposed future work.

- The further experimental studies of different catalysts appear to be very promising.
- The emphasis on completing the synthesis and characterization of  $B_{20}H_{16}$  should be a top priority.
- Plans build on past progress and generally address overcoming barriers. Synthesis and characterization of a pure phase of  $B_{20}H_{16}$  should be completed before the project ends next year. Hopefully, the synthesis will be completed in time to allow for sufficient characterization. The computational efforts to find low-lying eutectics look interesting.
- NMR is a good start, but mass spectroscopy would provide more detail about the complexity of the products. High-resolution EI, CI, or Maldi approaches should be investigated. NWU must have some very good mass spectroscopy facilities and expertise. It is unclear if there is a good reason that the team does not start with a mixture of  $Li_2B_{12}H_{12}$  and  $MgH_2$  and pressurize with hydrogen to learn if the reaction is indeed reversible. The same can be suggested for the  $B_{20}H_{16}$  if the products are boron and hydrogen. The team should do the reverse reaction first. All of these reagents are readily available and do not require complex synthetic reaction schemes.
- Future experimental work includes three materials:  $B_{20}H_{16}$ , the LiBMgH system, and  $LiBH_4$ /carbon. This appears to be a considerable dilution of effort on the experimental side. Perhaps the team should focus on two of the three. Alternatively, the team should plan on a cursory examination of  $B_{20}H_{16}$  because it does not sound like the project is going to get its hands on a lot of this material. If hydrogen release is slow or yields a significant number of BH end products, then perhaps the team should look at where the modeling went awry, but then focus on the two remaining systems. The team should fail fast and move on to more promising systems.
- Because this project will end within a few months without a no-cost extension or new funding, it is unlikely that all of the planned tasks shown on slide 26 can be performed, let alone completed. However, continuing the theoretical modeling of the behavior of the  $B_{20}H_{16}$  along with its synthesis and properties assessment seems worthwhile. In a short period, researchers can also probably look into the reversibility of the LiBMgH system, including hydrides within carbon composites via NMR, and model the diffusion parameters of eutectic phases of borohydrides for which there are recent results in the literature. The researchers need to focus on chemical mechanisms and on cost. This is not in their plans.

#### Project strengths:

- This project's strength is its computational expertise.
- This project features excellent synergy between theory and experiments. The project is well focused on the most promising reactions. There are well-coordinated collaborations.
- The PI has good computational skills and a reasonable knowledge of hydrogen storage phenomena. Adding NMR and material synthesis at the request of last year's review was favorable.
- This project features a strong team with background in materials, boron chemistry, theory, and SSNMR. This strength could be improved by adding an experienced complex metal hydrides experimentalist.
- The two theoretical groups at NWU and UCLA have developed very insightful and effective computation procedures for performing the prediction and modeling of potential storage materials. The involvement of qualified researchers for preparation of novel borane compounds (OSU) and solid-state NMR measurements (Caltech) to this project added increased capability to the experimental scope.
- This project has no strengths—the material is irrelevant in terms of cost and the researchers are not pursuing the important issues.

#### Project weaknesses:

- The synthesis of  $B_{20}H_{16}$  seems slow.
- This project suffered from a lack of adequate experimental activities.
- This project involves a good experimentalist, but it is not apparent that the experimentalist and the team are having critical conversations.

- This project features a lack of strength in complex metal hydrides experiments. Researchers could improve the project by reconciling project results with other existing research results in a convincing manner.
- Most hydrogen desorption behavior observed in this project during the experimental studies was for materials with limited or no reversibility. These are unlikely candidates for nearly all applications. Unfortunately, connecting first-principles calculations of defect formation and migration barriers often involves convoluted routes to establish reaction pathways and kinetics because numerous other more likely rate-determining processes are neglected. It appears that Ford played a much smaller role in this project during the past year than previously.
- The computational work should focus on the release kinetics, not on hydrogen transport in an idealized material. They also need to focus on materials that have practical costs.
- The utilization of catalysts/additives clearly has a positive effect, but it is not yet clear whether this effect is purely kinetic or whether it involves a change in mechanism. Simulations have suggested a range of meta stable magnesium borohydrides. It would be desirable to have more experimental data that could support the existence of some of these boranes, although that is extremely challenging. The team should also consider utilizing Raman spectroscopy for identification of the higher borane samples produced.

### Recommendations for additions/deletions to project scope:

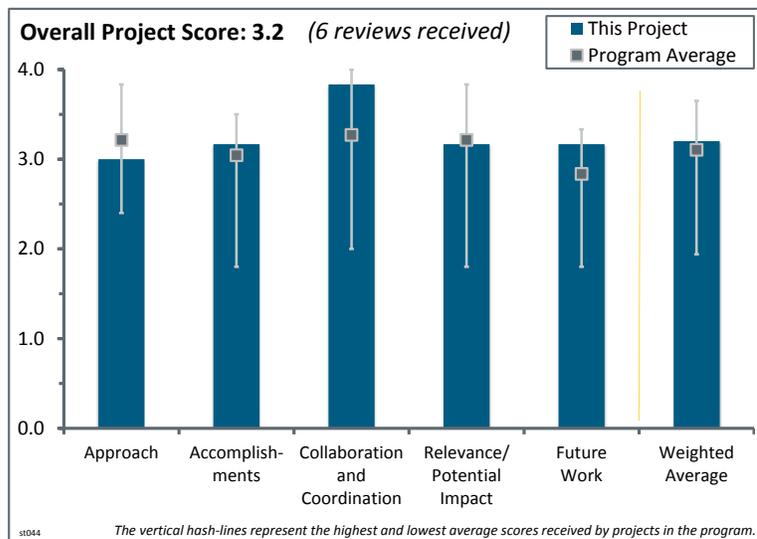
- The team should focus on  $B_{20}H_{16}$  synthesis and characterization. This project should not be continued past the current budget period.
- Because this project is scheduled to finish by the end of fiscal year 2013, there are only a couple of suggestions regarding its future scope. It would be valuable if  $B_{20}H_{16}$  could be successfully synthesized and if characterizations of its hydrogen desorption behavior along with NMR studies of the product phases could be completed within the scope of the project and reported to the hydrogen/fuel cell communities.
- The community seems to be in some agreement on the stability of the  $B_{12}H_{12}$  anion and its role not as an intermediate but as a terminal borohydride sink in complex metal hydride systems. Perhaps the researchers should conduct modeling work on this to discover if there exist potential pathways out of this thermodynamic well or develop suggestions as to how to avoid this sink. This would seem to be a valuable contribution this team could make. Perhaps a challenge to this team is to come up with new methods to measure species diffusion rates through the materials that do not require national user facilities to accomplish the work. This might not be achievable, but it is worth brainstorming.

## Project # ST-044: SRNL Technical Work Scope for the Hydrogen Storage Engineering Center of Excellence: Design and Testing of Adsorbent Storage Systems

David Tamburello; Savannah River National Laboratory

### Brief Summary of Project:

The objectives of this project are to: (1) develop and apply an adsorbent acceptability envelope, (2) conduct component adsorbent experiments, (3) design components and experimental test fixtures to evaluate the innovative storage devices and subsystem design concepts, (4) validate model predictions, and (5) improve both component design and predictive capability. Savannah River National Laboratory (SRNL), in cooperation with its research partners, is evaluating solid-state hydrogen storage systems for vehicle application. Storage device design has been investigated through modeling and experimental development.



### Question 1: Approach to performing the work

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

- Understanding how heat and gas flow through beds/pellets of storage material is and should be the key driver behind the entire Hydrogen Storage Engineering Center of Excellence (HSECoE, the Center)—it was the whole reason for advocating for the creation of the Center. Knowledge gained from this project will undoubtedly lead to improved material level targets and alignment with research needs/resources.
- For the review period, the “Specific, Measurable, Achievable, Relevant, and Timely” (SMART) milestones include analyses to demonstrate sorbent and system capabilities exceeding the HSECoE system targets of 4.1 wt.% and 20 g/L. These targets are lower than the 4.1–4.4 wt.% and 24–25 g/L gravimetric and volumetric capacities of commercially available 700-bar compressed hydrogen systems.
- The approach used by SRNL involved heat simulations.
- This approach is generally effective but could be improved; it contributes to overcoming some barriers. It is unclear what the difference is between a SMART milestone and a Transport Phenomena Technology milestone. It seems the former all involve reports of some type, but it is unclear how more reports are going to solve the key problems of volumetric density and loss of useable hydrogen. This seems like an easy way to meet all of the milestones without having any skin in the game. Milestones should be quantifiable and relevant. A “report on the ability to develop and demonstrate a 3 minute refueling ...” is essentially useless. Milestones are needed that state “Demonstrate a 3 minute refueling....”
- A well-developed and sensible approach has been adopted for modeling, designing, and testing engineering prototypes for adsorbent systems. The approach that was employed to rapidly down-select four system options from a huge number of possible system combinations is especially impressive. It would have been helpful to include an explicit statement of outstanding obstacles and challenges that must be addressed in the remainder of the project. Without that information, it is difficult to fully assess whether the approach focuses clearly on the critical remaining problems.
- The adsorbent acceptability envelope, combined with other models, clearly defines the properties needed for successful materials and systems. The Center’s approach of using “idealized” materials to guide materials discovery clearly shows the difficulties in materials design and synthesis. There is no apparent

analysis of the impact of the technologies on forecourt configuration and costs. This is likely to lead to suboptimal solutions.

### Question 2: Accomplishments and progress toward overall project and U.S. Department of Energy (DOE) goals

This project was rated **3.2** for its accomplishments and progress.

- The team has made tremendous progress in the last year. It feels like the effort and coordination of the previous years is bearing results and providing direction to the team. The team is beginning to learn the important trade-offs in heat and gas flow management associated with different material packing configurations.
- This project has achieved a significant improvement in cost (HexCell).
- Defining required properties for sorbents is a good development.
- Excellent progress has been made in 2012–2013 on developing an “acceptability envelope” for integrating material properties and system design. This will be critical for formulating an optimized solution for an adsorbent storage system. Good progress has also been made on developing solutions for effective flow-through cooling and heat exchange. Likewise, a comprehensive parametric analysis of a huge array of possible system options resulted in the identification of four adsorbent system designs optimized for heat transport and efficient hydrogen delivery. It would have been helpful to include some specific details concerning the sensitivity of overall system performance on variations in bed uniformity.
- Four systems have been evaluated; the updated spider charts show expected improvement in cost but little other improvement (for HexCell and modular adsorption tank insert [MATI]). The team has made significant progress toward meeting some of the barriers; however, a few key barriers remain (loss of useable hydrogen, and volumetric and gravimetric capacity). The team has also achieved accomplishments on idealized materials, including predicting an idealized material based on metal-organic framework-5 (MOF-5) using the desired system properties. Flow-through cooling with liquid nitrogen shows clear benefits, and tests at the Jet Propulsion Laboratory confirm improvement with liquid nitrogen, although not as much as predicted. It is unclear what the cost penalties are associated with liquid nitrogen cooling and how this impacts infrastructure at the forecourt.
- The SRNL/University of Quebec Trois Rivieres (UQTR) team has developed adsorbent acceptability envelopes for MOF-5-like materials assuming an 80 K storage temperature. For the next round of material discovery, attention must be paid to meeting the targets for not only system weight and volume but also energy efficiency (80 K is likely not acceptable) and cost. The decision to go with an all-metal, Type-1 aluminum tank should be revisited. Slide 17 shows that the metal tank in the four design options weighs between 80 and 110 kg and accounts for 53%–59% of the system weight. It is unclear how this design can lead to a go decision for Phase III. It is also unclear if this thermal mass can be cooled from 180 to 80 K in 3 minutes and what the penalty is in system efficiency due to this amount of cryogenic cooling.

### Question 3: Collaboration and coordination with other institutions

This project was rated **3.8** for its collaboration and coordination.

- The collaboration is very convincing.
- This project is clearly well coordinated with activities at other institutions in the Center.
- The principal investigator (PI) is part of the HSECoE—this is the best collaboration in the U.S. Department of Energy (DOE) Hydrogen and Fuel Cells Program. Other DOE programs should emulate this model.
- The presentation lists close-knit collaborations with other members of the HSECoE. No interactions were mentioned with people and organizations outside of the Center.
- The Center has assembled a strong team with good collaboration between original equipment manufacturers, national laboratories, and the Center. It is unclear whether material target properties are being communicated to material developers.
- A hallmark of the HSECoE is the positive impact that inter- and intra-organization collaborations have made on the overall success of the Center’s activities. This project is no exception. Fruitful and technically

important collaborations have been established with multiple partners in the Center and with external organizations. These collaborations have served to significantly leverage the SRNL activity.

#### Question 4: Relevance/potential impact on advancing progress toward DOE research, development, and demonstration (RD&D) goals

This project was rated **3.2** for its relevance/potential impact.

- This project fits perfectly into the Hydrogen and Fuel Cells Program (the Program). It is relevant and necessary.
- This project is a critical component of the overall HSECoE effort. The project incorporates innovative design concepts and system integration approaches for a storage system based on high-surface-area adsorbents. It addresses the principal DOE goals and targets and is directly relevant to DOE RD&D objectives.
- There is excellent trade-off analysis between the MATI and Hexcel designs—these systems will likely have different applications for different materials. The project team should keep refining work on both systems and highlight the advantages and disadvantages of each.
- For Phase II, this project is developing an adsorbent acceptability envelope, conducting adsorbent experiments, and designing components and test fixtures.
- Because none of the materials being studied by the Center appear to be viable, its relevance is certainly limited. Knowledge gained may or may not be applicable to viable materials.
- The project is focused on the Program’s goals and objectives delineated in the *Fuel Cell Technologies Office Multi-Year Research, Development, and Demonstration Plan*, but it is not clear how much advancement will be made. The loss of usable hydrogen and volumetric capacity remain far from targets and should be addressed. The value of systems engineering seems to have run its course and it is clear the remaining barriers cannot be addressed by optimizing the system. Engineering efforts should be coordinated with materials research efforts and should be limited to small prototypes until new materials are identified that may meet the volumetric/gravimetric and hydrogen loss targets.

#### Question 5: Proposed future work

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

- The project team should carry on with its work.
- The proposed future work should be done as planned.
- The future work builds directly on the current efforts, especially in the areas of thermal transport/cooling and experimental validation of system models. Unlike the situation with a more complex chemical hydrogen system, the integration, scale-up, and testing of a practical system based on a cryo-adsorption medium seems far more straightforward. The pathway and plans for prototype development in Phase III follow directly from the Phase II effort and seem appropriate and reasonable.
- The future work may need clearer definition; for example, “additional model development (as required)” needs to be more specific.
- The PI clearly laid out the future work in support of the Phase III prototype design. Because of the complex interactions and relationships with other teams, it is difficult to judge the contributions of the SRNL/UQTR team.
- Plans may lead to improvements, but they need to be better focused on overcoming barriers. Future work includes “Increase Material Capacity to 140% and ultimately 200% of Powdered MOF-5”—it is not at all clear how this will be accomplished.

#### Project strengths:

- This project has strong collaboration with UQTR and other members of the Center.
- The project has made good progress toward reducing system cost for both Hexcel and MATI.
- This project features a strong industry/laboratory/university team.

- The project is being conducted by a well-qualified team with background and expertise in all areas relevant to the development of a successful prototype system for a cryo-adsorbent storage system. The technical approach is solid and plans for future work build directly on the excellent progress that has been made in the Phase II effort. The technical effort by the SRNL team is augmented by useful collaborations with Center partners and external organizations.

### **Project weaknesses:**

- It is not clear if the best decisions have been made about flow-through cooling, 80 K storage temperature, Type-I tanks, interim weight and volume targets, etc. The net result is that the adsorption system does not look very viable.
- The project is far from meeting key barriers to the loss of usable hydrogen, volumetric density, and gravimetric density. It is unclear from the future work how these barriers will be addressed.
- There is no consideration of forecourt costs and implications. Optimization of an onboard system without considering the impacts on hydrogen costs and overall greenhouse gas issues may result in sub-optimal solutions.
- It is highly unlikely that a system based on MOF-5 will meet the DOE targets for hydrogen storage. However, the development of a prototype system based on the best available surrogate material(s) (e.g., MOF-5) will hopefully provide information that will translate directly to an optimized system based on a storage medium with improved properties.

### **Recommendations for additions/deletions to project scope:**

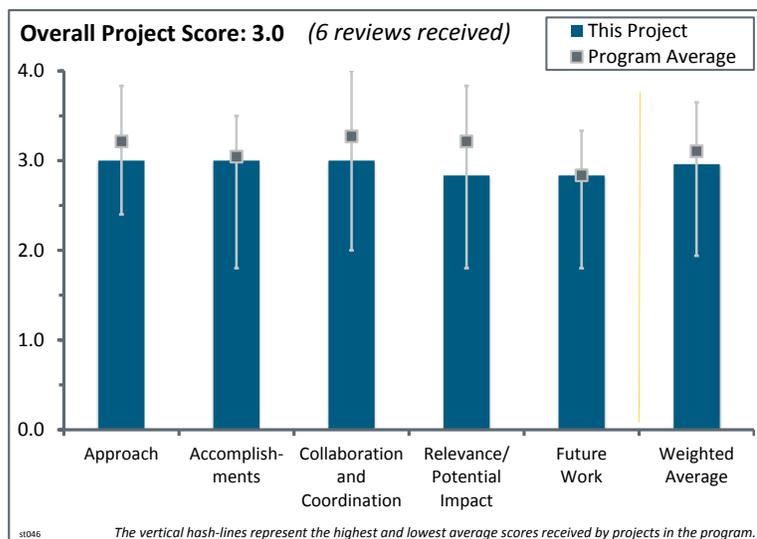
- Validation of the models is planned and is required. System scale-up and future system predictions are planned and are also required.
- It may be too late to add or subtract tasks. DOE needs to make sure that the data and methods are properly documented and available to organizations outside of the HSECoE.
- System optimization is unlikely to change issues associated with hydrogen loss and volumetric/gravimetric densities. Only MOF-5 is currently being considered—this is understandable because the project is focused on engineering a system—however, more materials research is needed to address key barriers.
- A more explicit and detailed statement of the remaining risks and challenges should be provided. Without that information, it is difficult to assess whether the technical effort is focused on the critical problems that really need to be solved.

## Project # ST-046: Microscale Enhancement of Heat and Mass Transfer for Hydrogen Energy Storage

Kevin Drost; Oregon State University

### Brief Summary of Project:

The objectives of this project are to use the enhanced heat and mass transfer available from arrayed microchannel processing technology to: (1) reduce the size and weight of storage, (2) improve the charging and discharging rate of storage, and (3) reduce the size and weight and increase the performance of thermal balance of plant (BOP) components. Arrayed microchannel processing technology has the potential to reduce storage system size and weight; offer a high degree of control over the process; maintain the optimum performance attained in a single cell; add complexity without increasing cost; allow rapid start-up and response to transients; and provide attractive high-volume, low-cost manufacturing options.



### Question 1: Approach to performing the work

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

- The Oregon State University (OSU) project addresses system volume and weight, hydrogen charging/discharging, and BOP. The work is tightly focused on microchannel-based concepts for managing hydrogen storage and thermal energy balancing. Modeling and bench-scale research are effectively carried out to provide a sound basis for evaluating the engineering and economic tenability of a microreactor-based approach to onboard hydrogen storage. The overall approach still needs engineering-scale vetting before a convincing argument can be made for raising this concept to the top of the list of candidates.
- The microchannel processing technology approach that has been adopted in this project is unique and innovative. It specifically addresses systems in which diffusion-limited processes inhibit thermal transport. The approach provides a potentially novel and elegant solution to improving charging/discharging rates and reducing the weight and cost of critical BOP components required for the prototype storage subsystem. The approach comprises a good combination of modeling/simulation and experimental validation. The use of microchannel assemblies for thermal transport together with modular adsorption tank inserts (MATI) is especially interesting because it can be used to enhance media conductivity and to facilitate use of a wider range of cooling options.
- OSU is a partner in the Hydrogen Storage Engineering Center of Excellence (HSECoE, the Center). The primary objective of the HSECoE is to address critical engineering issues that impede the development of materials-based hydrogen storage systems from meeting the U.S. Department of Energy (DOE) targets for fuel-cell-powered passenger vehicles. The role of OSU is to employ microchannel technology (MT) that enhances heat and mass transfer within components to reduce the weight, volume, and cost of the storage systems. This project does not directly influence the selection of composition of the storage materials themselves. The present focus is on adsorption hydrogen storage.
- The project's approach features MATI. Both experimental validation of model pellets and compaction have been completed.
- The project uses both simulation and experimental investigations to identify, prioritize, and evaluate the best novel microchannel designs for onboard applications. Test results are then used to validate the predictive tools.

- The project would be improved by having a well-defined baseline for conventional heat exchanger technology.

### Question 2: Accomplishments and progress toward overall project and U.S. Department of Energy (DOE) goals

This project was rated **3.0** for its accomplishments and progress.

- Good progress was made on this project in 2012–2013, especially in the fabrication and testing of the single- and multi-module MATI assemblies and the initial work on thermal conductivity enhancement in densified metal-organic framework-5 (MOF-5) cryo-adsorbents. The “needle insert tests” provide a useful methodology for improving thermal conduction in densified MOF-5 (“hockey puck”) samples. However, the final engineering embodiment of this approach is unclear. The design and testing of the 1 kW microchannel combustor for hydrogen heating during cold-start simulations and experimental results validated the concept and provided a straightforward pathway to further development and improvement of the thermal transport subsystem in the next phase of the project.
- The OSU presentation reported modeling and experimental results in a host of areas related to the microchannel reactor concept. Most of the critical issues are being addressed in a clearly thought-out and well-orchestrated manner for both the MATI and the microchannel combustor/recuperator. Qualification of aluminum as a suitable material for microlamination led to a significant cost reduction. Good agreement was achieved between modeling results and experimental measurements during Phase II adsorption bed tests.
- Work is in progress to revise the MATI design to accommodate a multi-modular stack for adsorption bed testing. Simulation of hydrogen charge/discharge cycles indicates that additional heat conduction is needed to meet the DOE target for hydrogen refueling rate. The principal investigator (PI) has proposed inserting solid pins in the MOF-5 bed to promote conduction enhancement. The project has tested a 1 kW microchannel combustor/heat exchanger for hydrogen heating during cold starts. Results meet the “Specific, Measurable, Achievable, Relevant, and Timely” (SMART) goals for 85% efficiency, 0.9 kg in mass, and 0.6 L in volume. Aluminum-6061 has been qualified for use as a construction material for both the MATI and the combustor/heat exchanger.
- During their Phase II efforts within the HSECoE, OSU researchers have been working on two applications for their MT capabilities: (1) MATI and (2) microchannel combustor-recuperator for hydrogen conditioning (MCRHC). The MATI could facilitate heat transfers within the tank using compacted adsorbents while the MCRHC could burn portions of hydrogen released at temperatures circa 200 K or lower to supply the fuel cell power system with hydrogen gas heated above minimal operating temperatures. OSU has designed, analyzed, and built simplified prototype configurations of the MATI and MCRHC. Feasibility testing of a simple prototype of the MATI has started. Cost projections for mass manufacturing of these devices were made, although there is still a need for refinements in designs and manufacturing. Specific configurations for Phase III development and testing have not yet been completed.
- The amount of work done does not seem to justify the \$2 million DOE spent on this project when compared with other projects with similar funding. Although the system can deliver 0.41 g/s, it is not obvious that this meets the target requirement (0.02 g/s/kW). This would supply a 20 kW fuel cell, but that is much smaller than a typical automotive fuel cell.

### Question 3: Collaboration and coordination with other institutions

This project was rated **3.0** for its collaboration and coordination.

- OSU is a member of the HSECoE and it has strong collaborations with other members of the Center.
- OSU has interacted with several of the HSECoE partners to determine what roles are best suited for the MT. These interactions led to design refinements of the MATI and MCRHC components. With input from Pacific Northwest National Laboratory and others, OSU has provided predicted manufacturing costs and configurations for adsorption storage systems.
- Strong collaborations with other technologists in the Transport Phenomena and Enabling Technologies groups in the HSECoE are reinforcing and augmenting the work in the OSU project. Several collaborators

are providing useful input to the MATI heat exchanger and enhanced puck conductivity efforts. The microchannel combustor work is being conducted in close cooperation with Savannah River National Laboratory and the Jet Propulsion Laboratory. These collaborations are ensuring that the OSU work remains closely connected to the overall HSECoE mission and provides important industrial and government laboratory perspectives to the university-led activity. Closer collaboration with the General Motors thermal management activity is recommended.

- Collaboration and coordination of research and development (R&D) activities at OSU with other HSECoE partners is reported to be appropriate and well established. Slide 30 contains a reasonably detailed summary of OSU's connections with several of the other Center partners, but this connectivity is not obvious in the results slides. It seems that OSU plans and conducts its own research, then reports to the other partners. It would be useful to clarify how the collaborations listed on slide 30 actually work. This is important because the devices being developed by OSU need to fit seamlessly into the overall system architecture evolving within the HSECoE.
- Strong interaction with some HSECoE system groups has been discussed. An even stronger interaction with the Adsorbent System group is suggested as optimization of compaction and system should go hand in hand.
- Collaboration is limited to the HSECoE.

#### **Question 4: Relevance/potential impact on advancing progress toward DOE research, development, and demonstration (RD&D) goals**

This project was rated **2.8** for its relevance/potential impact.

- This project is focused on applying MT for heat and mass transfer enhancement to reduce onboard system weight and volume and to improve hydrogen charge and discharge rates.
- The MATI and MCRHC can potentially reduce the mass and volume of adsorption storage systems while enhancing thermal performance. The unresolved issues include the added costs of these components and their durability during extended operation. The issues of fabrication of the internal structures using aluminum materials and the assembly of the MATI within light-weighted storage vessels have been incompletely addressed.
- The OSU message regarding relevance is that microchannel approaches can solve most (if not all) of the nagging barriers confronting onboard hydrogen storage, hydrogen delivery (to the fuel cell), recharging, and thermal energy management for fuel-cell-powered vehicles. OSU's modeling results support this message. What is currently needed is an appropriately scaled demonstration with a convincing outcome.
- This project employs microchannel processing technology to enhance thermal transport rates in specially configured (MATI) cryo-adsorbent media assemblies and to increase the performance of thermal BOP components for improved cold-start applications. This project addresses two important problems in cryo-adsorbent prototype storage system development. It supports the mission of the HSECoE and it is directly relevant to the DOE RD&D objectives.
- Without baselines for conventional heat exchanger designs, it is impossible to rate the relevance of this project.

#### **Question 5: Proposed future work**

This project was rated **2.8** for its proposed future work.

- OSU's plans for the coming year seem to be right on target. These plans are not extensive, but they are the next logical steps to take toward a definitive demonstration of the microchannel approach. Issues with respect to refueling time and heat transfer in the bed remain to be resolved.
- The proposed future work is a continuation of the work in progress and an improvement of the MOF-5 hockey puck to meet the hydrogen charging rate.
- The proposed future work is a direct extension of the current effort. The future plans for assembly and testing of the multi-cell microchannel/MATI assembly are straightforward. However, the plans are unclear for enhancing the conductivity in a MOF-5 puck beyond the levels measured in the current work. It would have been helpful if more detail had been provided. Likewise, remaining obstacles, challenges, and

potential problems have not been presented. It is difficult to adequately review the future plans without knowledge of the specific problems that must be addressed.

- During Phase III, fabrication issues and laboratory testing of the prototypes for both devices should be the researchers' major emphasis in order to verify their simulations of thermal performance. They also need to address issues and problems during component building and operating conditions. Based on the extent of testing performed at OSU during the past four years, it is not clear that sufficient assessments of thermal performance will be completed on new prototype devices during the duration of the project. For example, OSU has not yet built or tested devices that scale from a single unit of a compacted adsorbent to more highly integrated versions during Phase II.

### **Project strengths:**

- This project team features sound knowledge and capability in microchannel devices.
- The PI has a long history of research in MT. The project is well focused on meeting the technical objectives and targets defined by DOE and the HSECoE.
- The OSU project is directed by a bona fide expert in the field of microchannel device development. The research addresses a wide range of issues cleverly and effectively.
- OSU has experience with developing and fabricating MT devices for various purposes that suggest these assemblies can be suitable for those hydrogen storage components requiring improved heat and mass transport.
- This is an innovative project that is being conducted by a well-qualified R&D team. Good collaborations with other HSECoE groups are ensuring that the project remains focused on important goals for subsystem development.

### **Project weaknesses:**

- There is a lack of a clear baseline for comparison with other technologies.
- The current MATI design will not meet the target charging rate because of limited thermal conduction.
- Stronger interaction with the materials groups would be desirable. Optimization of the MT should go hand-in-hand with materials optimization.
- There is much that still needs to be verified in regard to the microchannel-based approaches under study at OSU. These include the robustness of the beds, gas distribution within the beds, and the final story on manufacturability at an acceptable price. Also, it is hard to accept the notion that flow path plugging will not be a problem at some level.
- A detailed statement is needed concerning specific technical obstacles, challenges, and risks. More detailed plans for enhancement of MOF-5 thermal conductivity that are consistent with a prototype engineering system should be provided.
- It is not apparent whether the as-conceived MATI and MCRHC will operate reliably under the pressure and temperature conditions that will be necessary for long-life components in hydrogen storage systems. In particular, leaks between the different fluids could lead to very serious problems. It is one thing for models to predict high-performance behavior under idealized scenarios in contrast to fabrication and assembly of the suitable components for testing.

### **Recommendations for additions/deletions to project scope:**

- The proposed future work seems to be the best path forward for OSU. The experimental system tests planned for the coming year need to demonstrate sustainable/robust microchannel device performance.
- OSU should continue to verify its conceptual designs for the MATI and MCRHC devices via experiments. In particular, demonstrations should show complete and reliable separations (i.e., no internal or external leaks of heat exchange fluids) during operation. Because heat transfer and gas permeation with their compacted carbon samples appear to be issues, proposed improvements should be evaluated via laboratory testing.
- Permeability and thermal conductivity are key issues in the optimization of such a design. The influence of compression on the achievable permeability and storage densities could be easily measured by having

collaboration in the area of in situ neutron imaging. For example, using a single compact that was compacted inhomogeneously, materials properties could be optimized easily.

- Because it is unlikely that MOF-5 will meet the overall DOE storage targets, it will be important to understand the extent to which the concepts and test assemblies developed here can be extended to other (hopefully improved) cryo-adsorption media.

## Project # ST-047: Development of Improved Composite Pressure Vessels for Hydrogen Storage

Norman Newhouse; Hexagon Lincoln

### Brief Summary of Project:

The objectives of this project are to: (1) identify appropriate materials and design approaches for the composite container; (2) maintain durability, operability, and safety characteristics; and (3) develop high-pressure tanks for hydrogen storage. The project will also identify pressure vessel characteristics and opportunities for performance improvement. High-pressure tanks should contain appropriate materials and operate safely and effectively at defined pressures and temperatures.

### Question 1: Approach to performing the work

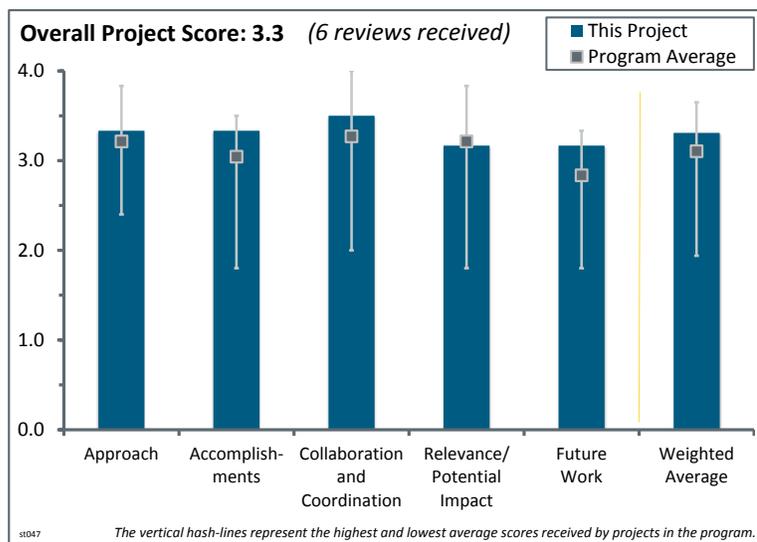
This project was rated **3.3** for its approach.

- Barriers are directly addressed in this project.
- The project employs a systematic approach to addressing the design and cost aspects of storage development.
- The approach is well thought out and consistent with the objectives of the Hydrogen Storage Engineering Center of Excellence (HSECoE, the Center). The switch from Type 4 to Type 1 tanks reflects the revised pathway for Phase 3 being adopted by the HSECoE.
- Hexagon Lincoln (HL) is sharply focused on crucial aspects of onboard hydrogen storage issues. The barriers addressed and the stipulated targets with respect to system weight, volume, and cost are the areas where gaps are the largest and most uncertain. Clearly, pressurized gas is at the top of the hydrogen storage method-of-choice list for good reasons. It is less complex (e.g., fewer components), less costly, and has less built-in uncertainty than the storage-materials-based approaches. The level of feasibility appears to be very high. HL is at center stage in the tank development part of the HSECoE.
- HL is a partner in the HSECoE. The primary objective of the HSECoE is to address critical engineering issues that impede the development of materials-based hydrogen storage systems from meeting the U.S. Department of Energy (DOE) targets for fuel-cell-powered passenger vehicles. The identified role of HL is to develop lighter weight and less expensive containment vessels that can meet the pressure and temperature requirements for these storage systems. This project does not directly influence the selection of the composition of the storage materials themselves. The focus of HL during Phase II was on the cryogenic properties of composite tanks being considered for adsorption hydrogen storage.
- It should be clearly mentioned that this project is dealing with pressure vessels for cryo-absorbent systems only. Test procedures should be described. For a better understanding, the correlation between a specific barrier, the approach, and the result should be described.

### Question 2: Accomplishments and progress toward overall project and U.S. Department of Energy (DOE) goals

This project was rated **3.3** for its accomplishments and progress.

- There has been good progress with the tests and the approved design approaches.



- Vessels have been designed, manufactured, and successfully tested. Selected vessel types will be available to other HSECoE partners for subsidiary component testing during Phase 3. Performance improvements in regards to weight, available volume, and cost have been realized through HL's achievements. Problems with the liner and boss junctions persist, but HL has plans to address these matters.
- Cryo-testing of subscale Type 4 tanks showed that the liner leaked at >3,300 psi. Cracks initiated at the boss/liner interface where stress level was high and there was a mismatch in the coefficient of thermal expansion between boss and liner materials. The Type 1 subscale tank was fabricated and tested at ambient temperature and at 80 K. The tank was cycled 200 times to service pressure at 80 K. It is necessary to cycle the tank to 5,500 cycles to be in compliance with SAE J2579. Hydrostatic pressure burst tests should be conducted at 3.5 times service pressure for Type 1 welded containers (FMVSS 304). There was no data presented on carbon fiber (CF) composite properties for the Type 4 tanks. It would be very useful to DOE if HL reports its findings on the translation efficiency, composite tensile strength, and modulus.
- For the development of adsorption hydrogen storage tanks, HL evaluated the cryogenic behavior of both Type 4 cylinders (i.e., CF wrapped with polymeric liners) and Type 1 (aluminum metal). The impact of extreme operating temperatures on these cylinders at cryogenic conditions was demonstrated from low-temperature leak, cycling, and burst tests. HL showed that no current polymeric liner material is suitable for Type 4 tanks that are to be operated at cryogenic conditions, although aluminum-based Type I tanks are adequate and sufficiently robust when pressures do not exceed about 100 bar. So far, there has been minimal consideration by HL of how the interior of these cylinders are loaded with sorbent material and enhanced heat transfer internal structures.
- Challenges arose with Type 4 designs at very low temperatures and it is not yet clear if these can be overcome for some applications. The Type 1 design shows promise with simpler media loading aspects. The weight penalty associated with the Type 1 design could be acceptable for some systems.

### Question 3: Collaboration and coordination with other institutions

This project was rated **3.5** for its collaboration and coordination.

- The partners represent a broad pool of top talent.
- It seems that all relevant partners for cooperation are involved.
- HL maintains good collaboration and interaction with HSECoE partners.
- The project has adapted to the changing parameters arising from the work of the well-coordinated collaborators.
- HL interacted with several HSECoE partners on the cryogenic properties of Type 1 and Type 4 vessels during Phase 2. A separable Type 1 aluminum metal vessel was developed to permit Phase 3 tests on a metal-organic-framework-5 (MOF-5)-based adsorption prototype, which can include internal structures for thermal management.
- HL's tank work is important to the entire HSECoE. Collaboration within the HSECoE on tank issues seems to be close and effective, as indicated on slide 17. A patent application with Pacific Northwest National Laboratory is in progress for the external vacuum insulating vessel concept. Vessel criteria are reached by consensus within the HSECoE.

### Question 4: Relevance/potential impact on advancing progress toward DOE research, development, and demonstration (RD&D) goals

This project was rated **3.2** for its relevance/potential impact.

- Cryo-storage will deliver a significant improvement in capacity.
- The project is addressing an important element for several developing onboard hydrogen storage technologies.
- Pressure vessel development is at the top of the relevancy list for the HSECoE. Everything HL is doing and will do in Phase 3 is as relevant as it gets because it looks like pressurized hydrogen gas will be the top choice for full system validation.
- This project is dealing with the vessel for an adsorbent system. The first step is to develop the adsorbent material itself, so this project is assessed only as "good."

- Characterization of the limitations of using Type 4 vessels for hydrogen storage at elevated pressures and cryogenic temperature is important information to share with the fuel cell community. While HL has not identified a solution to the issues of using polymeric liners in cryogenic vessels, it has shown the need for discovery of materials to meet these conditions.
- HL develops both Type 1 and Type 4 vessels in support of sorbent storage options selected by the HSECoE. The work on Type 4 vessels is relevant to meeting DOE's 2017 targets for system weight and volume. However, systems using Type 1 vessels will have no chance of meeting the DOE weight target.

### Question 5: Proposed future work

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

- The proposed work is straightforward.
- The project has identified multiple paths forward as contingencies for storage development.
- Three types of tanks are at various stages of design/manufacturing/testing. The Type 1 tank already looks pretty interesting. Things can only get better. Specific performance improvement needs have been identified and will continue to be addressed in Phase 3.
- The future plans shown on slide 18 would be useful for the Phase 3 activities of the HSECoE partners involved with adsorption storage. Namely, continuing work would be on identifying and characterizing materials for operation at cryogenic temperatures along with assessing the consequences of cycling. Development of designs that facilitate the filling and sealing cylinders with sorbent materials is also important. The large mass of the sealing region for the Type 1 Phase 3 tank is an issue that should be examined closely to see if other configurations with reduced mass can be designed.
- The characterization of fatigue in Type 1 tanks needs to be addressed as part of pressure cycling at cryogenic temperatures. Switching to Type 1 tanks has increased the system weight significantly, making it practically impossible to meet the DOE gravimetric capacity target. Further development of Type 4 tanks at 80 K should only be continued after successful qualification of the materials (e.g., tensile impacts) at service temperatures.
- There are a lot of tasks planned for future work. There are tests planned with different vessel types (Type 1, Type 3 and Type 4). It is difficult to understand the strategic approach behind these tasks.

### Project strengths:

- The testing involves actual hardware.
- A vessel manufacturer that has a lot of experience with regard to vessel behavior is doing this project.
- HL has substantial experience in developing and manufacturing high-pressure tanks for onboard hydrogen storage.
- The project brings deep experience in storage design to the development of tanks for challenging operational characteristics.
- HL is a commercial vendor of high-pressure gas cylinders for a range of applications. This background has been helpful during the HSECoE assessments of costing and manufacturing issues for hydrogen storage vessels along with clarifying safety requirements and procedures.
- The project's strengths include a knowledgeable principal investigator, very good connectivity and consensus building within the HSECoE regarding tank issues, and a high probability that further performance improvements will be forthcoming during Phase 3.

### Project weaknesses:

- Hopefully HL has enough resources left to take tank performance parameters to yet another level during Phase 3.
- The requirements for the tests are not clear (e.g., references to SAE, ISO, etc.). The test descriptions should be attached in the backup.
- HL does not appear to consider possible contaminations issues due to outgassing or decomposition of the storage materials, or how tanks need to be constructed and loaded with these sorbents. There seems to have been very limited publication on the work performed during Phases 1 and 2 of this project. Dissemination

of the cryogenic properties and limitations of Type 4 vessels would be valuable to the entire hydrogen energy community.

#### **Recommendations for additions/deletions to project scope:**

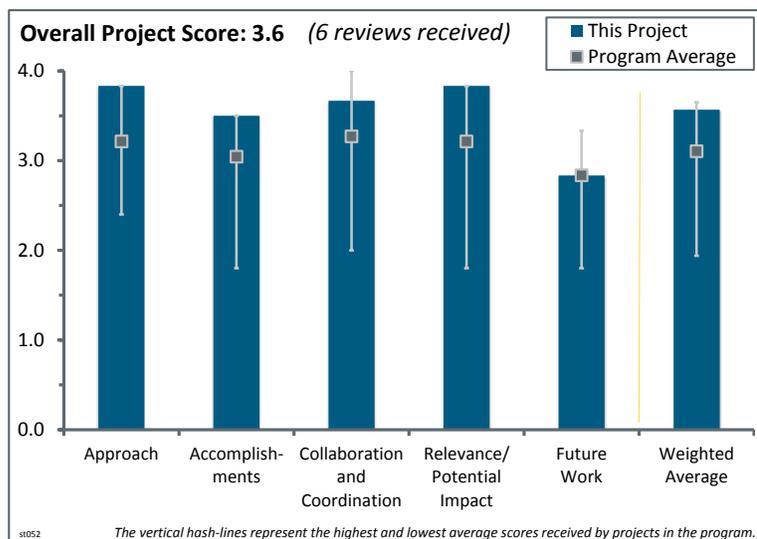
- The cryo-scope and comparison to alternatives could be better described at the start to give the reviewers a better sense of this technology.
- For the coming year, testing with hydrogen (instead of nitrogen) seems important. There may be embrittlement issues that are getting missed by using a surrogate for hydrogen. There is likely an extra “7” in the “Project Funding” total on the second slide; if not, the tanks must be more expensive than realized.
- HL should aggressively address design issues for assembling, filling, and sealing sorbent-containing vessels. This includes looking at chemical compatibility as well as conducting extensive pressure and temperature cycling. In addition, more effort should be made to find and characterize polymers that would reliably serve as liners in Type 4 tanks operating at cryogenic temperatures over the pressure range of 1–350 bar.
- The researchers should consider pressure cycling tests for up to 5,500 cycles to meet SAE guidelines. They need to quantify the fatigue characteristics of Type 1 tanks (a plot or at least a few data points of burst pressure versus number of cycles would be nice). Further development of Type 4 tanks at 80 K should only be continued after successful qualification of the materials (e.g., tensile impacts) at the service temperatures. Investigation of Type 3 tanks is recommended as a compromise between weight and cost. The team should report data on the translation efficiency, composite tensile strength, and modulus for Type 4 tanks.

## Project # ST-052: Best Practices for Characterizing Engineering Properties of Hydrogen Storage Materials

Karl Gross; H2 Technology Consulting LLC

### Brief Summary of Project:

The objective of this project is to prepare a reference document detailing best practices and limitations in measuring the hydrogen storage properties of materials. The reference document will be a guide to reduce errors and improve efficiency in measurements, improve reporting and publication of results, reduce the need for extensive validation, and allow experience and knowledge to grow and expand in the field of hydrogen storage. This project's goal is the establishment of uniform practices in the measurement and presentation of hydrogen storage materials performance.



### Question 1: Approach to performing the work

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

- The reference document covers various aspects of hydrogen storage materials. The tasks and chapters have been broken down into very logical and easy-to-follow practical subject areas.
- The basic idea to prepare a reference document detailing best practices for a variety of relevant measurements, their limitations, and error propagation is extremely useful to the hydrogen storage research community. It is really good that this document is publicly available.
- This magnum opus represents a labor of love for Karl Gross, but it also serves as the definitive manual on best practices for scientists and engineers working in the area of hydrogen storage. Dr. Gross is a first-rate experimentalist and he has distilled and collected material from a wide range of external sources in addition to collating wisdom and know-how developed within the U.S. Department of Energy (DOE) Hydrogen and Fuel Cells Program over the past decade. The document is still a work in progress, but it already defines the state of the art and will do so for many years to come.
- The principal investigator (PI) has assembled a group of internationally recognized experts to assist in the writing and review of this document. The authors have described the techniques and best practices for measuring and characterizing the hydrogen storage properties of new and existing materials in a complete and comprehensive way. A careful and very thorough approach was used to prepare the document. It is well organized and includes both introductory material and more detailed information about each topic. A comprehensive resource document that discusses uniform practices and issues in the measurement of hydrogen storage material properties will be of great benefit to the research, development, and engineering communities. In many ways, it is unfortunate that this resource was not available 5–10 years ago.
- The major objective of this project is to identify the appropriate methodologies for obtaining reliable measured data on the critical physical and chemical properties of hydrogen storage materials. The approach is to describe the advantages and limitations of common methods being used to characterize the hydrogen capacity, reaction kinetics, thermal properties, and other engineering parameters necessary to develop materials with the potential to meet the corresponding DOE performance parameters. An especially important aspect is to avoid classifying poorly conceived or conducted experiments as the discovery of “outstanding” hydrogen storage candidates; this wastes resources and diverts attention from more realistic materials. Unfortunately, many researchers choose not to heed this information. The emphasis during the past year has been on engineering properties, including thermal management issues.

## Question 2: Accomplishments and progress toward overall project and U.S. Department of Energy (DOE) goals

This project was rated **3.5** for its accomplishments and progress.

- Over the past several years a comprehensive and reliable online treatise has been produced. The recent topics contain the same high-quality descriptions and illustrations of principles.
- A very useful document has already been created and the final part, focusing on thermal and mechanical properties, is in good progress.
- Both engineering thermal and mechanical properties are very important for practical application of the hydrogen storage materials.
- While it is true that several sections remain to be completed, the magnitude of the task and the importance of the final product indicate that progress this year has been excellent. Several key sections have been completed and the final few are well underway.
- This document is the culmination of a multiyear effort. Although some additional work on selected sections remains, the document is essentially complete. The project represents a tremendous amount of work by a large number of highly skilled experts in the field. All of the major hydrogen storage material properties and characteristics (e.g., kinetics, capacity, and thermodynamic stability) and measurement methods are discussed in detail, and well-reasoned recommendations for best measurement practices are provided. Given the difficulties and confusion in making accurate physisorption pressure, concentration, temperature (PCT) measurements, the addition of a section (at DOE's request) that provides more in-depth analysis of the sources and propagation of errors in those measurements is useful and important.
- It is not uncommon for a project with so many stakeholders and reviewers to be somewhat cumbersome to make final versions, and it has been true in this case. This is particularly true for the error analysis section, which is one of the more crucial sections for this document to be an authority. It is not clear how much work beyond literature surveys and previous work has actually gone into engineering and mechanical properties—the subject of much of this year's work.

## Question 3: Collaboration and coordination with other institutions

This project was rated **3.7** for its collaboration and coordination.

- This is a document by consensus. Many of the experts in the relevant areas have been included in its drafting. The collaboration and coordination are exceptional.
- This project has a large group of collaborators from various fields in hydrogen storage materials; each brings in different expertise and makes this project a well-coordinated effort.
- Dr. Gross has recruited recognized experts to assist with and contribute to the project, such that each section represents the consensus of several leaders in the field.
- Numerous world experts in the field have contributed to the writing and review of this document. The PI has done a first-rate job of soliciting their input on specific sections and utilizing their considerable talents to create a comprehensive, well-organized, and eminently readable document. In addition, an important chapter on best practices for physisorption PCT measurements is being prepared in (an official) collaboration with the National Renewable Energy Laboratory (NREL).
- While a larger number of contributors were involved in the preparation of most of the earlier chapters, it appears that much of the last two chapters was based on the literature as well as some contribution from a staff member at Savannah River National Laboratory.
- Currently, there is much focus on low-weight element borohydrides for hydrogen storage. A huge number of recently published scientific literature describes the structure and reactions with other hydrides. But there is limited knowledge about the decomposition reactions and virtually no information about the mechanism for re-hydrogenation. This highlights that the project presented by Dr. Gross is highly relevant. There is a significant lack of general knowledge and understanding of the exact thermodynamic, kinetic, and “system” data. This project provides the fundament for performing systematic investigations, potentially worldwide.

**Question 4: Relevance/potential impact on advancing progress toward DOE research, development, and demonstration (RD&D) goals**

This project was rated **3.8** for its relevance/potential impact.

- This work will define best practices in hydrogen storage for years to come.
- The goals and aims of this project are extremely important. The only potential issue in creating a best practices guide is having the myriad of researchers actually use it.
- This document provides the community with some common measurement tools that can reduce the measurement error, improve the efficiency, and reduce the cost of extensive validation.
- It is very important to include engineering aspects such as thermal and mechanical properties as planned. Hopefully, it can be accomplished within the limited time this project has left.
- All of the thermal properties and engineering parameters being included in this project are relevant to the design, analyses, and operating behavior of hydrogen storage devices. Collecting this information within one document, albeit nearly 300 pages, should be beneficial to the purposes of the Fuel Cell Technologies Office's Hydrogen Storage program.
- Unlike other projects in the Hydrogen Storage program portfolio that focus on developing either materials or systems that meet the DOE targets for onboard hydrogen storage, this project is aimed at creating a comprehensive guide to metrics and best practices for measuring hydrogen properties of storage materials. Given the disparate and sometimes erroneous results that have been obtained by the hydrogen storage community (even on the same samples), there is a great need for a resource document that can be used to ensure that measurements are being made correctly and are in line with best practices. The best practices document prepared by the PI and his collaborators is well written and comprehensive and should provide both new and experienced workers in the field with a common basis for conducting measurements on the hydrogen storage properties of materials.

**Question 5: Proposed future work**

This project was rated **2.8** for its proposed future work.

- The PI and all of the co-authors are very skilled scientists; furthermore, a long list of high-profile international collaborators are also involved. This proves that the project is extremely well organized and productive.
- The project is at a stage where the remaining tasks define themselves.
- Finalizing the document is a fair goal and needs to be done. The timescale for this is not outlined, nor is the amount of effort it will take.
- The engineering mechanical properties chapter seems to not include the pelletized hydrogen storage material property analysis.
- All of the topics relating to future tasks shown on slide 22 are worthwhile tasks to be included in the best practices document. However, neither the gas permeation nor the materials compatibility tasks warrant the in-depth treatment that was given to the thermal and mechanical engineering areas. However, brief overviews of key issues, some representative examples, and references probably would be sufficient at this time.
- The future work includes completion and review of the section on engineering mechanical properties and the integration of the results from NREL's work on sources and propagation of errors in PCT measurements on physisorption materials and on methodologies and best practices acquired from NREL's project on spillover characterization and evaluation. These will be useful and important additions to the already comprehensive resource document.

**Project strengths:**

- This project features excellent work from a universally respected practitioner. Key experts and specialists have been involved in and provided input for each section.
- The community involvement is outstanding and will help to create an authoritative document for best practices in the broad fields of hydrogen storage.

- This effort provides an independent assessment of the methodology being used to evaluate hydrogen storage materials. It has heavily involved outside contributors and reviewers to provide both depth and balance in various subject areas. Much of the first chapters are based on the personal research and professional experiences of the PI. The contents are extremely comprehensive and contain good illustrations of key concepts and limitations in the conduct of measurements.
- This project has a large number of collaborators from various fields in hydrogen storage materials; each brings in different expertise and makes this project a well-coordinated effort. This document provides the community with a valuable tool for hydrogen storage materials research.
- The PI and all of the co-authors are very skilled scientists; furthermore, a long list of high-profile international collaborators are also involved. This proves that the project is extremely well organized and productive. The document produced, so far, is very well written, informative, and useful.
- This multiyear effort is a “tour de force.” No other single text can compare with the scope and breadth of the resource material that is given here. The author has assembled a team of world experts who have contributed to writing and reviewing the document. It will be extremely valuable for the research and development and engineering communities.

#### Project weaknesses:

- It is unfortunate that this resource was not available 5–10 years earlier.
- The timescales and project effort are not delineated; bottlenecks are not identified.
- In the engineering property chapter, there is a need to add more in-situ measurement techniques.
- The time taken from commencement to completion is significantly longer than initially anticipated. This may be seen as a drawback, but it comes at no extra cost and represents value in the final product.
- As the online best practices document has grown to more than 800 pages, it has become more difficult for the reader to digest all of the topics and contents. In other words, it has become challenging “to see the forest for the trees.” Because several chapters were written 5 or 6 years ago, many of the cited references have become dated, while relevant—but more recent—publications and books are not mentioned. As examples, papers reporting round-robin testing involving several international laboratories on hydrogen-carbon and MgH<sub>2</sub> reference materials were published in 2009 and 2013, respectively. From examinations of these papers, it is clear that serious errors are being made because researchers are not following proper methods to produce reliable data. Although the “Best Practices” document has been available for years, it does not improve the quality of the reported data unless the actual researchers read and adapt the recommendations.

#### Recommendations for additions/deletions to project scope:

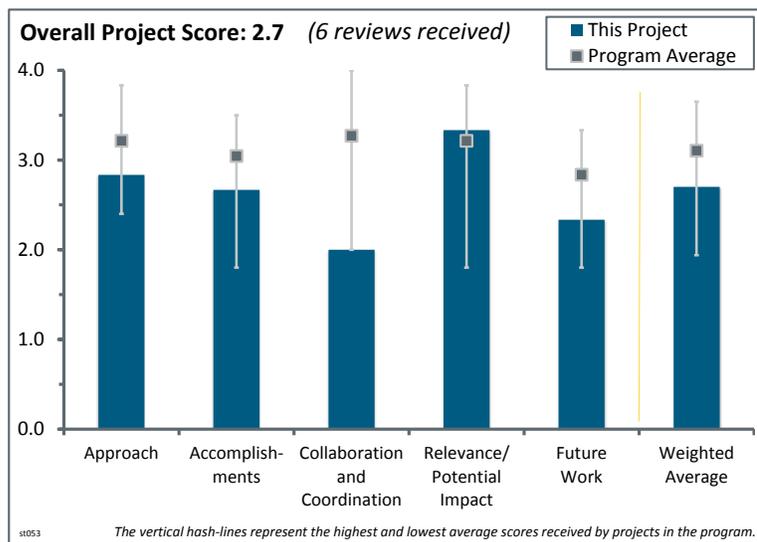
- This best practices project should be supported through the completion of Chapter 7, which is entitled “Engineering Mechanical Properties”; however, additional, new topics should not be added to its scope. Instead, the first chapters should be revised and updated with brief supplemental additions focusing on more recent research papers and books on hydrogen storage technology.
- The researchers should add the in-situ measurement tool to the engineering thermal properties chapter and add pellet mechanical properties to the engineering mechanical properties chapter.
- Complete and reliable measurements on engineering properties will be crucial for the next stage of hydrogen storage system development. The last chapters should also be completed and reviewed. Researchers should continue this project and include other experimental techniques as well, such as thermal analysis and spectroscopies.

## Project # ST-053: Life Cycle Verification of Polymer Liners in Storage Tanks

Barton Smith; Oak Ridge National Laboratory

### Brief Summary of Project:

The objectives of this project are to perform thermal cycle durability qualification measurements on polymeric tank liner specimens and assess the ability of liner materials to maintain the required hydrogen barrier performance. The project will devise and publicize test procedures for temperature cycling tank liner specimens, establish standardized test methods, and provide durability data on various materials. Permeability data will be used to develop an understanding of mechanisms for changes in liner permeability during thermal cycling. A test methodology for assessing liner behavior and durability with the liner attached to the composite reinforcement shell will be developed.



### Question 1: Approach to performing the work

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

- The general approach to develop a testing method of thermal cycling and permeation measurement of polymer specimens is effective.
- The approach to develop a standard protocol for testing tank liners and then publishing the protocols and results is good. It is also good that Oak Ridge National Laboratory is conducting tests called for in existing safety standards for fuel cell electric vehicles (FCEVs), such as SAE J2579. Planned testing with specimens that are sectioned out of actual tank liners is much better than testing coupon samples. Planned testing of integral liner/composite overwrap samples is also good, although this will likely require adjustments to the test procedures/equipment and analysis. However, it is not clear how this approach differs from the methods being used by the tank manufacturers to qualify the tanks that they produce. The presentation did not appear cognizant of prior work in this area or of what testing is being carried out by the tank manufacturers. The project needs to ensure that there is minimal overlap and duplication.
- Using disks might allow researchers to be able to predict the materials properties for diffusivity in some conditions; however, it is likely not a good method to evaluate the performance of liners in actual systems. Liners in systems will be exposed to different flexural and tensile conditions as well as interactions with the surrounding walls, bosses, etc.
- The original approach was valid and continues today, but progress has been slow. The ability for the project team to overcome obstacles throughout this project has resulted in slow but steady progress. The approach needs to focus solely on developing and providing to the industry a testing technique that can be used soon by tank and liner manufacturers. This is a key technology but it is at risk of being surpassed by industry that is using less technical approaches such as submerged leak testing. The approach by industry will not gather key durability aspects such as the ones this project is developing. The effects of temperature cycling with the liner are very important and require a repetitive testing approach such as the one this project is working to develop.
- The name of the project refers to “Life Cycle Verification”; however, this project is dealing with permeation only. The tests are dealing with permeation based on temperature cycles at specific pressure levels. Other parameters (e.g., liner buckling) are not mentioned. The project team should describe which real tank operation parameter could have an impact on permeations and which one will be applied at the

tests and why. It is unclear what the worst case parameters are for permeation. One test operation point is 700 bar at  $-40^{\circ}\text{C}$ . This is not a real tank operation point. It should be assessed if this could have an impact on the performance of the specimen. The expected potential failure mechanisms should be listed. It is unclear how these failure mechanisms are addressed. The impact of rapid depressurization on the specimen itself should be assessed (researchers should compare the depressurization rate during the test with real depressurization rates in tank systems).

### Question 2: Accomplishments and progress toward overall project and U.S. Department of Energy (DOE) goals

This project was rated **2.7** for its accomplishments and progress.

- Given the size of the budget the team has made good progress, particular in addressing the high-pressure seal for different types of polymers.
- The accomplishments in fiscal year 2013 look to be the best accomplishments for any year of the project. However, the progress is very slow and after five years one would expect the barriers and obstacles to be overcome, especially when dealing with sealing issues for which there are experts in the industry who could assist.
- Much time and effort was spent on sealing the disks to the apparatus—this seems like a distraction to the overall goal of characterizing different liner materials. The process was very much trial and error—it was very laborious without much strategy. Consultation with tank original equipment manufacturers (OEMs) or other partners could have significantly helped to mitigate this effort.
- There are no measured permeation rates within the past five years (the project started 2008), based on the assumption that the plots in the backup come from the literature. There was no information given about progress (percent rate) on the “overview” slide.
- One finding that has emerged is that permeation appears to be dependent on polymer compressibility. This is an important finding because storage tanks will likely undergo many compression/decompression cycles during the lifetime of an FCEV. In addition, the temperature of the liner can vary in the extreme from  $-40^{\circ}\text{C}$  to  $85^{\circ}\text{C}$ . The accomplishments are somewhat lacking because of difficulties with the experimental equipment, specifically, in getting a robust seal around the edges of the sample. There may be other delays ahead because of the need to accommodate integral liner/composite samples for testing.

### Question 3: Collaboration and coordination with other institutions

This project was rated **2.0** for its collaboration and coordination.

- The project team worked with other tank OEMs; however, the team did not seem to benefit from the OEMs’ knowledge in designing test apparatuses or understanding the critical areas of a tank where liners could have permeability issues (joints, bosses, etc.).
- A partner should be identified and contacted to review the general approach to measuring permeation.
- The project is important to the DOE Hydrogen and Fuel Cells Program (the Program) because it works to ensure the safety of compressed hydrogen storage on board FCEVs. Collaborations with tank manufacturers are mentioned but not enumerated. The project should interact with the manufacturers to ensure that the focus is on issues considered to be important by the manufacturers, even if permeation studies are not. Many tanks from different manufacturers have been in service for a number of years and permeation has not been reported to be a significant issue. Of more importance are the interactions between the tank and the liner under the extremes of ambient temperature and pressurization/depressurization cycles.
- The collaboration and coordination were not well articulated.
- It is not clear which Type 4 tank manufacturer has been involved in this project or how the manufacturer’s testing method is integrated into the project.
- There does not appear to be good collaboration. The collaborators listed are tank manufacturers, but they look to only be supplying liner samples. The real collaboration should be high-pressure test equipment manufacturers that can address the sealing issues and high-temperature fluid experts who can assist in the temperature cycling. None of these experts look to be consulted and thus progress is slow.

#### Question 4: Relevance/potential impact on advancing progress toward DOE research, development, and demonstration (RD&D) goals

This project was rated **3.3** for its relevance/potential impact.

- This is an important study to bolster the understanding of this particular subcomponent.
- The life cycle of polymer liners in high-pressure storage tanks is very important and critical for the industrial application of a practical hydrogen storage system.
- The permeation rate of the liner is one of the main performance criteria for a Type 4 vessel. The definition of the test procedure is also important, but it is not included.
- The project is important to the Program because it works to ensure the safety of compressed hydrogen storage on board FCEVs as they are introduced into the market. Many tanks from different manufacturers have been in service for a number of years and permeation has not been reported to be a significant issue. Of more importance are the interactions between the tank and the liner under the extremes of ambient temperature and pressurization/depressurization cycles. The project is wise to undertake some work in this area.
- This is clearly an important task in the development of improved liners for storage vessels. The principal investigator, however, was bogged down with a non-ideal test apparatus and seems to have lost focus on the end goal of understanding the overall system issues with the liners, not just material permeability.
- The relevance of this project is that it is developing a key technology that is truly needed by the industry. Liner durability is very important and is yet to be determined in a long-term storage system where high pressure and potential risk are present. As time passes, however, industry is advancing and the relevance is diminishing, so the slow progress is impacting the overall relevance of this project. It is important enough that it must be finished.

#### Question 5: Proposed future work

This project was rated **2.3** for its proposed future work.

- The proposed future work follows from the work to date.
- The testing of the polymer liner with the interaction of fiber wrapping is very important. The team needs to come up with a practical method to do this.
- Researchers should review the test procedure before continuing with the tests. Three additional specimens are scheduled to be tested within the next five months (project end is scheduled for October 2013). This is an optimistic schedule.
- The project team should deemphasize the work on repeating tests with 350 bar—there is likely not as much to be learned because conditions are not as challenging. The team should also increase its emphasis on understanding liner interactions with composite layers in real tanks.
- The planned work for the remainder of 2013 and for 2014 is reasonable. The planned work on sectioned tanks is definitely needed to develop an understanding of the interaction between the tank and the liner. Understanding failure mechanisms would be an important contribution to the community. Where possible, testing should be carried out under “real-world” conditions or as close to those as possible given the limitations of the test equipment.
- The outlined future work is too broad. All efforts should be placed on completing the testing protocol and proofing the testing equipment. Testing other materials is much less important than actually delivering an accurate, repeatable test procedure and equipment. The one area of future work that does not belong in this project is the work targeted to understand the region between the liner and the composite as well as the hydrogen absorption in the composite. This is very important to storage vessel performance and a project needs to address this aspect, but not this project. This project needs to complete the testing approach and publish its work for industrial use.

#### Project strengths:

- The testing technique represents a good approach.
- This project features a good selection of materials and treatment.

- The team has a very good material level understanding of the polymer liner and how to quickly screen its cycling behavior.
- The test facilities appear to be very capable of producing quality results on test sections of liner materials. Hopefully, the equipment will be able to test actual tank sections in a similar manner either with or without modifications.
- The accomplishments in the testing protocol and apparatus are showing progress and could lead to a standard testing method that would be a key element for the industry. The strength of this project is that the outcome is important and appears to be relatively close to completion.

#### **Project weaknesses:**

- This project features a poor test apparatus and lacks a plan to translate results into overall system validation.
- The team has not shown a valid method of testing the interaction between the polymer liner and the fiber wrapping, which is very important for a practical high-pressure Type 4 system.
- Tank/liner interactions under extreme conditions may be a more important issue to examine than permeation. The presentation did not discuss past efforts to study permeation through tank liners or ongoing efforts by the tank manufacturers. It is difficult to determine possible overlap and duplication.
- The progress has been very slow and the lack of “expert” collaborators appears to be a root cause of this. The weakness is the appearance that the work was focused internally and that help was not requested from industry.
- More effort should go into describing plans to approach the study of delamination of the liner from the composite overwrapped pressure vessel (COPV) shell.

#### **Recommendations for additions/deletions to project scope:**

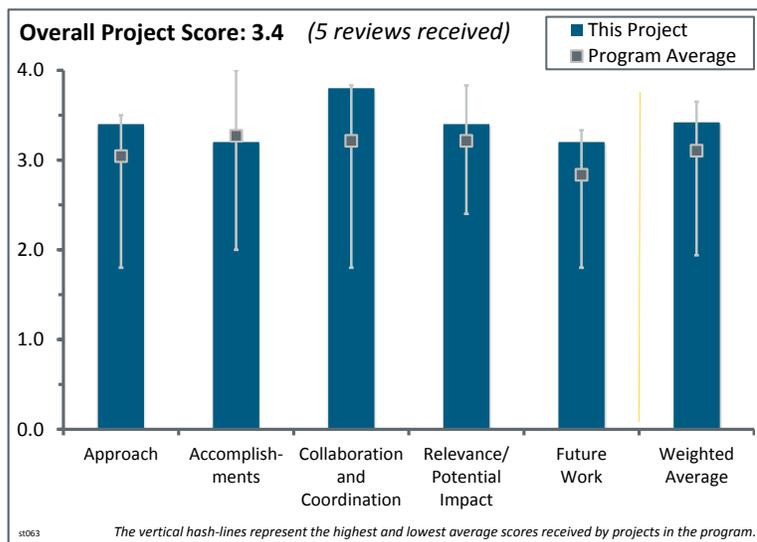
- The team should reevaluate the test methodology.
- The team should elaborate on how to study delamination of the liner from the COPV shell.
- The project should include the analysis of interaction between the polymer liner and metal joint at the cylinder neck, which accounts for a significant portion of the Type 4 tank failure mode.
- The research team should quickly establish a plan to understand areas of potential concern in different parts of the tank with regard to material durability (not just permeability) and test for those conditions where the material may experience additional stress.
- The project team should increase efforts in understanding tank/liner interactions under pressure and temperature cycling to the expected extremes in pressure and temperature. The project team should also look for new and novel tank liner materials for testing. A good outcome from this project would be establishing a standardized test procedure that could be used for qualifying liner materials in a consistent manner.
- The communication of a test procedure, standards, and results needs to be completed soon. These findings should then be given to a testing equipment manufacturer for collaboration on building a first-generation device. This work is important and the team needs to look outside for industrial partners to build a turnkey system and more aggressively overcome the obstacles, such as sealing and temperature control.

## Project # ST-063: Electrochemical Reversible Formation of Alane

Ragaiy Zidan; Savannah River National Laboratory

### Brief Summary of Project:

The overall objective of this project is to develop a low-cost rechargeable hydrogen storage material with cyclic stability, favorable thermodynamics, and kinetics fulfilling the U.S. Department of Energy (DOE) onboard hydrogen transportation goals. Specific objectives for the project include avoiding the impractical high pressure needed to form alane ( $\text{AlH}_3$ ), avoiding the chemical reaction route of  $\text{AlH}_3$  that leads to the formation of alkali halide salts, and utilizing electrolytic potential to translate chemical potential into electrochemical potential and drive chemical reactions to form  $\text{AlH}_3$ .



### Question 1: Approach to performing the work

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

- This project has made progress in some key areas over the past year. Most notable are the development of a closed cycle involving regeneration of metal alanates ( $\text{MAIH}_4$ ) to serve as a source of  $\text{AlH}_3$ , and the production of high-purity alpha  $\text{AlH}_3$ , as evidenced by powder x-ray diffraction.
- This project is positively evolving toward what could likely be a practical regenerable  $\text{AlH}_3$  process that would be important as a hydrogen storage source for fuel cell electric vehicles and to numerous other near-term fuel cell applications. Because the process is electrochemical, its broad scalability may prove to be very important.
- The research team has sharpened the focus of the approach over the last year. Now it is well focused on chemical efficiency. The approach is also being better communicated. It is unclear whether the approach should include defining which of the many half reactions shown are operating under regeneration conditions.
- The project is moving in the right direction toward  $\text{AlH}_3$  regeneration. So far, the researchers have been able to increase the reaction rate of  $\text{AlH}_3$  regeneration by increasing the conductivity during electrochemical regeneration. Likewise, the researchers have investigated barriers to this process by examining morphologies of the product phase. They have been able to avoid the formation of  $\text{Li}_3\text{AlH}_6$  dendrites that short-circuit pathways during the regeneration reaction by changing the cell geometry. Although this is not one of the stated goals of the research, one of the useful project outcomes is that the investigators also suggest a reaction pathway to regenerate  $\text{LiAlH}_4$ .
- The research group utilized electrochemistry combined with organic and physical chemistry to develop new experimental approaches for cycling the  $\text{Al-AlH}_3$  system in a solvent. There is a strong focus toward closed materials cycles and obtaining high actual measured energy efficiency. The number of partners is suitable compared to the amount of funding, and each partner brings in different expertise. The approach is a more direct conversion of renewable electricity to chemical energy and has a huge potential for possible applications, both mobile and stationary.

## Question 2: Accomplishments and progress toward overall project and U.S. Department of Energy (DOE) goals

This project was rated **3.4** for its accomplishments and progress.

- Good progress has been made in several key areas.
- Aluminum is abundant and cheap, and its hydride contains large and usable amounts of hydrogen both measured volumetrically and gravimetrically. The research consortium has already discovered a new catalytic approach that increases the yield of  $\text{AlH}_3$  and provides higher electrochemical cell efficiency.
- With a small amount of funding, the team continues to make progress that impacts overall  $\text{AlH}_3$  regeneration efficiency and cost. Finding ways to improve cell conductivity has led to improvements in  $\text{AlH}_3$  production rates. The team has produced prototype cell designs that demonstrate mitigation of dendrite formation. It also demonstrated  $\text{LiAlH}_4$  electrolyte regeneration, albeit at an 80% recovered yield—there is room for improvement here.
- The team has successfully addressed issues with the reactor evolution as they arose. Key features include the highly saturated electrolyte that enhances the precipitation of  $\text{AlH}_3$  adduct to aid in physical recovery. Additional important accomplishments include the move toward a separator such as Nafion, tripling electrolyte conductivity, and regenerating the electrolyte.
- The investigators are clearly making progress toward their stated goals (and those goals are aligned well with the DOE goals). For example, the investigators have developed alternative designs to the electrochemical reactor based on the formation of deleterious products (e.g.,  $\text{Li}_3\text{AlH}_6$  dendrites that caused short circuits in the prior reactor design). Product yield, cost, and safety were considered during the development of the regeneration process. However, the work lacks discussion of  $\text{AlH}_3$  regeneration reaction rates (as a function of cell voltage). This is also an important consideration for practical applications of this electrochemical approach.

## Question 3: Collaboration and coordination with other institutions

This project was rated **3.2** for its collaboration and coordination.

- Sensible collaborations have been established with key institutions and laboratories. These collaborations are well managed and appear to contribute in a meaningful way to the overall project.
- The investigators list collaboration with two other institutions on slide 3 (i.e., Brookhaven National Laboratory [BNL] and the University of Hawaii), but all of the technical accomplishments described were performed at Savannah River National Laboratory (SRNL). The investigators suggest the development of new, industrial collaborations on slide 21.
- This project is very well coordinated. The number of collaborators is relatively small. The information on the poster indicates that there are already new discoveries that will be patented.
- The project shows good coordination among current and past efforts in  $\text{AlH}_3$ ; the project team has a good handle on where the state of the art lies. The project may improve if some communication occurs between the Argonne National Laboratory (ANL) systems modeling effort to ensure that the research priorities are set appropriately with the small amount of funding available.
- It is unclear how responsibilities are exactly shared among collaborators.

## Question 4: Relevance/potential impact on advancing progress toward DOE research, development, and demonstration (RD&D) goals

This project was rated **3.8** for its relevance/potential impact.

- The successful development of a low-energy electrochemical route to  $\text{AlH}_3$  from aluminum and hydrogen gas would redefine the whole direction of the Hydrogen Storage program going forward.
- This project has a huge potential for future high-energy-density storage. The actual, measured energy efficiency of 68%–75% has already been achieved and is approaching the ideal value of 83%. The project approach has great novelty, specifically in employing direct electrochemical energy storage.

- Chemically and energy-efficient regeneration of off-board regenerable materials is highly relevant to DOE RD&D objectives to reduce the cost of off-board regenerable hydrogen storage systems. The potential impact of this project is high if a well-integrated, chemically efficient, and energetically efficient process can be defined and demonstrated in the laboratory.
- Because  $\text{AlH}_3$  has a 10 hydrogen wt.%, this approach creates a pathway to onboard storage that can be potentially critical for hydrogen's success in transportation. The methodology also creates significant technical opportunities in many other fuel cell applications that may see commercial growth in the nearer term than the fuel cell electric vehicle.
- Because  $\text{AlH}_3$  is one of the most promising metal hydrides for meeting DOE's targets, the goal of low-cost regeneration is extremely relevant. The researchers have demonstrated that the electrochemical regeneration approach being developed is also relevant to other hydrides (e.g.,  $\text{LiAlH}_4$ ); however, a cost comparison with other methods to form  $\text{LiAlH}_4$  has not been made. Such a comparison would have been useful to demonstrate that the electrochemical approaches, when generalized, are beneficial across a variety of hydride systems.

### Question 5: Proposed future work

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

- The proposed work for the coming year is sensible and builds on this year's progress.
- The future work (slide 21) is detailed and lists items that seem to be both measurable and achievable.
- The improved electrochemical cell design and  $\text{AlH}_3$  separation are very important to realizing the potential of this process.
- It would be very interesting to investigate the possibilities for scaling up the synthesis to obtain, for example, 100 g  $\text{AlH}_3$ .
- The proposed future work contains a significant amount of work to accomplish at SRNL for only \$400,000. The project has shown success in providing proof of principle. The principal investigator (PI) should consider whether to continue to invest in improving cell designs or instead focus on areas that have potentially more impact on overall efficiency/cost issues, such as separations (of  $\text{AlH}_3$ , of catalyst components, etc.), and the recycle of aluminum from spent fuel to anode formation. Feedback from systems analysis experts would be helpful here. It is unclear whether the future work should anticipate another round of "cost estimation" by ANL. If so, then the researchers may want to prioritize future work to address process cost estimation needs in concert with ANL input. For example, the impact of the future work may be improved by considering how the returning aluminum spent fuel enters into the regeneration process; for example, how one takes spent aluminum to form the anode efficiently. The future work might profit by including tracing where the "dopant" in  $\text{AlH}_3$  ends up, and how/when/if it needs to be separated from the process and recycled.

### Project strengths:

- This project features a genuinely original approach to a challenging technical problem.
- The project partners collaborate well and efficiently, as demonstrated by the amount of results already achieved and in light of the modest amount of funding.
- This project is focused on overcoming a significant barrier to off-board regenerable hydrogen storage materials.
- This project features a knowledgeable and capable team, a Cooperative Research and Development Agreement (CRADA) with an industry partner, and a good semi-empirical approach.
- The project lays a platform for developing electrochemical methods for  $\text{AlH}_3$  regeneration (and organic adduct removal). If this can be done efficiently, this is a relevant goal for meeting DOE targets. The approaches taken involve engineering (reactor design) and materials science (understanding the role of morphologies in the product phases formed). Clearly, this team of researchers is capable of driving the project toward the end goal of low-cost and efficient  $\text{AlH}_3$  regeneration.

**Project weaknesses:**

- The project would likely be helpful with more focus on the actual mechanism for electrochemical hydrogen uptake and the function of the additive/catalyst. It is unclear if there are some intermediates involved; for example, similar to those suggested for the alanate system ( $\text{Al}_2\text{H}_7$ ). However, that may require increased funding support.
- It is still not clear how much real assistance is provided electrochemically to the reaction  $\text{MH} + \text{Al} + 1.5\text{H}_2 = \text{MAlH}_4$ . This reaction was shown to work perfectly well using conventional energy inputs (temperature/pressure) both by Dr. E.C. Ashby at Georgia Tech in the '60s, and more recently by Dr. Jason Graetz at BNL.
- The project could be improved by incorporating input from systems analysis to focus the limited resources on highest priority topics.
- There is a clear lack of participation by the collaborating institutions (i.e., BNL and the University of Hawaii).

**Recommendations for additions/deletions to project scope:**

- The project began with a focus on  $\text{AlH}_3$  and has shown a lot of progress in that regard. However, the electrochemical methods being developed here for  $\text{AlH}_3$  may be more generally applicable to other light metal hydrides. An analysis and further thought/comment about the cost benefit to applying this process to other hydride systems would be useful.
- The research team should follow the proposed plan; utilization of a "low-boiling-point" solvent (DME) may be more efficient for the synthesis of  $\text{AlH}_3$ , along with further optimization of the activation process for aluminum and utilization of efficient additives/catalysts. The team should also investigate the possibilities for scaling up the synthesis to obtain larger amounts of  $\text{AlH}_3$ .
- Given the limited dollar resources this project has, it may be helpful to focus prioritized areas on systems analysis feedback. Because proof of principle of cell design has been demonstrated, perhaps postponing/delaying the improvement of the electrochemical cell design activity would provide more resources to focus on separations issues, for example. Separations tend to be the most costly portion of integrated chemical processes.
- The project team may also want to look into Zirfon as a cell separator. It is a separator used in many alkaline electrolyzers. It is zirconia particles in a polysulfone matrix. THF, like the DME used earlier, is highly flammable. Its auto-ignition temperature in air is  $321^\circ\text{C}$ ; this is not expected to occur unless an anomaly happens in the cell to raise the temperature or create a spark in the presence of air. This is unlikely, but it may lead to scale-up and production-level codes issues. It is unclear if any more benign solvents have been considered. The overpotential cited on slide 9 is for the specific experiment and its design. It is unclear if there is design latitude for reducing it. In a commercial system, the cell design will be driven at some aerial current density and should have an ohmic varying with current density. This may contribute to higher fractional energy consumption. It may be worthwhile to add an effort to understand the cell design and current as a function of energy consumption to optimize the efficiency.

## Project # ST-093: Melt Processable PAN Precursor for High-Strength, Low-Cost Carbon Fibers

Felix Paulauskas; Oak Ridge National Laboratory

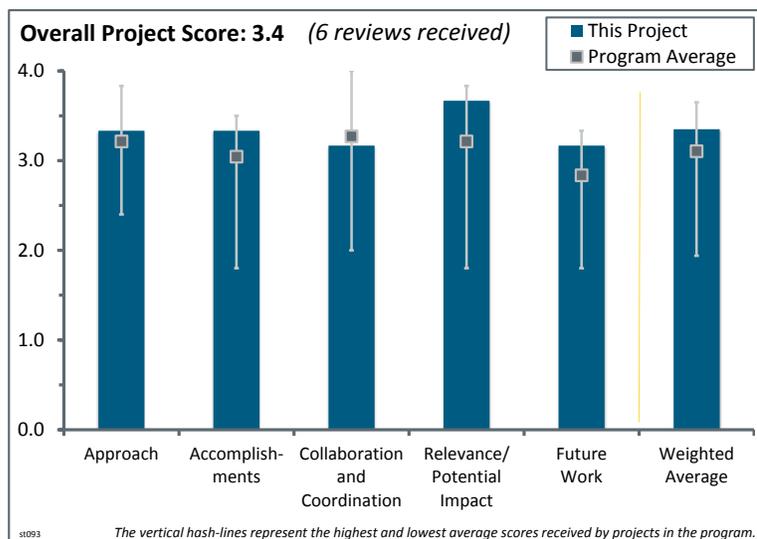
### Brief Summary of Project:

The objective of this project is to reduce the manufacturing cost of high-strength carbon fibers (CFs) by means of significant reduction in the production cost of the polyacrylonitrile (PAN) precursor via hot melt methodology and the utilization of a polyacrylonitrile-vinyl-acetate (PAN-VA) polymer. This technology has the potential to increase the throughput in the production of the PAN precursor and decrease the cost of precursor production.

### Question 1: Approach to performing the work

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

- Because the precursor is the main cost driver of a CF vessel, it is a very good idea to investigate a different production process.
- The team is effectively addressing barriers as they are discovered. The project is as well designed as it can be for the large scope and associated limited funding. Demonstrating a compelling reduction in manufacturing cost does not appear feasible during the remaining period of performance. The team's integration with other efforts is consistent with work being performed and is acceptable.
- The approach for this project is well focused. The analysis of former work by BASF has led to a refined approach that addresses the issues and concerns of the previous work. Much work has been accomplished in fiscal year 2013 as a result of the focus that this project contains.
- Melt processing of a PAN precursor is projected to result in lower cost precursor fiber than is currently produced by solution processing. The approach is simpler and more environmentally friendly than the current process. The approach is to improve the PAN melt stability by reducing the temperature below the degradation temperature. The approach builds on the past work by BASF that was abandoned for economic reasons. Because the impact of small changes in processing conditions is not easily predictable, a high level of experience and expertise in polymer processing is required to investigate the process space in a reasonably efficient manner. The team excels in this area.
- The overall approach of the project is good because it pursues the melt-spun processing as an alternative to the solution processing. The approach could be improved by including quantified metrics for evaluating the fiber surfaces rather than simply a subjective assessment. It would also be appropriate to cross-section the fibers to evaluate the internal porosity rather than just on the surface. Additional information on the steps that were used and could be used to improve the fiber properties would add value to the approach in order to highlight the science rather than the "art" of the processing. The project should transfer to a polyacrylonitrile-methyl acrylate (PAN-MA) rather than a PAN-VA because the properties will not be achieved with the PAN-VA. Finally, a cost model needs to be developed in the near term to confirm the potential savings of the process. The previous cost estimates were from a study from five years ago and need to be updated.



## Question 2: Accomplishments and progress toward overall project and U.S. Department of Energy (DOE) goals

This project was rated **3.3** for its accomplishments and progress.

- The accomplishments are good, especially the significant improvement in mechanical properties. The progress provides a step toward gaining confidence in the feasibility of the melt-spun processing precursor. It would be useful to quantify the specific cause and effect that facilitated the progress.
- The conversion of a current sample into CF results in a tensile strength of 150 ksi. Current aerospace-grade CF used to manufacture tanks has a tensile strength of approximately 700 ksi. The project is on a good path, but it is not clear whether tensile strength values (approximately 700 ksi) will be reached. The addressed barrier is the high cost of CF. It is stated that the production cost can be reduced by 31%–33%. However, there is no correlation to the DOE vessel target costs.
- The project achieved significantly greater progress than last year. The Oak Ridge National Laboratory (ORNL)/Virginia Tech (VT) team produced PAN CF that has very good outside surface characteristics with no detectable damage, notching, or cracking. Numerous trials met or surpassed their March milestone of 15 Msi modulus and 150 ksi strength. This progress was possible because of the concerted efforts of ORNL and VT to modify precursor chemistry and processing conditions in an effective manner. The fact that some of the success was fortuitous does not diminish the accomplishment.
- The accomplishments over the last year are impressive, with key advancements made in the spinning, post-spinning treatment, and carbonization of the fiber. The improvements to the pressure chamber and winding mechanism are very good and the incorporation of the steam stretch has resulted in a very good VA-based precursor, as noted in the scanning electron microscopy analysis. The “outstanding” rating suggests that barriers “will” be overcome. The progress over the last year would easily be rated as “outstanding,” but scale-up barriers still exist and need to be better addressed.
- After somewhat slow progress in previous years, this project has made some nice advances this year.
- Progress has most certainly been made in advancing this potentially impactful work, but an unequivocal connection to DOE goals is unclear.

## Question 3: Collaboration and coordination with other institutions

This project was rated **3.2** for its collaboration and coordination.

- The collaboration between ORNL and VT is very effective and helped the researchers overcome some significant obstacles this year.
- The degree to which this project interacts with other entities and projects has been dictated by necessity and is optimized for the work and limited funding available.
- Collaboration is mainly between ORNL and VT, which is important because of their individual expertise. With some initial success, additional manufacturers have been approaching ORNL; further collaborations could increase the chances that the process will be commercialized.
- It is understood that this project is dealing with a very specific technology; however, more partners would be preferable. Please continue looking for more partners.
- The collaboration with VT seems to be useful, but further collaboration should be considered with a U.S.-based chemical or fiber company that could assess the potential of the melt-spun processing for a commercial precursor. A chemical company partner could also assist in the development of a realistic cost assessment based on its knowledge of capital and operational costs, or another cost consultant should be added to the project.

## Question 4: Relevance/potential impact on advancing progress toward DOE research, development, and demonstration (RD&D) goals

This project was rated **3.7** for its relevance/potential impact.

- Because CF is the main cost driver, this project has a high potential to reduce CF costs significantly.

- While still at risk of success, the potential relevance is extremely high to the DOE Hydrogen and Fuel Cells Program (the Program) goals and objectives.
- The project is very relevant to the Program because early fuel cell electric vehicles will use compressed hydrogen storage systems. Lowering the cost of CF is crucial to the success of the vehicle launch. Lowering the cost of precursor fiber is a step in the right direction, but lowering the cost of carbonizing precursor fiber into finished fiber is also needed.
- The project is highly relevant because it is focused on the main cost factor (precursor) associated with the CF, which is clearly the highest cost driver in the compressed hydrogen tank system. The potential cost saving of 31%–33% would have a high impact on reducing the cost of the tank system and fuel cell vehicles. However, an updated cost model is needed to confirm the potential savings.
- This project is focused on meeting the cost-savings target of the Program. It is not addressing, however, the increasing movement toward a higher-strength CF. The technology that this project is developing is a key component of addressing a lower-cost CF, but it may not be well positioned to meet the needs of the Program. The importance of this project cannot be understated, because its successful development will certainly make a commercial impact in the use of CF.

### Question 5: Proposed future work

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

- It is crucial to see how properties and cost/process change with use of methyl acrylate.
- The project has naturally experienced barriers commensurate with developing a manufacturing process and material. The planning has been as logical as allowable with such an endeavor. For this reason, it is acceptable that discrete decision points are lacking; there has been and will continue to be discovery. Equally commensurate with this type of effort was not knowing the alternate pathways in advance, but this did not stop the team from addressing issues as they encountered them.
- The tensile strength target is 600 ksi. The tensile strength target should be comparable with CFs that are currently used in a 70 MPa system (i.e., 700 ksi). It is unclear if 600 ksi is enough to manufacture a 70 MPa Type 4 vessel.
- Future work plans for the remainder of 2013 focus on scalability and increasing mechanical property values. Alternative co-monomers, particularly methyl acrylate, need to be investigated; the project team has listed this area for future work.
- The general plan for future work was provided, but the specific plan for improving the strength would be useful. The ultimate goal would be to produce a low-cost carbon composite that should include an assessment of the fiber with the resin to ensure the translational strength. A high-level cost assessment should be included to verify the main benefit of the project.
- The future work for this project continues to address the barriers associated with melt spinning. However, more effort could be placed in optimizing the pressure chamber and spinning process, as well as developing an in-line steam stretch and treatment process. A fully integrated process is a critical step in being able to develop a commercial process. The future work is also aimed at improving the CF properties, but it falls short in being able to afford the necessary time to optimize the carbonization process for improved properties.

### Project strengths:

- The greatest strength of this project is in its potential impact on DOE goals and the proof of progress that the project team has made.
- This project's strengths are the project team's extensive knowledge and expertise in CF production and polymer processing and the excellent facilities for producing CF.
- The project is focused on the key cost driver for compressed hydrogen tanks and is making good progress with the mechanical strength properties.
- The collaboration between ORNL and VT and the accomplishments in the last year are notable and represent the strengths of this project. The approach and passion of the principal investigator are also strengths.

**Project weaknesses:**

- The project’s weakness is inherent in the scope of work that was proposed and the inherent risk typical with the level of manufacturing and material development required for quantifiable success.
- The project team needs to explain additional aspects of the science rather than the “art” of the process. The team also needs to update the cost estimate based on the current assumptions.
- The relation between the properties of the precursor and the finished CF is not clear. Understanding fundamental materials properties and their relationship is beyond the scope of this project. The project will have to rely on repeated trials to define the process conditions to ensure acceptable CF performance.
- This project is making substantial headway but appears to be significantly underfunded. This is important work and the funding does not fully provide adequate access to resources and time to fully develop this precursor.

**Recommendations for additions/deletions to project scope:**

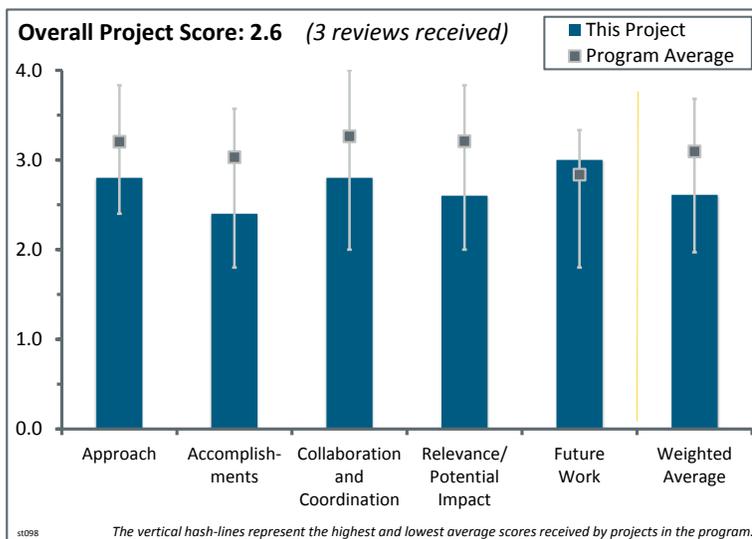
- The project team should continue to seek industrial collaborators to provide process knowledge and facilities.
- There is certainly no recommendation to de-scope in terms of funding. However, it would be good to see a re-expression of metrics and a clearer roadmap to reaching DOE’s goals. A breakdown of manufacturing costs and associated risks with each step would help in evaluating progress and focus.
- The project team should add a partner or effort in the area of cost estimating—it should consider including a consultant or an individual in the fiber industry to ensure that precursor development will have a high potential of delivering the needed attributes for a commercial high-strength fiber.
- The project team should consider a better application within the DOE umbrella where additional funding can be made available. The impact of a successful project in expanding the use of CF in industrial and automotive applications could be substantial. Efforts to light-weight automobiles could benefit from this project more than the Program could. DOE should provide the necessary funding to more quickly and thoroughly develop this precursor.

## Project # ST-098: Development of a Practical Hydrogen Storage System Based on Liquid Organic Hydrogen Carriers and a Homogeneous Catalyst

Craig Jensen; Hawaii Hydrogen Carriers, LLC

### Brief Summary of Project:

The objectives of this project are to identify the most versatile liquid organic hydrogen carrier (LOHC) for hydrogen storage and to design an LOHC containment system to interface with a fuel cell. The LOHC chosen should give the best combination with the pincer catalyst for high cycling capacity, rapid dehydrogenation kinetics, and no degradation of LOHC upon cycling. The LOHC tank and reactor system should be space-, mass-, and energy-efficient and should facilitate hydrogen release through an easily interfaced connection to a fuel cell.



### Question 1: Approach to performing the work

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

- The project has taken a logical, well-planned approach to this problem. The investigators should have looked at possible advantages that could have been achieved by using single isomers (i.e., cis vs. trans hydrogen addition across double bonds). Theoretical calculations could quickly show if improvements would be possible by using a single isomer.
- The project is generally well designed and addresses the U.S. Department of Energy (DOE) goals and barriers. Liquid carriers are likely to offer balance-of-plant and infrastructure benefits, especially compared to solid chemical hydrides.
- The approach to hydrogen storage using reversible, low-temperature, and pressure liquid organic carriers addresses several barriers that currently exist for onboard storage of hydrogen. In particular, liquid regenerable systems could, in principle, provide many advantages to an engineered system. The project is focused on proof-of-principle demonstration using low pressure, 1 bar experiments for the release of hydrogen from a low-capacity carrier.
- This is a unique project that is designed to test the benefits of using homogeneous catalysis in liquid carriers. The catalyst would be carried in the liquid and used to release hydrogen as well as regenerate hydrogen. It might not meet the vehicular targets, but the insight developed here could benefit near-term market strategies of the DOE Hydrogen and Fuel Cells Program (the Program).
- The approach is to develop catalysts for dehydrogenating organic compounds. There is no originality in this work. The researchers are using well-established organic compounds that are basically the same as what is in the big Air Products patent. They are using a catalyst developed by the Jensen group a number of years ago. They are interacting with General Motors (GM) and are considering the engineering issues with their approach. They have the catalyst loading down to 100 ppm, which is good because they are using a rare metal, iridium, as the catalyst. It would have been good to see an attempt to use a catalyst based on a first-row transition metal. The helical reactor is very nice. It would have been good to see a cost analysis of the catalyst. The bladder storage tank is nice. The researchers are developing a liquid chemical hydrogen storage fuel.

## Question 2: Accomplishments and progress toward overall project and U.S. Department of Energy (DOE) goals

This project was rated **2.4** for its accomplishments and progress.

- The researchers have made good progress toward meeting their goals. They have not completed their catalyst cycling studies, but good progress is being made. It is unclear whether they can scale this process up and whether they can meet the weight percent needed to be viable. The 100 ppm level for the catalyst is a real accomplishment.
- This project has not shown a great deal of progress over what was shown the previous year. Notable progress was found in the area of identifying LOHCs that are liquid in both hydrogenated and dehydrogenated forms. Dehydrogenation rates were termed “adequate,” but they took 18–20 hours to run to completion. This time to completion seems at odds with the characterization “adequate.” The experimental apparatus limited dehydrogenation kinetics studies to around one atmosphere; these are conditions not on par with DOE requirements for the inlet pressures of hydrogen for fuel cell applications. The recyclable capacity was not demonstrated. While expected to be low due to material ultimate capacity limitations, such a demonstration would have been valuable.
- Accomplishments this year have gone some way toward DOE goals, but a substantial gap remains. The volumetric and gravimetric capacities remain at the levels of prior years for this project, and although another catalyst and several LOHCs have been tested, no new systems appear to have been developed. The rate of dehydrogenation of BPHP may be faster than other compounds tested, but this still takes 20 hours at 13 degrees below the boiling point. It is unlikely that this compound will present a practical LOHC. The measurements of hydrogenation rates (with a 100 ppm catalyst) and the commencement of cycling studies show useful project progress.
- Despite determined efforts and a good approach, no viable combination of chemical hydride and pincer catalyst was found.
- It was obvious, appreciated, and appropriate that the principal investigator (PI) and coworkers used cost as a primary “filter” for the liquid carriers they considered. They appeared to eliminate a number of potential materials based on the cost of the material on a gram basis from a research chemical supplier. As the project is coming to a close, it would be valuable to have a similar cost analysis for the catalyst. Even if it is based on “Aldrich” costs, it will be valuable for others that come along after and consider homogenous catalysts for liquid carriers. The reviewer tried to estimate a back-of-the-envelope cost, assuming one used a 100 ppm iridium catalyst. One hundred ppm is 0.01 mol %, assuming 100 ppm is on a mole basis. For the liquid carrier used in the present study using MPHI, the researchers were able to get 2.9 wt.% hydrogen. For a 5.6 kg usable hydrogen system, they would need about 194.6 kg MPHI (1,400 moles MPHI) at 100 ppm; this would require approximately 0.14 moles of catalyst. For the pincer catalyst, this is about 60 grams of catalyst. If this is incorrect, the researchers could provide a worksheet to provide the grams of catalyst required for a tank of fuel. There is some confusion over the turn-over number (TON); it is listed as 250–300 on an earlier slide (perhaps slide 8), and then the later slides suggest a TON of 100,000. It is unclear what the differences are in the two experiments. A TON of 300 is not so good for an expensive catalyst. A TON of 100,000 is excellent and one might get about 1,000 fills for the lifetime of the catalyst. One could spread the initial cost of the catalyst over the number of fills expected for the lifetime of the system. Also, detailed information is needed on how to get from an experimental rate to a “practical rate.” The Arrhenius parameters give a rate of  $4 \times 10^{-6}$  moles of  $H_2/s$  at  $180^\circ C$ . A “practical rate” is assumed to be five orders of magnitude greater—about 0.4 moles of  $H_2/s$ . It is also notable that the regeneration stops at approximately 89%. Perhaps this could be due to an established equilibrium ( $LQH_2 = LQ + H_2$ ). This might start to answer one reviewer’s reoccurring question about what the conversion is at 5–10 bar back pressure in a system for a fuel cell vehicle.

**Question 3: Collaboration and coordination with other institutions**

This project was rated **2.8** for its collaboration and coordination.

- The internal collaboration between Hawaii Hydrogen Carriers (HHC) and GM looks to be excellent, with both sides closely interacting. No other external collaborations exist and such collaborations could be helpful.
- The work seems mostly confined to the PI's institute and subcontractor, and there does not seem to be any outcome evident from the interaction with Oregon State University (OSU). An additional collaboration with the Hydrogen Storage Engineering Center of Excellence (HSECoE) has been leveraged to help with the reactor design and modeling.
- The collaboration with the GM PI seemed good on the surface. The communication between HHC and GM may not have been ideal because it is hard to fathom how a member of DOE's Storage Tech Team and a member of the HSECoE apparently did not communicate the desired engineering-based technical targets or requirements (rates, pressures, etc.) to the HHC team members.
- It is understood that the reactor modeling effort by GM was reduced this past year, but it was not very clear how the collaboration with OSU is working. The connection is unclear.
- There is limited collaboration. The researcher should have engaged with Air Products, which has extensive experience with these systems.

**Question 4: Relevance/potential impact on advancing progress toward DOE research, development, and demonstration (RD&D) goals**

This project was rated **2.6** for its relevance/potential impact.

- This project features a good, honest appraisal of using a homogeneous catalyst with liquid organic carriers.
- The project aligns with DOE interests. It is not an exciting project because it does not involve the use of new material or of a new catalyst. It is hard to see it having an impact on chemical hydrogen storage, but it was good to learn if this approach will have an impact or not.
- The approach this project took is in principle highly relevant, and liquid reversible materials offer many advantages to an engineered hydrogen storage system. The project's relevance suffered by not adhering to basic materials and testing requirements for release systems. Project outcomes would have been easier to judge had experiments been conducted at conditions relevant to DOE's technical requirements for fuel cell operations.
- Although the project is highly relevant to the goals and objectives of the Program, the potential to significantly advance progress does not appear to be strong. The project is nearly complete and many of the metrics (especially capacity and rate of release) remain short of DOE targets.
- None of the materials studied had any real potential for meeting Program targets.

**Question 5: Proposed future work**

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

- It will be very helpful to others thinking about this approach to see a mini-analysis of homogeneous catalysis in liquid carriers. Some more relevant chemical engineering input is needed; specifically, how "100 ppm," a "TON of 350–100,000," and "practical rates" translates to a system. A simple Excel spreadsheet could be used, where one could input the molecular weight of the organic carrier and the wt.% hydrogen (to know how 100 ppm of catalyst is converted to moles and grams of catalyst and how many liters of liquid carrier are required for 5.6 kg of usable hydrogen). Also, the optimum TON for a homogeneous catalyst at 100 ppm is unclear. Three hundred and fifty is likely too small and 100,000 is likely more than necessary for 500 fills of 5.6 kg hydrogen. One might add these liquid carriers to the DOE database of materials and include rate information in order to determine how much liquid carrier is needed at what temperature to give a rate of 0.2 g H<sub>2</sub>/s. It seems like this analysis would help this team as well.
- The project is essentially complete and the researchers are finishing the cycling studies on the catalyst. The modeling of the process and reactor at GM is being completed.

- This scoring section is not applicable because the project is very near completion.
- The proposed future work is not rated; the project is ending.
- Not applicable—the project is complete.

**Project strengths:**

- This project features a potentially relevant approach.
- Despite being short of DOE targets, the project has developed some of the best-performing reversible liquid compounds for hydrogen storage.
- This project's strengths include its use of known chemistry and its liquid fuel. The researchers have substantial experience with the chemistry. There are good interactions within the team, including having GM on the team. The catalyst loading and performance are reasonable. The helical reactor is nice. There is good modeling at GM.

**Project weaknesses:**

- The HHC project team did not have experimental facilities to demonstrate hydrogen release under relevant conditions.
- This project contains chemistry and technology that is not really exciting. It is unclear if the researchers can meet the weight percent requirements, what the real cost and lifetime of the catalyst are, and what it costs to regenerate the catalyst.
- The terms “practical” and “acceptable” appear to be used without justification regarding rates of both hydrogenation and dehydrogenation. The examples given take several days for either process, which hardly seems “practical.” The project should have defined what it meant by acceptable rates, tied these to DOE goals, and shown numerically how these were met.

**Recommendations for additions/deletions to project scope:**

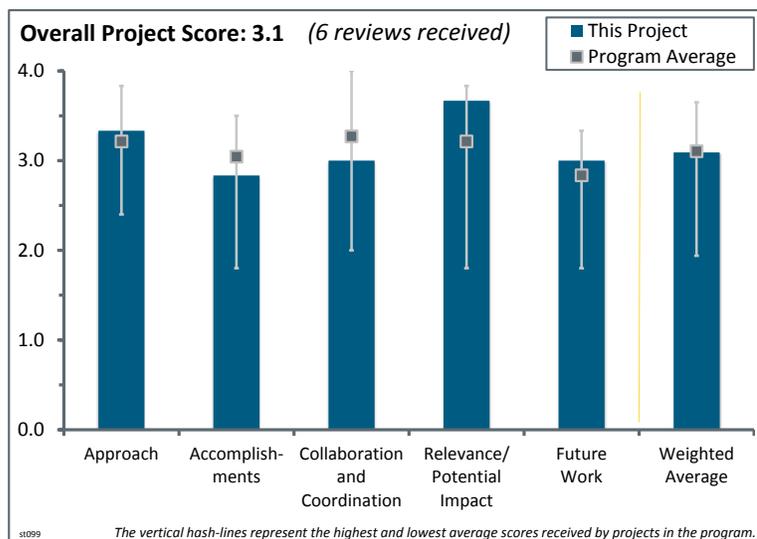
- This is not relevant because the project is near the finish date.
- There are no recommendations because the project is almost complete.

## Project # ST-099: Development of Low-Cost, High-Strength Commercial Textile Precursor (PAN-MA)

Dave Warren; Oak Ridge National Laboratory

### Brief Summary of Project:

The objective of this project is to develop a polyacrylonitrile-methyl acrylate (PAN-MA) formulation produced in a textile mill with as few changes to the precursor manufacturing as possible to achieve the performance requirements for hydrogen storage while preserving the high-rate, high-volume cost advantages of a textile mill. Carbon fiber (CF) composites make up 60%–80% of the hydrogen storage system, and the cost of the fiber accounts for the majority of the storage system cost. This project works to develop lower-cost precursors to meet performance requirements while preserving high-production-rate cost benefits.



### Question 1: Approach to performing the work

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

- The approach of using a low-cost commercial textile precursor is good. The project benefits from two previous projects funded by the U.S. Department of Energy (DOE) Vehicles Technologies Office.
- The project is well designed, shows feasibility, and appears to be integrated with other efforts. The project has a compelling approach to reducing the cost of CF.
- The overall approach is sound; development of low-cost fibers is essential for decreasing the cost of CF and, subsequently, the cost of high-pressure hydrogen storage tanks that rely on CF overwrap. The project leverages previous work done under the Vehicle Technologies Office to produce lower cost CF for vehicle structural members. Oak Ridge National Laboratory (ORNL) is working with a manufacturing partner, FISIFE, that brings manufacturing capability and expertise from the textile industry. This may result in the development of a potentially lower cost route to CF. The project hopes to improve the properties of the precursor and the manufacturing throughput to lower CF cost.
- It was a good idea to continue the work of two former projects. However, because a CF for 70 MPa systems was not the focus of the former projects, it will be difficult to reach the goals for a 70 MPa vessel.
- The overall approach of the project is good because it pursues a textile-based precursor as an alternative means to reduce the cost of CF. The approach could be improved by including quantified metrics for evaluating the fiber surfaces rather than simply a subjective assessment. Additional information on the attributes to quantify a quality fiber would be useful in order to highlight the key characteristics. Finally, a cost model needs to be developed in the near term to confirm the potential savings of the textile precursor for an aerospace CF.

### Question 2: Accomplishments and progress toward overall project and U.S. Department of Energy (DOE) goals

This project was rated **2.8** for its accomplishments and progress.

- The project accomplishments since the 2012 DOE Hydrogen and Fuel Cells Program Annual Merit Review (AMR) have been significant. The most promising precursor formulation was selected based on test results. Carbonized fiber properties up to 400 ksi tensile strength and 30 Msi modulus were achieved. The major

issue with fiber “fuzzing” was resolved by FISIFE by modifying the precursor manufacturing process. Delays in receiving precursor material from FISIFE delayed the optimization of the final oxidation step by about four months.

- It seems that the project is on a good path, but it is not clear if the expected tensile strength will be reached. There is no information about the expected mass and/or cost reduction. The team should add these numbers and correlate them to the DOE targets.
- The F2000 precursor was down-selected as the sole precursor for further development (down from three as of fiscal year 2012). This precursor has gone through four of the seven steps that convert precursor to final fiber. Two major issues encountered in previous years were resolved (or partially resolved); they were related to the size uniformity of fibers and shape deviation from “round fiber.” These problems underscore the importance of managing variability in fiber manufacturing because unintended variability reduces the effective strength of the CF.
- The team is making measurable progress toward DOE goals, which suggests that it is continuing to address the barriers encountered. Performance indicators were clearly presented in the form of attribute and cost impact. As is typical with most development projects, mitigation of barriers prior to them appearing was not feasible, leading to some delays.
- The accomplishments are good but the progress was not clear in the AMR presentation. Many of the same issues and down-selection accomplishment highlights were included in last year’s presentation. The current status for the fiber strength is slightly better than the previous year. A significant gap still exists regarding the strength requirements for aerospace fiber. The optimization effort is encouraging because it shows that further steps can be taken. It would be helpful to have further information regarding the potential of developing computational models to further improve the optimization in order to reduce the physical testing.

### Question 3: Collaboration and coordination with other institutions

This project was rated **3.0** for its collaboration and coordination.

- It seems that the project is in contact with all relevant partners.
- ORNL partners with FISIFE of Portugal. There is no collaboration with any partner in the United States.
- The collaboration with the precursor source has had challenges, but these have been well addressed.
- ORNL is partnered with FISIFE, which is headquartered in Portugal. FISIFE is responsible for precursor formulation and precursor spinning using textile-based processes. SGL Group recently purchased FISIFE and is a major CF producer. FISIFE is cost sharing by funding necessary plant modifications to produce the PAN-MA precursor by an air-gap spinning process. The role of SGL Group in this project is not clear.
- Because SGL Group has bought FISIFE, the collaboration is a concern. The project was delayed due to the formation of this relationship by four months. The future effect of the FISIFE integration into SGL Group is uncertain regarding the support for the project and the ongoing potential of commercializing the precursor.

### Question 4: Relevance/potential impact on advancing progress toward DOE research, development, and demonstration (RD&D) goals

This project was rated **3.7** for its relevance/potential impact.

- Success of this project would significantly advance progress toward DOE RD&D goals and objectives.
- CF is the main cost driver of a pressure vessel, so this project has the potential to reduce cost and mass.
- Reducing the cost of CF is one of DOE’s objectives for a 700-bar hydrogen storage option. Successful development of a low-cost commercial textile precursor can potentially help in meeting the DOE cost target for CF.
- Developing lower cost CF based on textile precursors is very relevant to the efforts of the DOE Fuel Cell Technologies Office to develop the technologies to enable the market introduction of fuel cell electric vehicles. CF accounts for about 65% of the cost of a CF overwrapped storage tank. Significant reductions in the cost of CF would enhance the prospects for commercialization.

- The project is relevant because it is focused on the main cost factor (precursor) associated with the CF, which is clearly the highest cost driver in the compressed hydrogen tank system. The potential cost saving for the textile precursor was not specified, so the potential impact can only be speculated for a compressed hydrogen tank. An updated cost model for the aerospace fiber is needed to confirm the potential savings.

### Question 5: Proposed future work

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

- The plans appear to be logical and based on previous results.
- Given the technical issues encountered over the past two years, the future plans appear to be reasonable. It is very important that variability in fiber size and shape be reduced as much as possible.
- The goal of this project is to manufacture a fiber with 650 ksi. This is a little bit lower than a T700 CF. Tank manufacturers should be asked now if this tensile strength is sufficient to build a 700 bar vessel.
- Future work plans are logical and seek to maximize the material properties in the conversion protocol through refinements in time, temperature, and tension. Other possibilities mentioned in the presentation, but not in the scope of the project, include investigating existing sources of precursor materials and possibly developing a new precursor supplier.
- The general plan for future work was provided, but the specific plan for improving the fiber would improve the future work. The ultimate goal would be to produce a low-cost carbon composite; this should include an assessment of the fiber with the resin to ensure the translational strength. A high-level cost assessment should be included to verify the main benefit of the project. Also, an effort should be included to evaluate additional opportunities to develop FISIFE or another precursor supplier toward a commercial product.
- There remains a large gap between current fibers (approximately 400 ksi) and the target of 650 ksi. It is not clear whether the plan for future work has the potential to close this gap.

### Project strengths:

- ORNL has many years of experience from previous projects in the development of low-cost CF.
- The project has made reasonable progress with measurable success, and it has sufficient funding.
- The project is focused on the key cost driver for compressed hydrogen tanks. The project has a high potential of influencing CF costs in the near term.
- Basing the project on textile manufacturing approaches appears to be an effective way to reduce the cost of CF by taking advantage of commercial processing technology. The partners have the materials expertise (ORNL) and processing know-how (FISIFE) to effectively carry out the proposed research.

### Project weaknesses:

- Part of the work to optimize the conversion process and precursor production is not exact science, but instead it simply relies on tedious trial and error.
- While the project was well planned and understood, the critical innovation that would presumably lead to the return on investments was not easy to understand.
- Other avenues to cost reduction include materials substitution and increasing manufacturing rates that were not mentioned in the presentation.
- The project team needs to include specific metrics for developing a high-quality aerospace CF. The team needs to have an update on the cost estimate based on the current assumptions.

### Recommendations for additions/deletions to project scope:

- The research team should add a partner or effort in the area of cost estimating. It should also consider including others in the fiber industry beyond FISIFE to ensure that precursor development will have a wider impact rather than simply to SGL Group before the project is complete.
- It would be good to develop a better understanding of the impact on final materials properties of polymer dope filtration as well as other aspects of the spinning process that could reduce the number of large-scale

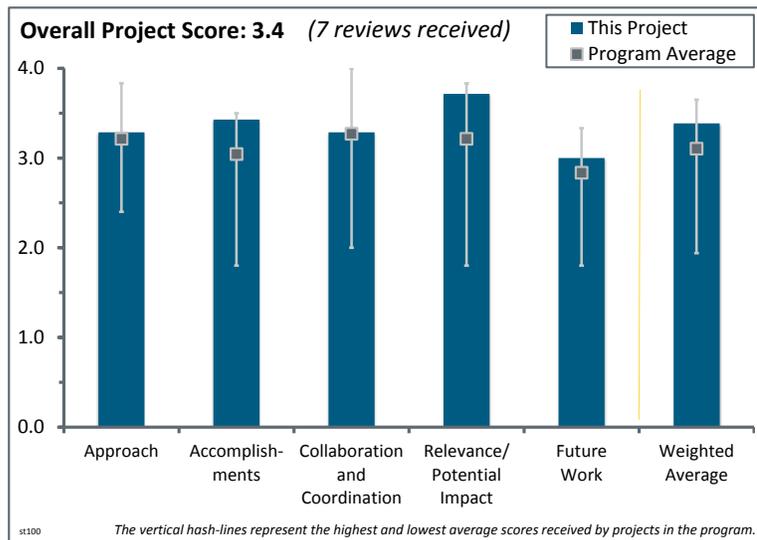
pilot trials. It is unclear if SGL Group plays a role in the project. If so, its role should be described. It has manufacturing expertise that can be brought to bear on this project.

## Project # ST-100: Hydrogen Storage Cost Analysis

Brian James; Strategic Analysis, Inc.

### Brief Summary of Project:

The objectives of this project are to perform process-based cost analysis of current and future hydrogen storage technologies and to validate the cost analysis methodology so that there is confidence when the methods are applied to novel systems. Sensitivity studies will determine the cost impact of specific components on the overall system. Analysis should identify the most fruitful research paths to cost reduction, including system technology and design parameters, system size and capacity, balance of plant (BOP) components, and materials of construction.



### Question 1: Approach to performing the work

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

- The project should add the significant variable of percent yield (both initial production and regeneration) to the sensitivity studies.
- Using Design for Manufacturing and Assembly (DFMA) is a very good approach to identify potential risks and cost factors. The project features a very good overview of 70 MPa system costs.
- The DFMA approach is a robust method for cost estimating for vehicular systems.
- The approach is logical and encompasses the necessary information. The influencing factors are highlighted and appropriately addressed.
- The approach makes sense but the reviewer has no background to evaluate it further.
- Overall, the approach is good because it utilizes DFMA along with industry best practices to develop relevant cost estimates. It is clear that the BOP for the compressed hydrogen tank system is a significant portion of the cost at lower volumes. The approach could be improved by including further cost details on certain BOP components. Also, further cost sensitivity analyses would be useful to highlight the key cost drivers within the tank and BOP, including the effects of certain design assumptions such as pressure and burst factors.
- A clarification on the correlation of vessel length to diameter (L/D) ratio with cost is required. There is a correlation, but costs of BOP dominate at low volumes. The principal investigator (PI) should provide more insight to show why both L/D cost curves are equal. The PI has improved the overall system layout—it is more reflective of a real-world system—and has provided different configurations of L/D, single/multiple setups, etc. This is beneficial to understand the different packaging trade-offs, etc.

### Question 2: Accomplishments and progress toward overall project and U.S. Department of Energy (DOE) goals

This project was rated **3.4** for its accomplishments and progress.

- Progress and refinement of models continue to improve every year.
- The baseline physical assumptions are very reasonable.
- The progress described seems reasonable.

- The project appears to properly address the goals and is focused on achieving the targets in the appropriate time frame. The progress is therefore on a proper time frame.
- The revision of the compressed tank cost estimates provided by this project is important to guide the U.S. Department of Energy (DOE) Hydrogen and Fuel Cells Program (the Program).
- The accomplishments and progress with this project were significant since last year's status. The schematic of the compressed hydrogen system was improved, and the cost estimates for this system were better developed at the various volume levels. The project also was able to accomplish and provide results for the regeneration of ammonia borane (AB).
- The project incorporated more up-to-date information from partners of the Hydrogen Storage program, including industry and design and analysis partners. Sensitivity analyses are important in helping to identify future focus areas. The project team should examine the sensitivity to economy-of-scale assumptions such as learning rate(s). Costs for off-board recycling of alane and AB systems may need to be examined as packaged systems rather than one-of-a-kind (typically site-built) systems.

### Question 3: Collaboration and coordination with other institutions

This project was rated **3.3** for its collaboration and coordination.

- All relevant partners for cooperation are included.
- The project team is consulting with the right combination of tank manufacturers, suppliers, and original equipment manufacturers (OEMs).
- The project team has incorporated information from national laboratories, the Hydrogen Storage Engineering Center of Excellence (HSECoE), and a number of industry integrators and suppliers.
- Strategic Analysis, Inc., has a high level of collaboration with others in hydrogen storage research. It has collaborated with the HSECoE and many others in the industry. The analysis coordination with Argonne National Laboratory (ANL) appears to be beneficial for both organizations, while the formal contribution of the National Renewable Energy Laboratory within the project is uncertain.
- The PI is working well with ANL in incorporating ANL's modeling results into cost models. The PI should consider partnering with an engineering, procurement, and construction contractor in the chemical process industry for the project's efforts to estimate off-board regeneration costs of hydrogen carriers. The off-board regeneration work should be reviewed by the delivery and/or production tech teams, where the Program's chemical processing experience resides.
- It appears that collaboration exists, but it is difficult to ascertain the extent of the collaboration. The partners are listed and properly noted. Their areas of expertise are also noted. It would be helpful to determine the extent of the work of each collaborating partner on the pertinent slide where that partner provided information and research.
- More collaboration could be sought.

### Question 4: Relevance/potential impact on advancing progress toward DOE research, development, and demonstration (RD&D) goals

This project was rated **3.7** for its relevance/potential impact.

- Accurate, unbiased cost analysis is vital in guiding Program research to maximize the return from research investments.
- This effort provides a consistent basis for cost estimates across the variety of storage development efforts in the Hydrogen Storage program.
- This remains a very important project because there are not many high-pressure storage systems to understand costs available on the market. These systems do not have tremendous deviation in design (as compared to fuel cell engine cost modeling), so results are likely to be more useful and accurate to OEMs. Understanding the cost and potential future savings due to volume and technology improvements will play a critical role in aiding OEMs to make decisions on when/how many hydrogen vehicles to launch in the future.
- This project provides very important information for near-term storage technology (35 and 70 MPa systems) for DOE, OEMs, and suppliers to evaluate their potential business cases. High expected AB off-

board regeneration costs should lead to a higher focus (in other projects) on off-board technology compared to onboard systems.

- The project is highly relevant because it is critically important to have a cost analysis for the various hydrogen storage options. Because it is difficult for researchers to develop cost projections and inappropriate for OEMs to provide their cost estimates, this cost analysis project provides DOE and others with a baseline understanding of the economic potential of the various storage options for both the vehicle cost and fueling cost.
- The approach and layout of the project addresses the relevance of the DOE goals well. The project is developing the appropriate cost analysis to direct DOE efforts and also is effective in determining the directions that need not be pursued. Overall, the project is effective and providing the information needed to support the Program.

### Question 5: Proposed future work

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

- The project has a logical path forward in continued support of the Hydrogen Storage program.
- The proposed future work elements seem reasonable, but the reviewer is not an expert in this area.
- This project features good, comprehensive proposed future work packages to predict system costs. The system layout represents the current state of the technology. It is unclear what an advanced system layout could look like and what the impact would be on the BOP costs.
- The scope of the future work looks acceptable, but much of the work is validating previous assumptions and work. The future work needs to be focused on advancing the project, ideally by taking the advancements of associated hydrogen projects to provide ongoing cost impacts and potential improvements. The cost analysis of onboard hydrogen storage meets the requirements of effective future work, but the other items noted do not advance the project and should be improved.
- The project team should provide more detail on why L/D cost curves overlap, as well as itemize some of the BOP components to highlight the fact that they dominate the cost curve.
- The plan for the future work was relatively vague. It could be improved by highlighting the key areas of uncertainty for the compressed hydrogen system and proposing a list of other onboard storage systems to be analyzed based on their potential commercialization from industry interest or previous analysis. For example, a cryo-compressed system may be useful to analyze as the next onboard storage system due to a significant interest from BMW. A further validation step would be useful in the future to compare the model projections to actual tank or BOP costs.

### Project strengths:

- The approach and logistics undertaken look to be the strengths of the project. The project organization is also excellent.
- This project is covering a good combination of system configurations. It is useful to OEMs for packaging requirements.
- The experience of the project team, particularly with DFMA for onboard systems, provides a solid basis for consistent estimates across the Hydrogen Storage program.
- This project plays a key role in understanding the impact of cost for the various hydrogen storage systems. Strategic Analysis, Inc., is highly capable and works well with other organizations.

### Project weaknesses:

- It is not clear how the barrier “system lifetime assessment” is addressed.
- The future plans or next steps were not clearly defined. Comparisons and validation of the cost analysis projections should be included in order to promote confidence in the values.
- Based on the questions following the presentation, the technical content could be questioned. The questions were pointed toward some assumptions that appeared to not be technically or commercially feasible. Other data, such as carbon fiber pricing, were very conservative and may not completely reflect the current market situation. Consequently, the technical approach and some assumptions could be improved.

- The AB cost analysis did not take into account the impact of handling hydrazine, a toxic, highly flammable compound that requires substantial use of personal protective equipment. Exposure must be monitored and kept below 0.1 ppm. This is not trivial.

**Recommendations for additions/deletions to project scope:**

- The input parameter of the cost model should be checked regularly in order to be sure that the assumptions are correct and up to date.
- The hydrazine recharging of the AB cycle probably would make this system uneconomical.
- Cost targets need to be brought to a more current basis year. This is a Program issue that will flow down to the programs and projects. The hydrazine-based AB recycle path, given current hydrazine prices, seems very unlikely to approach the cost targets and should not be pursued further.
- Researchers should accelerate the cost projections of other hydrogen storage systems for comparison to compressed storage systems.
- The project scope could be improved by incorporating the advancements of other hydrogen projects into the costing model. This would in effect allow this project to keep up on technological advancements and not reflect a dated state of the art. Also, industrial partners could be better utilized and provide input for creating such assumptions as labor, production rate, material costs, etc.

## Project # ST-101: Enhanced Materials and Design Parameters for Reducing the Cost of Hydrogen Storage Tanks

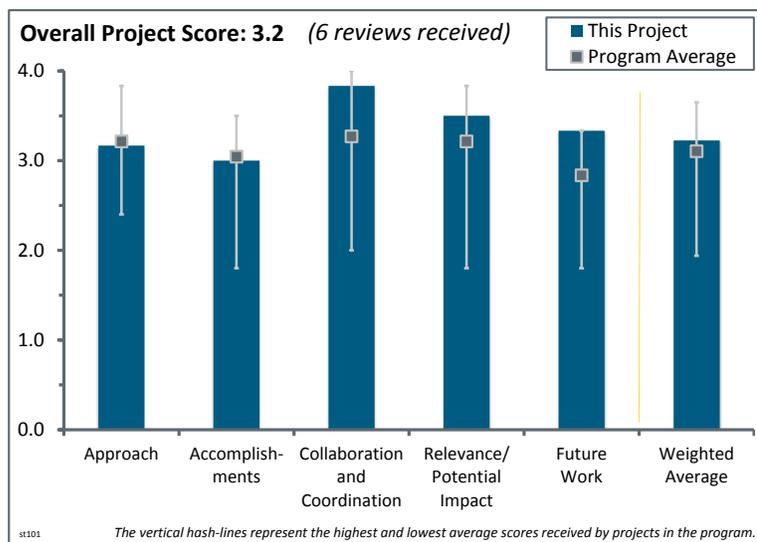
Kevin Simmons; Pacific Northwest National Laboratory

### Brief Summary of Project:

This project works to improve the individual constituents of hydrogen storage tanks for synergistically enhanced tank performance and cost reduction.

Planned project milestones include: (1) developing a baseline cost model for an onboard vehicle capacity tank and comparing cost against prior U.S. Department of Energy (DOE) studies; (2) designing and modeling a new tank with enhanced operating parameters of pressure and temperature for an equivalent tank with alternate fibers and/or a new fiber placement technique and developing a cost model for the new improved tank; (3) developing a feasible pathway to achieve at least a 10% cost

reduction for a compressed hydrogen storage tank through detailed cost modeling and specific individual technical approaches; (4) demonstrating integration of modified carbon fibers (CFs) and alternate/modified resins; and (5) conducting a baseline subscale prototype tank and burst test.



### Question 1: Approach to performing the work

This project was rated 3.2 for its approach.

- This project is straightforward work.
- It is a very good approach to create a model, simulate some improvements, and validate these simulations with hardware.
- The project is taking a comprehensive look at many approaches to reduce tank costs and is supported by strong modeling efforts.
- Barriers were clearly addressed and explained in the presentation. The project is well designed, appears to be feasible, and is well integrated with other efforts.
- The work to establish a baseline cost and reduce tank costs and mass through engineered material properties via the efficient use of CF is very good. The main cost drivers are the fibers; nevertheless, the project seems to strongly focus on the resin, where only a limited cost improvement is expected.
- The organization of this project is excellent. The principal investigator (PI) has developed specific tasks for each collaborator and set appropriate goals and follow-up activities. This is the best organized project that this reviewer has had the opportunity to review. The modeling task stands out as a highlight of the project. However, the approach does not adequately address innovative ways to meet the DOE Hydrogen and Fuel Cells Program's (the Program's) aggressive goal of reducing tank costs by 50%. Replacing epoxy resin with vinyl ester (VE) resins is a good step, as is working with a fiber supplier to create a sizing that is compatible with VE resins. By combining these efforts with the fiber type modeling, the project can reach the 10% target milestone for year 1. There exists, by the project's own declaration, a cost savings of 40% still to be realized, but there are no innovative ideas or plans on how to achieve this goal. Simply stating that the remaining savings can be realized by reducing the performance of the tank has merit; however, one would think that if this is then the goal, the overall project is overstated and should be focused on developing the optimized pressure vessel design that shows the most efficiency in capacity, performance, and cost. The model that was developed can greatly assist in this effort. If all pressure vessel projects are aimed at producing a 700 bar tank and it is determined by this project that the ideal tank is

different than the 700 bar design, then an overall directive should be issued to focus on modeling the optimum tank size and performance. The best outcome and value for this project is to determine what the optimum tank design should be for hydrogen storage. Working on optimizing resin, fiber, and wind patterns is something every pressure vessel manufacturer does on a daily basis and may not be providing benefit to the Hydrogen and Fuel Cells Program.

### Question 2: Accomplishments and progress toward overall project and U.S. Department of Energy (DOE) goals

This project was rated **3.0** for its accomplishments and progress.

- The project team has made significant progress.
- The project appears to be making clear progress toward DOE goals. The clarity of the presentation indicates that barriers will be overcome.
- Several potential cost-saving strategies have been identified. “Waterfall” charts showing potential system improvements should be accompanied by credible strategies for achieving targeted improvements or some idea of how likely improvements are. The basis for the improvements should be explained and justified by preliminary experimental accomplishments.
- The work to optimize resin, fiber, and winding efficiency is good and nicely done. The development of the modeling program is also a notable accomplishment and will provide a tool for future work. The milestones for year 1 have been met and should set the basis for future work, but the overall project goals are still very distant.
- The project team developed a feasible pathway to achieve at least a 10% (\$1.5/kWh) cost reduction, compared to a 2010 projected high-volume baseline cost of \$15/kWh for 350-bar Type 4 pressure vessels, through detailed cost modeling and specific individual technical approaches. The data collected so far is very good, but it has to be validated.
- The predicted cost savings of 10% are good; however, it is not clear how the total cost savings of 37% will be reached.

### Question 3: Collaboration and coordination with other institutions

This project was rated **3.8** for its collaboration and coordination.

- The project is exemplary in terms of the degree to which it interacts with other entities and projects.
- All relevant partners are involved.
- The collaborative effort of each partner appears to be very well coordinated and executed. The PI is doing a nice job of keeping the partners on task and focused.
- This project’s active collaborations with Hexagon Lincoln; Ford Motor Company; Toray CFA; and AOC, LLC include round-robin tests.
- The project is utilizing the expertise of fiber, resin, and tank manufacturers and original equipment manufacturers.
- The partners are competent.

### Question 4: Relevance/potential impact on advancing progress toward DOE research, development, and demonstration (RD&D) goals

This project was rated **3.5** for its relevance/potential impact.

- This project features a comprehensive approach to bring costs down.
- This project involves reducing pressure vessel cost, mass, and volume.
- A broad study such as this one will advance progress toward the Program goals in terms of understanding the general connection between materials and cost.
- Because compressed tanks appear to be the leading technology for hydrogen storage, accurate modeling of cost and performance is a vital competence for the Program.

- The project's goals and ideals of removing 50% from the cost of the hydrogen storage tank are very aggressive. This project, however, will struggle to meet those goals in its current format. The relevance of this project lies in its development of a modeling technique that can compare cost and performance of a pressure vessel. This model can then have a significant impact on the Program given its appropriate use. The manufacture and testing of pressure vessels are important to validate the model, but they will not provide the necessary impact relative to the high funding level of this project.

### Question 5: Proposed future work

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

- This project features a very good approach by validating modeling results with real hardware and tests.
- The validation of predictive models with experimental data is necessary and should be done.
- The team has effectively planned its future in a logical manner and has a clear understanding of DOE barriers.
- The project has a clear path forward aimed at achieving and validating additional incremental advances to lower tank costs.
- The future work of the project as planned does not add value to the overall outcome of the project or allow the project to advance beyond the 10%–15% cost savings already identified. The most valuable aspect of this project will be the ability to utilize its modeling technique to identify the optimized tank geometry and performance level. This modeling effort could provide the necessary input for all storage projects because it either defines a new optimized tank or validates that the 700 bar design is the best for overall capacity and cost. Once the ideal tank geometry and working pressure are identified, the Program can model the most efficient design parameters and fiber arrangements.

### Project strengths:

- This project features a good approach and accomplishments.
- If simulations turn out right, this project represents a very good advance in cost reduction.
- The project is very well planned and managed.
- There was a very good visualization of project structure, assignments, and accomplishments (compare slides 6, 7, 8, and 14).
- The project's organization and follow through are impressive. The modeling work is also a strength that has led to an opportunity to further define the project scope.

### Project weaknesses:

- So far the project has focused on simulations. Experimental verification is missing, but it is planned for the future.
- Due to the potential impact the material study could have on structural performance, a more involved material study may be warranted, such as testing for an additional weight percent. This could help distribute the performance of the different additives.
- The future work looks to be a weakness because the efforts do not appear to further address the remaining 40% cost reduction goal. The effort to optimize the use of different fiber types is the right approach. However, the future work does not appear to leverage the success of the modeling effort with an optimized pressure vessel geometry and ultimately the efficient use of different fiber types.

### Recommendations for additions/deletions to project scope:

- Funding should be diverted from manufacturing and testing pressure vessels in order to concentrate efforts on determining the optimum pressure vessel size and performance. This recommendation is based on the PI's comment that by reducing the working pressure design to 500 bar, the remaining 40% savings could be realized. If this is the case, then all efforts should be focused on validating this comment so that all other storage projects can be recalibrated to a new, optimized hydrogen storage pressure vessel design. Only then should a tank be manufactured and tested to validate the findings. This new standard could be the biggest

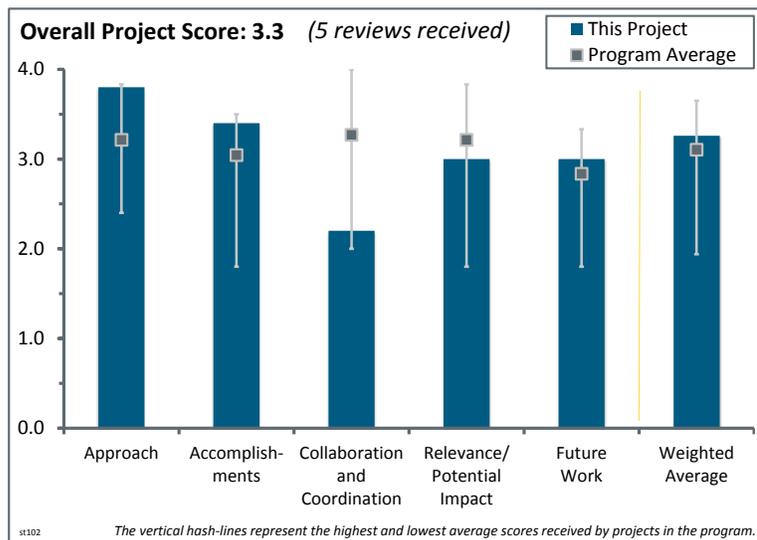
benefit to the overall Hydrogen Storage program because there would be many ways to build this optimized tank using alternative fibers, mixed fiber types, or modified resins, and several manufacturers would be able to commercialize their own cost-effective solutions. Refining the scope of this project to a narrower task could provide an opportunity to reduce the funding to an appropriate level.

## Project # ST-102: Room Temperature Hydrogen Storage in Nano-Confined Liquids

John Vajo; HRL Laboratories, LLC

### Brief Summary of Project:

The objectives of this project are to: (1) develop hydrogen storage materials that are compatible with the vehicle engineering and delivery infrastructure for compressed gas storage and (2) use measurements and simulations to characterize, understand, and optimize the (enhanced) hydrogen storage capacity of nano-confined liquids (liquids confined within nanoporous scaffolds). The project also works to establish procedures for measuring hydrogen sorption (solubility) in liquids and liquid-based composites at pressures up to approximately 100 bar, validate procedures with bulk solvents, determine the enhanced solubility of nano-confined liquid composites, and develop a simulation scheme to understand the enhanced solubility effect.



### Question 1: Approach to performing the work

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

- The principal investigator (PI) has used accurate measurement techniques to measure hydrogen capacities of nano-confined liquids.
- The quality of research is excellent and work has been focused on capacity targets. The PI has carried out careful measurements and has verified these with repetitions and assessment of errors.
- The project is focused on looking at novel sorbents, notably, liquids confined in nanopores, building on a set of papers from the National Center for Scientific Research (CNRS) in France. The experimental work and approach is truly outstanding. The computational work is less so as that is not the researchers' domain of expertise. They should collaborate with an external group for the simulations and not focus on this aspect.
- This project has a great degree of novelty. It may be fruitful with a slightly stronger focus on experimental science and by utilizing theoretical methods to verify the physical measurements.
- The approach to the project is adequate.

### Question 2: Accomplishments and progress toward overall project and U.S. Department of Energy (DOE) goals

This project was rated **3.4** for its accomplishments and progress.

- The researchers have made excellent progress in showing that it is unlikely that this approach will work. They clearly show that the French work is not correct or that it is not the same material with which they are working. They may find a material that works by September 2013, but this will be difficult. However, they have built a unique screening capability that is perfect for testing whether an approach will work or not. This provides a critical testing capability to the DOE Hydrogen and Fuel Cells Program's storage projects.
- Although the research results are opposite to those expected, the presented work explored another interesting idea, which unfortunately did not work out. The project deserves a rating of "good" because negative results are valuable ones.

- Accurate measurements of solubility effects appear to show no enhancement effect. Confirmation that the effect is not real is a valuable contribution to the DOE Hydrogen and Fuel Cells Program (the Program), allowing it to refocus on more promising technologies.
- Good progress has been made on project goals; however, the results and accomplishments do not contribute significantly to DOE goals. The results appear to indicate that the initial reports of enhanced hydrogen solubility in nano-confined liquids are at best grossly exaggerated and at worst false.
- The experimental measurements are challenging and ongoing.

### Question 3: Collaboration and coordination with other institutions

This project was rated **2.2** for its collaboration and coordination.

- The project appears to be well coordinated. The project is based on completely new ideas, and there is little other similar or relevant ongoing work elsewhere, which naturally limits the possibilities for collaborations.
- There is limited collaboration, but this is not a significant weakness for this project.
- There were only a limited number of collaborations; however, in this particular case, an extensive collaboration would not help anyway.
- The work seems to have been done completely at the sponsoring organization, although the PI has reached out to other institutions in discussion. Attempting to obtain a sample of the scaffolds used by CNRS researchers would have addressed the remaining discrepancy between U.S. and French results. A more active collaboration with the CNRS group is recommended.
- It does not appear that the researchers are collaborating as closely with others as they could be. They need to be more closely linked to the French group in terms of materials. It is unclear what material the French group really had. They also need to collaborate closely with a good theoretical/computational group. The current theory work is quite naïve, and they are not using the best potentials for the molecular dynamics simulations. They need to collaborate in the experimental structural work as well to back up their really nice and carefully done work.

### Question 4: Relevance/potential impact on advancing progress toward DOE research, development, and demonstration (RD&D) goals

This project was rated **3.0** for its relevance/potential impact.

- This is an extremely interesting and important project based on novel ideas. It is a high-risk/high-gain project. The project will undoubtedly lead to new fundamental science insight.
- The impact could have been quite significant if the idea had worked out.
- Although the results so far are valuable in terms of establishing whether nano-confined liquids are useful storage media, they do suggest that the project will have little impact toward providing storage methodologies that meet DOE targets. If the scaffold without solvent has higher storage, then it is hard to see a path forward.
- The researchers' work is really excellent, even though they mostly have negative results. The work shows that this technology has real issues and that this can only be demonstrated by careful experimental work. Their go/no-go decision is likely to be a no-go based on their results, but the researchers should continue and explore other options with their very careful and high-quality experimental work. They have built a really nice experimental measurement system and this should be used to explore other options.
- Because the enhanced solubility effect is negligible, the value of additional work in this area is highly questionable.

### Question 5: Proposed future work

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

- The project is well organized and has a good research plan.

- Investigating different solvents and scaffolds is the best avenue open to see if this proposed solubility enhancement has any merit. There is less future in the simulations, especially because the PI indicates that he is unlikely to include hydrogen explicitly in these calculations. The project needs a successful result before simulation can be used to (a) verify that the simulation agrees with the experimental result, (b) give some insight into the mechanism of increased solubility, and (c) explore whether other systems offer better performance. Without a robust experiment to compare with, the value of simulations will always be called into question. Therefore, the PI should focus efforts on experiments that could meet the go/no-go decision later in the year.
- The experimental work is very good, but the computational work is not at the same level due to a lack of expertise. The researchers need to focus on being able to treat hydrogen in their MD simulations. Just looking at the vacant space does not provide much information. They need to use better potentials—such as CLAYFF or one of the force fields for silica—and combine these with the force fields for liquids as published by B. Smit and J. I. Siepmann or the force fields of Peter Cummings. They need to model hydrogen in hexane as the test case for their potentials. The CHARMM potential is probably not the best to use because it was developed for biomolecules such as proteins and DNA in aqueous solution, which is not what they are studying.
- The research project should be rethought based on the new results presented at the review meeting.
- Given the fact that the enhancement effect is either non-existent or much less than previously reported, DOE should consider termination of this project.

### Project strengths:

- A strength was the highly professional way in which the project was handled.
- This project features excellent experimental methods and quality of research.
- This project features excellent, high-quality experimental work and very careful measurements.
- The project is based on novel ideas; some preliminary investigations have already been conducted.
- This project features careful, accurate measurement capabilities and a strong understanding of hydrogen storage.

### Project weaknesses:

- Stronger preliminary studies should have been conducted before the proposal was submitted.
- Unfortunately, the effect reported by earlier workers cannot be reproduced and may be an experimental error. Engagement with the original group could have been given a higher priority.
- The computational aspects could be stronger. There is an issue with the chosen system based on CNRS reports. It is unlikely that it will work.

### Recommendations for additions/deletions to project scope:

- The project should be continued even if the go/no-go is not met in September 2013. The experimental capability should not be lost, because it is very important to the Program.
- It may be fruitful to focus more on experimental measurements and utilize modeling to verify and analyze the observations.
- The researchers should focus on experiment rather than simulation, but even here there is no reason to expect success. The work should be firmly focused on an experimental demonstration to set the go/no-go decision. The relatively low storage capacity measured is unfortunate because the PI has undertaken some excellent experiments and has developed valuable expertise for careful measurements of this type.
- The project should be closed, based on the progress results obtained to date.
- The project should probably be terminated at the September 2013 go/no-go point if no compelling evidence is observed for nano-confined enhancement.

## Project # ST-103: Hydrogen Storage in Metal-Organic Frameworks

Jeffrey Long; Lawrence Berkeley National Laboratory

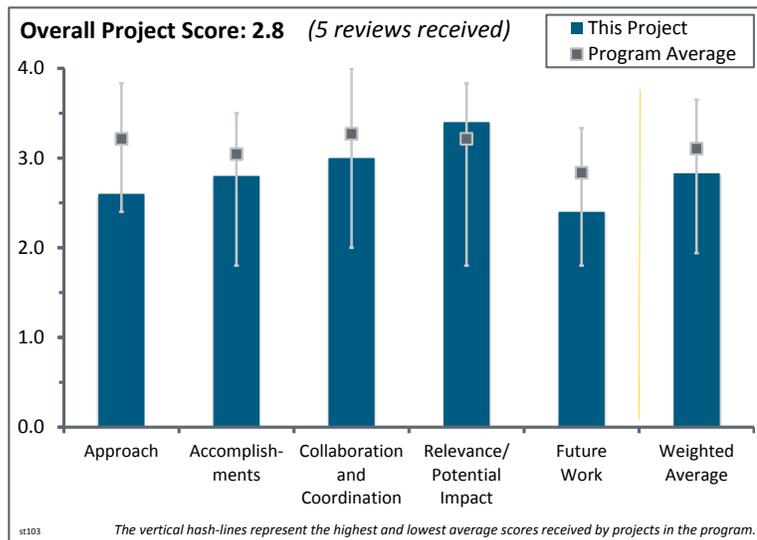
### Brief Summary of Project:

The objectives of this project are to: (1) research and develop onboard hydrogen storage systems that allow for a driving range of greater than 300 miles, (2) identify materials with the potential to meet the U.S. Department of Energy (DOE) mass and volumetric capacity targets for reversible uptake, and (3) synthesize new metal-organic frameworks (MOFs) capable of achieving the adsorption enthalpy required for use as hydrogen storage materials operating under 100 bar at ambient temperatures.

### Question 1: Approach to performing the work

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

- This project uses a combined synthesis, modeling, structural characterization, and hydrogen uptake measurement approach to develop new MOFs that will meet DOE objectives. The project team has the highest qualifications for achieving these goals. The modeling and characterization strategy for optimizing the search for the most promising MOFs is a good approach that will hopefully prove successful.
- This is a high-risk, high-reward project geared toward the synthesis and characterization of MOFs that have highly exposed metal cations that can, in theory, provide active sites for multiple hydrogen binding. This may increase the gravimetric capacity and operating temperature of sorption-based hydrogen storage systems; however, the recourse to higher-surface-area materials with larger pore sizes and extra volume to accommodate analogous ligands than can support the metal cation may lead to lower packing density and thus, lower volumetric density, which is already short of meeting DOE targets. The project should clearly show the advantages and disadvantages of the approach.
- This project has a rather DOE Basic Energy Sciences (BES)-program-level approach and tends toward addressing fundamental issues. Thus, its impact on obtaining the DOE Office of Energy Efficiency and Renewable Energy hydrogen storage goals suffers. The approach from a fundamental science perspective is good, but it may not have a substantial impact on overcoming the mass and volumetric barriers that the chosen materials class faces.
- The group is very good at making and characterizing MOFs. However, a convincing path for improving the enthalpy of adsorption was not provided. It appears that the team is pursuing several approaches without an overarching strategy in mind. Importantly, General Motors' work scope seems to be at odds with the major goals of the project. For example, slide 3 of the presentation states that one goal is to develop MOFs that will work at pressures below 100 bar. It is therefore unclear why the effort is devoted to developing a pressure, concentration, and temperature system that can measure uptake at pressures up to 350 bar. The Hydrogen Storage Engineering Center of Excellence (HSECoE) has shown that at pressures above approximately 200 bar (the "crossover pressure"), physical storage outperforms storage in MOF-5. It is unclear why these high-pressure capabilities are needed. This component of the project should be discontinued unless a clear rationale for its existence can be provided.
- The general approach seems good, with an appropriate balance of empirical and computational effort in developing sorbent materials for hydrogen storage. However, the need for Task 4, development of a high-pressure hydrogen adsorption measurement to 350 bar, is unclear. Previous studies have shown that the benefits of using a sorbent material occur below 200 bar, so a high-pressure measurement device beyond 200 bar is not necessary. The project should focus on demonstrating the feasibility of multiple hydrogens at



a single binding site, which should be further clarified in the approach. Also, the isosteric heat should be consistent throughout the adsorption curve, rather than accepting significant variations.

### **Question 2: Accomplishments and progress toward overall project and U.S. Department of Energy (DOE) goals**

This project was rated **2.8** for its accomplishments and progress.

- Considerable technical accomplishments have been achieved in a short period of time, and most of the milestones have been met. New MOFs should be tested for hydrogen uptake as they are produced, even if at lower pressures than 350 bar; this will be a good predictor of capacity and enthalpy values.
- The project demonstrated the ability to prepare functionality ligands, allowing for post-synthetic insertion of metal cations, and prepared two new MOFs containing coordinatively unsaturated high-valent cations. However, the results of cobalt and nickel analogues show that the higher hydrogen binding enthalpy only exists at low coverage (less than 1 wt.%) and drops sharply to its normal value at higher coverage; therefore, it is presently more of a penalty than an advantage.
- Scientific progress has been very good; however, progress toward overcoming the mass and volume barriers is coming along at a much reduced rate. The progress has been hindered by not having access to adequate, high-pressure measurement systems from the beginning of the project. This task is now only 30% complete, one year into a potentially three-year project.
- The accomplishments were outlined in the presentation, but it was difficult to evaluate if the completed tasks were making enough progress toward the objectives. The isosteric heat curves indicate the potential improvement in binding at the metal sites at low pressure before transitioning to traditional surface adsorption. This characteristic actually could be a negative characteristic because the sorbent material would benefit from having low binding energy at low pressures to maximize capacity.

### **Question 3: Collaboration and coordination with other institutions**

This project was rated **3.0** for its collaboration and coordination.

- The collaboration between the materials side and the neutron scattering effort is clearly going well.
- This project has a very well qualified group of researchers that have demonstrated that they communicate and work together as a productive team.
- The coordination between the project partners seems to be effective. The project could benefit from connecting directly with the effort on adsorbents within the HSECoE to develop a system perspective on the material targets and needs.

### **Question 4: Relevance/potential impact on advancing progress toward DOE research, development, and demonstration (RD&D) goals**

This project was rated **3.4** for its relevance/potential impact.

- The project is highly relevant to the overall DOE Hydrogen and Fuel Cells Program objectives.
- The higher operating temperature of physisorption-based storage will significantly advance progress toward DOE goals.
- This project could have a significant impact if it is able to increase the enthalpy of sorbent materials used as hydrogen storage materials operating at ambient temperatures.
- This project could, in principle, align with DOE RD&D objectives in hydrogen storage. However, the relevance of this project suffers due to the rather BES-like approach. While this results in very good science, the focus on advancing the state of knowledge to address the volume and weight barriers in the applied-research oriented Hydrogen Storage program falls short and limits the potential impact.

### Question 5: Proposed future work

This project was rated **2.4** for its proposed future work.

- The future work appears to have a focused plan. It would be helpful to identify the key steps that could potentially close the significant gap between the current status and the target.
- The volumetric storage capacity is as important as gravimetric, if not more, given the present drawbacks of compressed hydrogen storage. The project should concentrate on improving both, and not one at the expense of the other.
- The in silico screening technique seems very promising. There should be enough data on currently known MOFs to validate the concept. It was a little surprising that more validation of this search method was not presented in this year's work; it should be given a high priority with a go/no-go decision.
- Not many details were provided regarding future plans. It is unclear exactly how computation will be used to guide experiments. Thus far, computation has operated as a reactionary mechanism by calculating enthalpies of known compounds. It is unclear if and how predictive calculations will be performed.
- The proposed future work does not provide a well-designed pathway to address the weight and volume barriers the team has subscribed to toppling. The future plans could be improved by discussing, for example, the potential to improve the hydrogen absorption energies well beyond a few moles per gram of material, or a realistic plan for achieving far more than one mole of hydrogen/metal site in order to provide some relevant pathways to addressing the mass/volume barriers in a meaningful way.

#### Project strengths:

- The project features a good mix of capabilities and expertise for materials synthesis.
- This project features a team that is very good at approaching scientific problems.
- This project features a strong, very knowledgeable team.
- The project has both empirical and computational aspects to the project, which provides a strong validation aspect to the project.
- This project has a well-organized team with clear goals and the potential to meet DOE targets. Work has progressed rapidly, with a number of results to show in the first year. However, more hydrogen uptake and enthalpy data would have been expected at this point. The future work is in line with the strong progress of this project.

#### Project weaknesses:

- This project lacks an overall view of material-based hydrogen storage system requirements.
- More hydrogen uptake and enthalpy data would have been expected at this point.
- The overall direction/strategy is hard to see. The high-pressure measurements seem unnecessary.
- The project should confirm alignment with the system requirements. The project should avoid the development of high-pressure measurement equipment.
- Weaknesses include the lack of high-pressure adsorption characterization capability and the lack of a well-posed roadmap to address the volume/weight barriers in the remaining two years of the project.

#### Recommendations for additions/deletions to project scope:

- The in silico screening technique should be validated using the multitude of current data available, and hydrogen uptake measurements should progress rapidly.
- Once the researchers have an operable calibrated adsorption system, providing both adsorption and desorption data to demonstrate cyclic capacity would be most interesting to determine if the "20kJ/mole fraction" of hydrogen bound to the metal center upon adsorption of hydrogen is released upon pressure letdown under realistic adsorption system temperature ranges. This should be a requirement for all of the projects that are attempting to improve the capacity of adsorption systems by this pathway.
- It is unclear why there was so much effort to go to 350 bar with the characterization when the project objectives include achieving storage under 100 bar. The additional characterization of the volumetric capacity and the reversibility of the synthesized materials would definitely help the project.

- The research team should delete the high-pressure measurements.
- The researchers should delete the effort associated with the high-pressure isotherms or confirm that an adsorption system would still provide a benefit in comparison to a high-pressure compressed system.

## Project # ST-104: Novel Carbon(C)-Boron(B)-Nitrogen(N)-Containing Hydrogen Storage Materials

Shih-Yuan Liu; University of Oregon

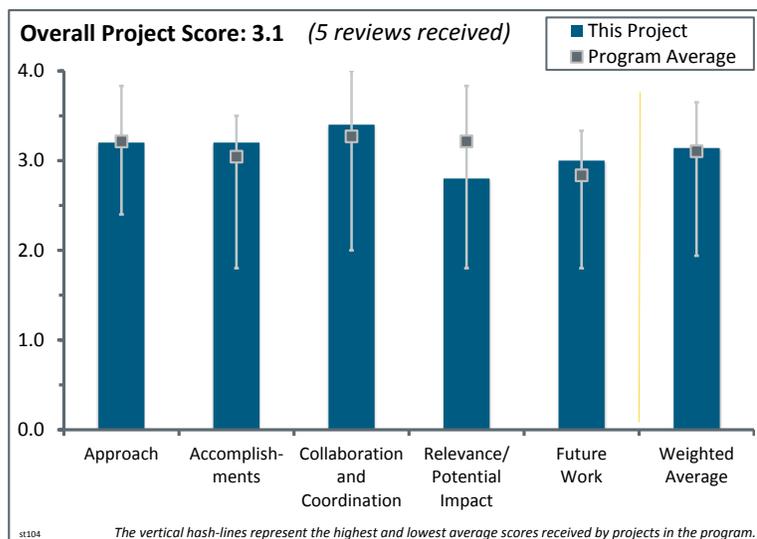
### Brief Summary of Project:

The objective of this project is to develop novel chemical hydrogen storage materials that have the potential to enable non-automotive applications and vehicular applications. The focus of the material development efforts is on compounds that maintain a liquid state while demonstrating reversibility and reasonable kinetics at moderate temperatures. Tasks in this project will address synthesis of proposed materials, characterization and scale-up of the synthesized materials, and fuel cell testing.

### Question 1: Approach to performing the work

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

- It is an interesting approach to attempt to meet sorption metrics with heterocyclic materials of variable structures and physiochemical properties.
- The University of Oregon is leading an integrated project to discover and characterize compounds with the potential to serve as liquid-phase hydrogen storage media. This approach is most appealing because it focuses on providing reactant and product species that can be handled throughout the hydrogen storage process as liquids to facilitate filling and discharging the fuel. The project includes an excellent combination of complementary capabilities that range from the work at the University of Alabama, which utilizes first-principles theory to identify viable candidates from both model thermodynamics and predicted reaction pathways, to the University of Oregon's innovative synthesis methods to synthesize the candidates. The project also characterizes key chemical and physical properties of original compounds and products following hydrogen desorption. The involvement of a fuel cell company to assess the performance of the more promising compounds is very useful in order to identify detrimental issues before committing time and resources to doomed materials.
- The initial approach to this project was excellent. An inspiration based on chemical intuition was backed by a first-rate computational study, which was followed by highly skilled synthesis and characterization of novel compounds. The more recent studies seem to be drifting away from the original goal of developing a hydrogen storage material that can meet the U.S. Department of Energy (DOE) H<sub>2</sub> Storage Light-Duty Vehicle (LDV) targets, but they could be applicable to the DOE H<sub>2</sub> Storage Portable Power targets.
- The project is well defined and contributes to overcoming some barriers. There is clear coordination between computational efforts and experimental synthesis. The project is nicely focused on three classes of compound liquids (in both states), as well as potentially reversible and high-capacity exothermic systems. However, the liquids and reversible systems are likely the most useful. The idea to use Compound B or other liquids as a carrier liquid for ammonia borane (AB) is a great idea and should be considered for other slurry systems (such as AlH<sub>3</sub> and LiAlH<sub>4</sub>) if there are no compatibility issues. The purpose of the polymer electrolyte membrane fuel cell demonstration is unclear. Running a fuel cell for 30 minutes does not really prove anything—it may be better to focus on the mass spectrometry of the released gas to determine impurities.
- The approach to onboard hydrogen storage using recyclable, liquid carriers provides opportunities for the engineering of onboard systems. While many of these “prototype” liquid carriers cannot meet current



gravimetric capacities, they provide an excellent platform for demonstrating the proof of principle of onboard storage systems. The team has demonstrated that hydrogen release from these CBN compounds can occur catalytically and that the catalyst may be a heterogeneous catalyst—a feature that is important both to an engineered hydrogen release reactor and to the contribution to the ease of separation of catalyst prior to regeneration. The approach the team takes is rational. The team aims to take advantage of the propensity of boron-nitrogen-containing compounds to rapidly dehydrogenate, and then to down-select to compounds that remain in the liquid state over the relevant range of conditions in both hydrogenated and dehydrogenated forms. The approach the team takes to develop potentially reversible systems by choosing the thermodynamically middle ground is a good first-order approach, but there is more to reversibility than cataloging compounds that have a delta-G of around zero. The team should better define the meaning of a more detailed analysis of the thermodynamics of practical reversibility. This would be useful guidance for current and any future liquid carrier projects. The approach of using the liquid carrier as a “solvent” for a higher capacity material is a good one, but this approach needs to also incorporate the additional complexity of regenerating an even more complex mixture.

### **Question 2: Accomplishments and progress toward overall project and U.S. Department of Energy (DOE) goals**

This project was rated **3.2** for its accomplishments and progress.

- This project has made excellent progress over the past year. Although there seem to be no clear winners yet, a number of interesting new compounds have been proposed and synthesized. Even if the reversible capacities of these materials remain low, they could be extremely useful as carrier liquids (although this may complicate regeneration somewhat). Experiments with Compound B and AB look especially promising because the spent fuel remains liquid even at room temperature. The isolation and characterization of intermediates that form during decomposition have shown nice progress.
- Much has been accomplished toward several, perhaps not all, of the barriers the team has chosen to address. Good progress has been made in the areas of compound synthesis and characterization. Good initial progress has been shown in providing proof-of-principle fuel cell testing, albeit for a very short time (it is assumed that materials limitations/costs are an impediment here). As usual, the theory component at the University of Alabama has been very productive and focused on the problem at hand—suggesting potential reaction pathways for hydrogen release from these molecular CBN compounds. It speaks to developing a more advanced knowledge of structure-function relationships in this class of hydrogen release compounds.
- Excellent progress has been made toward completing the proposed tasks. The majority of the target compounds have been prepared and characterized, and their dehydrogenation behaviors have been elucidated. A number of insightful mechanistic studies have also been carried out. Unfortunately, the work does not seem to be progressing toward the development of a material that will meet DOE’s targets.
- So far during this project, 9 of the 12 proposed candidates were prepared and at least partially characterized. However, only one (i.e., Compound B, shown on slide 9) appears to be a liquid-state hydrogen carrier and its likely hydrogen storage capacity is only 4.7 wt.%, which is below the 2012 DOE gravimetric target. Substantial characterizations of the relevant chemical and physical properties of Compound B were done at Pacific Northwest National Laboratory. Protonex also tested this material as a hydrogen source to operate a fuel cell. There are numerous issues with various properties, including thermal stability, reverse hydrogen recharging, and impurities in the released hydrogen gas that need further investigation. It is not clear whether these shortfalls can be overcome to provide a practical storage candidate that can satisfy the DOE targets for vehicle or other applications.
- The researchers found a very limited number of materials that had the physiochemical properties needed. However, they did conduct a thorough investigation. The principal investigator (PI) was not aware of the need to retest fuel cells after exposure to hydrogen stored in their materials. The impurities may greatly reduce the longevity of the cells, but a limited test is not adequate.

### Question 3: Collaboration and coordination with other institutions

This project was rated **3.4** for its collaboration and coordination.

- This project features excellent coordination with the theory partner and close, appropriate collaboration with other institutions.
- There appears to be excellent interaction among all four major partners involved in this project. Their activities are very complementary and appear to be highly coordinated. The work seems to be a model of cooperation for other teams to follow.
- The team continues to operate in a very collaborative, open format. The project continues to incorporate input on engineering-related issues such as viscosity, impurities, etc., and thus demonstrates good communication with the Hydrogen Storage Engineering Center of Excellence (HSECoE).
- There is good collaboration and coordination within the project team but no outside collaboration.

### Question 4: Relevance/potential impact on advancing progress toward DOE research, development, and demonstration (RD&D) goals

This project was rated **2.8** for its relevance/potential impact.

- This is one of only a few projects with the potential to significantly advance progress toward DOE RD&D goals and objectives. Similar to other projects of this type (focused on materials discovery), progress often seems slow because no new capacity records have been set. However, this is one of the more promising areas for hydrogen storage at the moment and this is an excellent team.
- The utility of liquid hydrogen carriers in addressing vexing engineering problems in onboard hydrogen storage systems has been well discussed. This project is relevant to providing proof of principle to addressing the utility of a liquid system that can be readily off-boarded for regeneration. The work this project does is relevant to all of the DOE technical barriers the PI has chosen to address, and there are several. The potential impact of the project suffers somewhat because of the rather low available hydrogen capacity, but the project has demonstrated catalytic hydrogen release capacities and kinetics that are more than competitive with other hydrocarbon-based systems. Their impact could improve if the team can demonstrate hydrogen release from the carbon backbone of these compounds, which would result in improved hydrogen capacity.
- The project is generally relevant in the sense that it explores a highly novel class of compounds that expands the horizon of potential hydrogen storage materials and represents the kind of original thinking that will be required to develop materials that meet the DOE targets. However, the dehydrogenation thermodynamics of these compounds prohibit their direct re-hydrogenation. Suitable physical properties are found only with derivatives with unsuitably low hydrogen densities; therefore, the class of compounds appears to be irrelevant to the DOE H<sub>2</sub> Storage LDV targets.
- The problems lie in the level of impurities and the extensive degradation of the materials.
- The team members appear quite aware of the properties and behavior required from both the reactant and products species in order for these hydrogen candidates to be acceptable for hydrogen storage. They should continue to look at all of the issues associated with producing and handling these materials, including hazard and toxicity potentials.

### Question 5: Proposed future work

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

- All of the planned future tasks shown on slide 31 are reasonable and consistent with the objectives of both the project and DOE performance targets. Completion of the efforts needed for the assumed go/no-go assessment at the end of Phase I should be emphasized, including the attempt to prepare Compound E and obtaining more thorough assessments of any other promising candidates.
- The plans clearly build on past progress and are sharply focused on barriers. Compounds E and F look somewhat promising, but full hydrogen removal is needed to access full capacity. It is worthwhile to continue investigations of liquid CBNs as independent storage systems and as carrier liquids with other

high-capacity hydrides (e.g., AB,  $\text{AlH}_3$ ,  $\text{LiAlH}_4$ ). The researchers may want to postpone the fuel cell studies and focus on investigating gas analysis.

- The strength of the PI is in the synthesis of new compounds, the catalysis of hydrogen release, and the regeneration of “spent” fuel, and the future plans largely take advantage of these strengths to continue to address the chosen technical barriers. The project team should either consider (a) the complexity of regeneration of “fuel blends” prior to expending effort in fuel cell testing of blends or (b) what the stationary or portable power requirements are to determine if the fuel blends approach makes sense for a “once-through” approach where maybe regeneration is not the main issue. The researchers should continue to improve the communication of this project with the HSECoE.
- The future plans are not directed toward the development of derivatives that will meet DOE  $\text{H}_2$  Storage LDV targets.

### Project strengths:

- This project is innovative.
- The project is exploring a highly novel class of compounds that expands the horizon of potential hydrogen storage materials.
- There is a good distribution of strong capabilities, as well as collaboration. In general, the plans to move forward are well thought out.
- This is an excellent combination of expertise and capability among the four partner organizations, spanning complementary disciplines. It is good that the researchers are looking at the behavior of Compound B as it supplies hydrogen gas to operate a fuel cell. Similar and longer term evaluations of fuel cell operation are suggested. The past assessments and characterization of AB and related chemical storage compounds are clearly evident in the approaches used with these materials.
- There is excellent coordination between computational and experimental efforts. This type of project can move quickly, using theory to guide the synthesis and materials discovery and further computational efforts to help identify intermediates and reaction pathways. CBN-H materials show good promise, especially the liquids.

### Project weaknesses:

- There are a limited number of materials that meet the physiochemical metrics that are needed to be considered viable. No reversible behavior has been reported yet. There is a lack of longer term testing in fuel cell systems.
- The fuel cell demonstration seems like a distraction because it is not really a good test of impurities or impact on fuel cell performance.
- The limited hydrogen storage capacities of nearly all of the candidates remain a major issue with this approach. More information on the stabilities and reversibility of these compounds is needed. The limited ability of the reactant and or product species to remain in liquid phase or solution at temperatures below 300–350 K could be in doubt. Preparation of sufficiently large batches of well-characterized material should be a concern, along with the quantity and composition of impurities released during formation of the hydrogen gas. Finally, the development of effective catalysts for both decomposition and reformation of the storage materials could be a major challenge.
- The project is narrowly focused on a prohibitively expensive family of compounds with the same structural core. Unfortunately, no derivative has been found or seems likely to be found that has the right combination of physical properties, dehydrogenation thermodynamics, and gravimetric hydrogen density to meet DOE targets.

### Recommendations for additions/deletions to project scope:

- The project focus should be redirected toward the development of a compound that will meet the DOE  $\text{H}_2$  Storage LDV targets.
- The project team should carefully examine the fuel blends issue with respect to regeneration if the main focus going forward is vehicular application.

- The scope of tasks and planned activities is sound at this time (for completing Phase I and transitioning into Phase II). The team should devote more time to searching for and identifying impurities released during the hydrogen desorption under conditions needed to operate fuel cells, as well as looking at intrinsic degradation and thermal stability.

## Project # ST-107: The Quantum Effects of Pore Structure on Hydrogen Adsorption

Raina Olsen; Oak Ridge National Laboratory

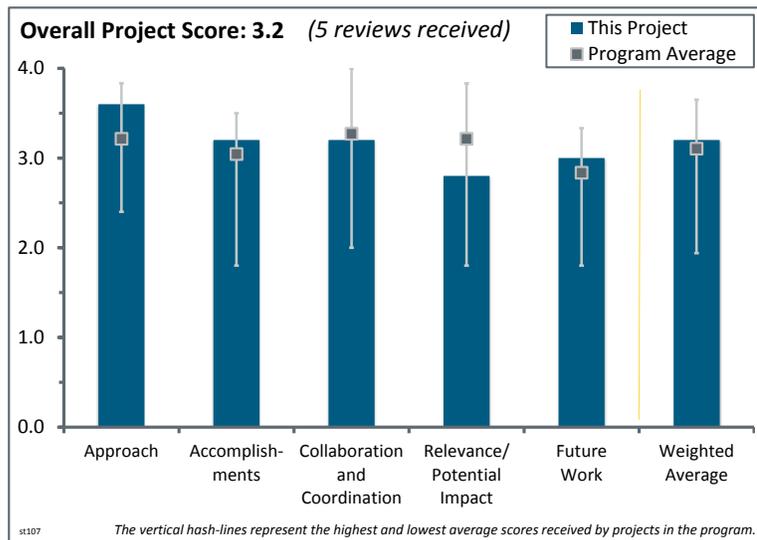
### Brief Summary of Project:

The objective of this project is to understand volumetric and gravimetric storage and hydrogen adsorption in a carbon adsorbent with volumetric storage larger than similar carbons, despite having smaller surface area. The research approach includes experimental study of carbon with high volumetric storage, neutron measurements of quantum states of adsorbed hydrogen, and theoretical calculations of quantum states and quantum adsorption effects.

### Question 1: Approach to performing the work

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

- The approach to interrogate the carbon adsorbent HS;0B appears to be sound.
- The approach demonstrates a good handle on the use of some theory in conjunction with neutron scattering to attempt to develop a working model of what may be an unusual adsorption site on a particular carbon sample.
- Inelastic neutron scattering is used for measurement of quantum states of hydrogen molecules while they are adsorbed on carbon samples. Computational work is performed in order to understand quantum states and propose a quantum model of adsorption. This is an interesting plan, which may lead to new fundamental science insight.
- This project seeks to explore the phenomenon of excess hydrogen absorption in activated carbons at low temperatures. Experimental evidence for the effect is presented, and a model based on the formation of a Bose-Einstein condensate (BEC) is advanced. Proving the existence of a BEC is no mean feat: preliminary evidence from neutron diffraction experiments is consistent with the phenomenon but key experiments remain to be conducted.
- The approach is generally sound and is directed toward important barriers in hydrogen storage capacity. The link between experiment and theory could be improved. A new BEC has been proposed that could help address the DOE goals, but the experimental evidence to support the existence of this BEC is somewhat tenuous. The inelastic neutron results show some features that are consistent with the proposed structures, but not fully convincing. The principal investigator (PI) noted that more and better DINS data are needed, for example. The proposed pores arising from defects between graphite layers are also somewhat speculative at this stage. It is understood that the flake morphology of the sample naturally aligns graphene layers perpendicular to the TEM viewing direction; nevertheless, the team did not find any of the proposed pores among the observable graphene sheets. It would also be possible (but admittedly more difficult) to prepare TEM specimens looking along the plane of the flakes by cross-sectioning specimens mounted in epoxy, for example, and/or by using FIB/SEM to cut out sections from flakes. In the long term, it would seem necessary to correlate the concentration of slit pores with observed INS features and increased adsorption if the theory is to have merit in addressing storage barriers.



## Question 2: Accomplishments and progress toward overall project and U.S. Department of Energy (DOE) goals

This project was rated **3.2** for its accomplishments and progress.

- Data has been measured and the analysis is in progress.
- The project is making good progress in identifying and characterizing BECs in an unusual hydrogen sorption site. The combination of sorption, Raman, neutrons, and microscopy appears to be well integrated and well thought out. The project addresses the very difficult problem of finding “the needle in a haystack” in these complex, highly heterogeneous materials.
- This is a technically challenging project for which there exist only a limited number of available techniques to explore the unusual behavior of hydrogen in the pores of the activated carbon. Significant progress has been made in characterizing the structural features of the carbon and with the neutron scattering experiments performed to date.
- The HS;0B sample was characterized by a multitude of techniques. Data was not seen in the slides on how many samples/batches were evaluated, but perhaps there was a comment on this during the talk. The researcher seemed well versed in all of the applied characterization techniques and their limitations.
- This is difficult to assess for this project, which is mostly concerned with quantum states in adsorbents and how these might lead to progress toward DOE goals. The accomplishments are in establishing a theory, and the experimental measurements presented are in support of this. The approach is in line with the stated objective of understanding the unusually high capacity of a particular carbon adsorbent. With this approach, progress shows no improvement in the DOE performance indicators (in this case, gravimetric and volumetric storage capacity). However, this does not seem to be the objective of the project, and capacity could improve in the long term as a result of the understanding obtained in the current project. Given the length of time remaining, however, it is unlikely that any improvement in the demonstrated storage capacity will result.

## Question 3: Collaboration and coordination with other institutions

This project was rated **3.2** for its collaboration and coordination.

- There is a strong network of collaborators compared to the small size of the project.
- Good collaborations have been formed within Oak Ridge National Laboratory (ORNL) and experience has been gained for postdoctoral research.
- Appropriate collaborations have been established with other researchers at ORNL and with the University of Missouri - Columbia.
- This project features good collaborative efforts with other ORNL groups, the PI’s graduate university, and Buffalo. These bring a wide range of different synthetic, analytical, and computational tools; however, some are a little cursory. X-ray diffraction of primarily amorphous materials is not especially illuminating unless a full Pair Distribution Function analysis is undertaken. The small Raman probe could be used to map the different features in the sample and give some quantitative idea of the heterogeneity. However, the real heterogeneity is likely on a finer scale than the Raman laser and the results obtained may relate to the physical orientation of flakes because Raman signals are sensitive to the relationship between bond direction and laser polarization.

## Question 4: Relevance/potential impact on advancing progress toward DOE research, development, and demonstration (RD&D) goals

This project was rated **2.8** for its relevance/potential impact.

- This is a highly relevant project, seen from a fundamental science point of view.
- The project is clearly relevant to DOE goals. Understanding physisorption, especially new mechanisms, is an important route for developing new materials with improved properties.
- This project is longer term and more speculative in its objectives than most of the others presented at the DOE Hydrogen and Fuel Cells Program Annual Merit Review; but, if successful, it would represent a

paradigm change in the approach to hydrogen storage and the capabilities of carbon-based (and other) porous materials. So, although it is not critical to the current activities in the Hydrogen Storage Engineering Center of Excellence, if successful, it would supplant much of the current work in this area.

- In principle, better understanding of the local structure that gives rise to the unusual adsorption phenomenon in the carbon materials studies can lead to new ideas in sorption studies that could be of potential relevance to improved overall gas sorption in solids.
- Slide 3 indicates a maximum of 4.39 wt.% stored hydrogen at 300 K. Although larger than MSC-30, this material clearly will not meet the near-term (2017) material target of approximately 11%. The characteristics of the HS;0B material are curious; they would make an excellent DOE Basic Energy Sciences project, but they do not have the potential to meet the DOE targets. A better understanding of this material, and the underlying phenomena, may allow a future material to be engineered.

### Question 5: Proposed future work

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

- This project features a good research plan.
- The proposed future work is sound and builds on progress to date. A hydrogen deuteride (HD) experiment should be conducted as a priority.
- The additional neutron scattering experiments planned will be very valuable in verifying the proposed quantum mechanism because the current results are consistent but not completely convincing. If the results are positive, then further experimental effort should be directed toward identifying the relevant features in the sample.
- The proposed graphene oxide frameworks may be a better way to verify the effect. The inter sheet spacing of these structures appears to be in the <1 nm range proposed and highly regular, judging from the diffraction peaks. These would therefore present a much larger and controlled area that relates more strongly to the theoretical systems studied.
- It is unclear what potential impact the impurities (rust, NaCl) might have on this material. It is unclear if it is possible to make this material in an inert atmosphere, using an acid-cleaned steel container, so as to avoid the “chunks of stainless steel” mentioned on slide 7. Phil Parilla mentioned that the most common impurity in hydrogen sources is H<sub>2</sub>O, due to a possible reaction with rust in the tank and subsequent reduction. Additional experimentation to evaluate the impact of water on the carbon performance seems warranted (and a subsequent reevaluation of the synthetic method).
- While the project is ending, the final activities described are good. Examining other “new” carbons for this effect is rational; also, it would be of interest to perhaps look at additional batches of HS;0B to examine whether there is a batch-to-batch reproducibility, particularly because there was apparently a good amount of iron oxides observed. Perhaps this could be related to or associated with the “unusual” porosity.

### Project strengths:

- This project features a good combination of experimental and theoretical work.
- This project features an original and ambitious approach.
- This project features good integration of many skills, particularly for a postdoctoral project.
- This project features good productivity, a high degree of novelty, and the possibility of impacting DOE goals.

### Project weaknesses:

- The experimental work is difficult and requires specialist facilities (this cannot be avoided).
- At present, much of the work is speculative or supported by experimental data that does not have an unambiguous or definitive interpretation.
- It is unclear how the hypothetical wt. % of stored hydrogen on slide 3 was calculated. In the future, the researchers should annotate the technical backup slides (especially slide 21) so the reviewers can be more quickly calibrated to the spectroscopies used.

**Recommendations for additions/deletions to project scope:**

- Measurement of the performance of HD under similar conditions is highly recommended. HD is a fermion and will not exhibit a BEC. This experiment could deliver definitive proof of the nature of the observed phenomena.

## Project # ST-108: Metallation of Metal-Organic Frameworks: En Route to Ambient Temperature Storage of Molecular Hydrogen

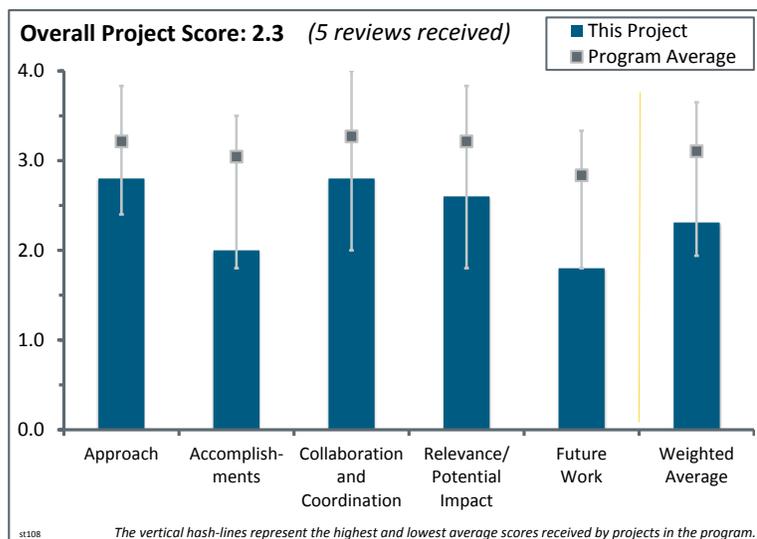
Joseph Mondloch; Northwestern University

### Brief Summary of Project:

The objectives of this project are to: (1) develop functionalized sorbents for metallation, (2) deposit metal ions by solution and atomic layer deposition, and (3) characterize materials and performance. The project adopts an iterative computational and experimental approach to depositing coordinatively unsaturated metal ions on functionalized sorbents.

### Question 1: Approach to performing the work

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



- This project has a combined experimental and theoretical approach, which is good.
- The project represents a good exploratory approach to improving sorption properties. The approach is rationally based and extends the work from prior observations that metal ions on frameworks interact with dihydrogen, increasing the sorption energy. The approach involved using several materials platforms to search for evidence of enhanced quantities and energies of sorbed hydrogen on modified materials. It would be valuable and instructive to carry out desorption experiments on such metal modified materials to ascertain whether or not the hydrogen bound at higher energies is desorbed under the “usual” conditions.
- The project has followed sound ideas to improving the storage capacity of metal-organic frameworks (MOFs) by attempting to add additional metal sites for hydrogen adsorption. There are other U.S. Department of Energy (DOE) Hydrogen and Fuel Cells Program (Program) projects that are exploring similar avenues. The barriers listed on slide 2 are project goals rather than Program-defined barriers. The investigators should use the Program barriers in the future to show how they are focused on DOE objectives, as suggested on slide 3, where reference to gravimetric and volumetric targets is made. The iterative experimental/computational approach has been overstated. Two slides were dedicated to this. Such an approach is fairly common and may be worth mentioning, but the investigators should focus more on the real approach and accomplishments. Aside from the  $Q_{st}$  figures on slide 8, there is little evidence of an iterative experimental/computational approach anyway.
- The experimental/computational synergy is a common approach. The reference article does expound on the method, but it only describes the synthesis of a single MOF to “validate” the method, and the resulting MOF did not perform substantially better than an already known MOF of similar structure (the authors claim the competing MOF has higher methane coordination than their model predicted—additional evidence that the model is poor). Nearly half of the slides are on the approach. Because the project is close to the end, a more concise overview (even though a presentation or poster from last year could not be found) was expected. The project team should convert its gravimetric densities into weight percent of hydrogen in the future. It is very difficult to gauge progress (or potential progress) when everyone uses a different unit in each talk. Also, a percentage excess of the target is a preferred value rather than absolute value.
- This is a postdoctoral research grant to examine the metallization of MOFs. It is clear that there is a very nice balance of autonomy for the postdoctoral researcher to lead the work and guidance/supervision from the mentors, Dr. Joseph Hupp and Dr. Omar Farha. The investigator tried two approaches to metallization of MOFs (i.e., atomic layer deposition and solution deposition). The result was that the metallization (or metallation) of the MOF PAF-1 by both approaches led to a decrease in surface area and has not resulted in

achieving the goal of unsaturated metal sites on the MOFs. However, the MIL-101 MOF was able to be metallated without significant loss in surface area. Other issues arose surrounding the loss in crystallinity in the MOF and the limited increase in the enthalpy of adsorption. This increase in adsorption enthalpy was predicted to occur computationally for  $Zn_{2+}$  and  $Mg_{2+}$  metallation. With further research, it is possible to overcome these barriers in the MIL-101 system.

## Question 2: Accomplishments and progress toward overall project and U.S. Department of Energy (DOE) goals

This project was rated **2.0** for its accomplishments and progress.

- The project made good progress, and the postdoctoral student gained great value in carrying out this work and forming collaborations to study and characterize the complex materials he was working with. While many of the results were negative results, this exploratory approach is valuable in setting out what can work and what may not work in future approaches to using highly metallated open framework materials as gas sorbents. Progress was made in demonstrating that small aperture materials present problems when involving molecular chemical approaches to the metallation of ligand sites within the void volume. In at least one system, improvements were made in enhancing the energy of hydrogen binding to (presumably) metal sites, with binding energies demonstrated up to 7 kJ/mol and with up to 2 mmol of hydrogen being bound with higher energy than the unmodified framework material.
- The researchers should include a single bullet point at the bottom of each slide indicating the take-home message. It is easier to evaluate progress this way, even for reviewers who attended the session. On slide 12, the researchers should annotate the plots. It is unclear if one data series represented a control. It is unclear if slide 14 is really an accomplishment or if it is an advertisement. If intellectual property issues prevent the researchers from sharing sufficient information to show progress, they should exclude these slides in the future.
- The research encountered a major and seemingly unexpected barrier in the difficulty of metallation (due to small pore sizes). Pore clogging is likely occurring for both techniques. Although progress has been slow, the decision to move to a different MOF (i.e., from PAF-1 to MIL-101) was a good one. The  $-NH_2$  and  $-OH$  functionalized MIL-101 remained porous. This is a step in the right direction. It is unclear whether the MIL-101 remained porous because of the  $-NH_2$  and  $-OH$  functionalization or because the pore sizes in the MIL-101 were larger than those in the PAF-1. This would have been useful to discuss (and might have guided this work a step further toward a different MOF structure for which the overall strategy of lowering the enthalpy of adsorption by metallization might have been accomplished).
- The project goal to achieve physisorption enthalpy in the range of 15–25 kJ/mol appears to be very optimistic. On one hand, the experimental improvements are small (60%) or about 7 kJ/mol, similar to other unmodified porous materials. On the other hand, the computationally predicted  $Q_{st}$  values are very high (and unrealistic) for physisorption of molecular hydrogen. There appear to be a significant discrepancy between the theoretical and experimental results.
- Although a substantial amount of work has been reported, the results have been somewhat unfortunate and it does not look like any Program barriers have been overcome. The investigators have addressed some of their own “barriers” by depositing metals inside an MOF. This does not appear to have resulted in a significant increase in hydrogen adsorption, even if a small increase in  $Q_{st}$  was observed (from a very low starting value). It would have been good to have seen a better presentation and analysis of some of the data. The data in slide 11 has no legend and so it is unclear whether functionalization has improved hydrogen adsorption. Using values related to the DOE targets (wt  $H_2$ /wt material, instead of  $cm^3/g$  or  $mmol/g$ ) would have made the adsorption more readily understandable in relation to the barriers. Also, the adsorption shown on slide 17 is normalized to surface area (although the units are not). Because the surface area of the copper-atomic layer deposition sample was not given, it is not possible to understand the absolute adsorption. The presenter did note this, but it gives the impression that the authors are trying to present the data in the best light rather than show understanding. For these data, perhaps it is possible to compare all of the materials on the basis of moles MOF rather than weight MOF. Maybe both could be given. Because metal:zirconium ratios are known, presumably the surface area, pore size, pore volume, and even adsorption could be compared for the same quantity of zirconium. This would then allow a quick understanding of how the properties have changed as a result of metal addition; for example, how much of the specific surface area change is a result of the increased weight of the MOF. Similarly, it would be good

to know how the increased  $Q_{st}$  shown in slide 17 correlates with the amount of copper in the MOF. It is unclear if the inflection or point where the two curves coincide corresponds to the amount of copper.

### Question 3: Collaboration and coordination with other institutions

This project was rated **2.8** for its collaboration and coordination.

- This project features a good range of collaborators from various institutions that are all contributing complementary information.
- The project appears to be well coordinated, and the number of partners and collaborators compares well to the funding for this project.
- This project features good collaboration at the postdoctoral level in the relevant areas of computation and modeling, materials synthesis and modification, and materials characterization, among others. It is likely that the postdoctoral student gained very valuable experience in performing multidisciplinary studies.
- Although many collaborators are listed on slide 18, the contributions of those collaborators are not highlighted well within the technical slides. The technical slides present work primarily accomplished at Northwestern University.

### Question 4: Relevance/potential impact on advancing progress toward DOE research, development, and demonstration (RD&D) goals

This project was rated **2.6** for its relevance/potential impact.

- The project is clearly focused on improving the storage capacity of porous frameworks and therefore supports the objectives of the Program.
- The project goal of tailoring the enthalpy of adsorption by metallation with unsaturated metal sites is well within the DOE objectives.
- Improving hydrogen sorption energies beyond what has been shown to be available in conventional sorbents is a goal of the Program's RD&D plan; the potential impact of this project's approach would be very high if a higher heat of sorption could be found at hydrogen loadings of greater than just a few mmole/g material.
- There is significant disagreement between theoretically predicted data and experimentally measured data. It is unclear to which extent the metallation will compromise the storage capacity by increasing the weight of the storage material and decreasing the surface area of the porous structure.
- Although it is evident that more hydrogen can be stored if a  $Q_{st}$  of 15–25 kJ/mol is achieved, it is not clear how much hydrogen can then be removed from the system. If a room temperature material can store 7–8 wt.% of hydrogen but only deliver three-quarters or one-half of that amount, it is unclear how these materials are better than cryo-compressed hydrogen. The researchers should see the previous presentations by Dr. Snurr for some data in this regard and present estimates of deliverable hydrogen in the future, directly beside the DOE targets, so that reviewers can quickly gauge the project's progress.

### Question 5: Proposed future work

This project was rated **1.8** for its proposed future work.

- The presentation indicates that the metallization leads to decreased surface area. It should be estimated how much the modification of the porous materials compromises the gravimetric and volumetric hydrogen storage densities, both due to the increased mass of the scaffold and the decreased surface area.
- While the project is ending at the conclusion of the postdoctoral student's tenure, the "future work" area was sparse, considering that six months still remain for the project. More details on what the final six months could entail would be useful.
- Even though this project is nearly complete, the "Future Work" section should be treated as what the researchers would do should the project continue, so that future researchers can learn from this work. It is unclear what exactly "iterative materials feedback" entails when the experimental techniques either failed

or resulted in no  $Q_{st}$  improvement. It is unclear whether the model will suggest new ways to metallate or suggest MOF precursors that will produce larger pore structures that you could not guess on your own.

- Although a clear solution to the problem of MOF metallation has not been achieved (the metallation process still has barriers), the investigators propose to move onward to examining other metals (slide 19 lists more than 60 metals of interest). This does not seem like a logical step forward. The investigators might first try to understand the role (if any) of  $-NH_2$  and  $-OH$  functionalization in the success of metallation for MIL-101. It is unclear how MOF pore size or surface area affect metallation. These are fundamental questions that should be tackled before moving on to other metals of interest. The study of hydrogen sorption dynamics (in situ) is good future work to pursue.
- The proposed future work was not described especially well and does not appear to be focused on overcoming barriers. It is concerning that insufficient time remains for “Iterative materials feedback” to produce significant results before the project finishes in November 2013. The summary slide indicates that future research will “use computational guidance to further metallate our functional MOF....” It is unclear whether the computation has been shown to make useful predictions in these systems. For example, the start of the presentation shows computed  $Q_{st}$  in unnamed MOFs to be  $-84$  kJ/mol for copper; the measured figure was  $-7$  kJ/mol (probably in a different MOF). There are at least three metallated MOFs shown on slide 16. It would seem sensible to compute and measure  $Q_{st}$  for all of these to see if the computational method is an accurate predictor before launching into new systems.

#### Project strengths:

- This project features an exploratory route to open framework materials modifications.
- The project objectives are clearly stated and important to meeting DOE goals for sorbent materials. If successful at developing an approach for adding unsaturated metal sites to MOFs (in order to change the enthalpy of adsorption), this project will have a very large impact on the future of hydrogen sorbent materials. The investigators examine two approaches to metallation. This is very good. The project is challenging because of the loss in surface area on the MOFs after metallation. This barrier was overcome by changing to a different MOF (specifically, a functionalized MOF).
- Some high-storage capacities for materials are under investigation.

#### Project weaknesses:

- There appear to be a significant discrepancy between the theoretical and experimental results.
- The path forward to developing better materials is not well focused. The project gives the appearance of trying a range of materials to see what works.
- There is poor evidence that theoretical methods will really help MOF development. There was no assumptions slide at the end.
- The investigators should take more steps in the direction of varying MOF type (i.e., pore size) and functional groups.

#### Recommendations for additions/deletions to project scope:

- The researchers should conduct desorption measurements on metal modified frameworks.

## 2013 — Fuel Cells

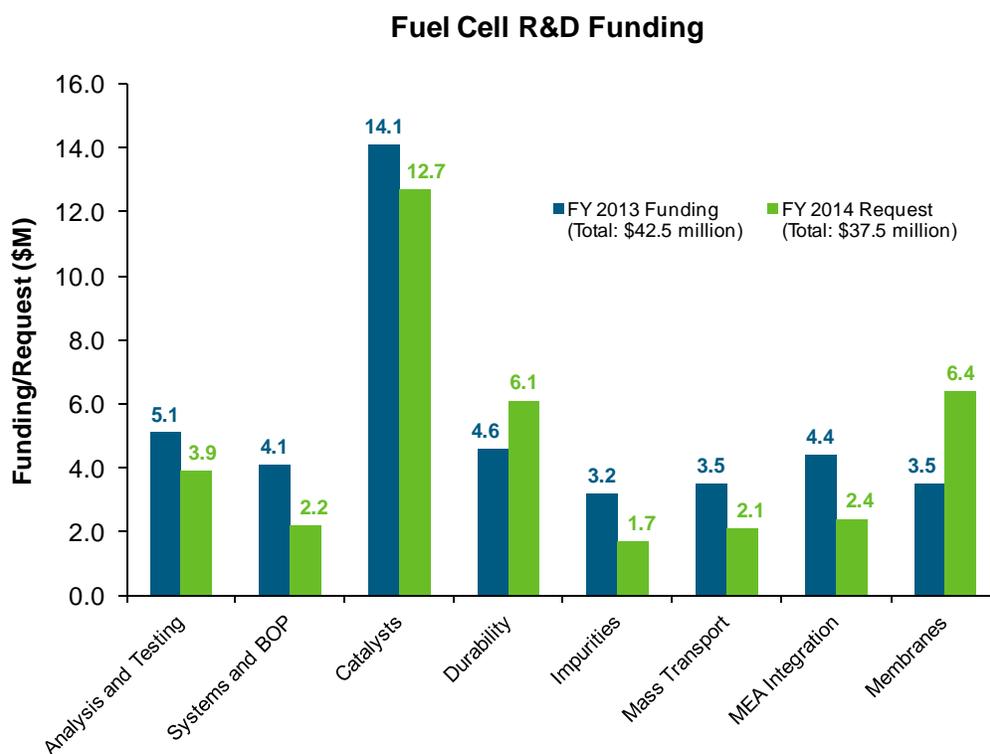
### Summary of Annual Merit Review of the Fuel Cells Program

#### Summary of Reviewer Comments on the Fuel Cells Program:

Consistent with previous years, reviewers commended the Fuel Cells program for being well managed and clearly focused, with annual progress demonstrated. They noted that key challenges were identified, a strategy was in place to address those challenges, and that the project portfolio was appropriate to address the key challenges. However, reviewers commented that certain areas of the portfolio need to be further strengthened and that fuel cell system cost projections are based on some high-risk components. They also expressed concern about the lag in new starts due to the recent shift in forward funding projects.

#### Fuel Cells Funding by Technology:

The Fuel Cells program received \$42.5 million in fiscal year (FY) 2013 and \$37.5 million is requested for FY 2014. The program continues to focus on reducing costs and improving durability, with an emphasis on fuel cell stack components. Efforts are balanced to achieve a comprehensive approach to fuel cells for near-, mid-, and longer-term applications. Three new projects were initiated in FY 2013 focusing on balance-of-plant (BOP) and catalyst improvements.



#### Majority of Reviewer Comments and Recommendations:

At this year's review, 47 projects funded by the Fuel Cells program were presented and 37 were reviewed. Projects were reviewed by between five and nine reviewers, with an average of seven experts reviewing each project. Reviewer scores for these projects ranged from 2.4 to 3.6, with an average score of 3.1. This year's highest score of 3.6 and average score of 3.1 were similar to last year's highest and average scores of 3.6 and 3.0, respectively. The lowest score of 2.4 for all projects reviewed in 2013 was an improvement over 2012's low score of 1.8 for all projects reviewed.

**Analysis and Testing:** Ten projects were reviewed and received scores between 2.7 and 3.6, with an average score of 3.3. According to the reviewers, the analysis and testing projects benefited from good collaboration, but the reviewers were concerned that the lowest-scoring project lacked focus.

**Systems and BOP:** Five systems and BOP projects were reviewed this year, with scores ranging from 2.4 to 3.5 and an average score of 3.0. Reviewers commended the highest-scoring project for making significant progress toward meeting its goals. The reviewers were concerned that the lowest-scoring project had technical challenges that hindered its success. They suggested adding additional modeling to help identify the best path forward.

**Catalysts:** The scores for the 12 catalyst projects ranged from 2.6 to 3.5, with an average of 3.1. The highest-scoring project was praised by the reviewers for being well organized and for making significant progress toward addressing degradation due to start-up/shutdown events. Reviewers expressed concern that not enough detail was included in the presentation for the lowest-scoring project.

**Durability:** The two durability projects received scores of 3.0 and 3.1. Reviewers praised the durability projects for being sharply focused and for making good progress toward a significant challenge. In some instances, the reviewers recommended studying durability at the molecular level; current studies are at the system level.

**Impurities:** The two impurities projects reviewed received scores of 2.7 and 3.3. Reviewers felt that the highest value of the highest-scoring project was its materials screening effort; however, they noted that the outcomes cannot be fully applied to improve fuel cell durability without better understanding the degradation mechanism. The reviewers had similar concerns for the lowest-scoring project, as well as concerns that impurity concentrations were not aligned with what would be observed under operating conditions.

**Mass Transport:** The three mass transport projects reviewed received scores ranging from 2.7 to 3.3, with an average score of 2.9. Reviewers considered the transport projects to be doing a good job of solving a complex modeling problem. The reviewers recommended performing sensitivity analyses to better understand the role of each variable.

**Membrane Electrode Assembly (MEA) Integration:** One MEA integration project was reviewed, receiving a score of 3.0. Reviewers considered the project to have a good balance of applied research and development. They recommended that the principal investigator address water management and low-temperature operation.

**Membranes:** The two membrane projects reviewed received scores of 2.4 and 3.1. The reviewers considered the highest-rated project to have a good approach and to be clearly focused, but they were interested in better understanding the cost impact and benefit compared to traditional supported membranes. The reviewers consider the approach taken for the lowest-scoring project to be good for increasing MEA area, but they doubt that it will be able to overcome the cost and performance barriers that this project is intended to address.

## Project # FC-006: Durable Catalysts for Fuel Cell Protection During Transient Conditions

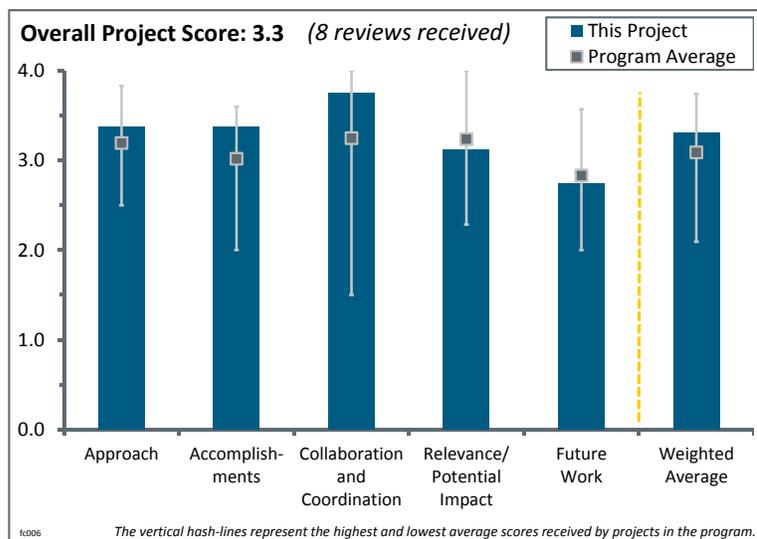
Radoslav Atanasoski; 3M

### Brief Summary of Project:

Developing catalysts that will enable polymer electrolyte membrane (PEM) fuel cell systems to weather the damaging conditions in individual fuel cells during transient periods of fuel starvation makes it possible to satisfy 2015 U.S.

Department of Energy (DOE) targets for catalyst performance, platinum group metal (PGM) loading, and durability. Fuel starvation could result in high positive voltages at the cathode during start-up/shutdown (SU/SD) or at the anode during cell reversal. This project develops a catalyst that favors the oxidation of water over the dissolution of platinum (Pt) and carbon (C) at voltages

encountered beyond the range of normal fuel cell operation and beyond the thermodynamic stability of water (greater than 1.23 volts).



### Question 1: Approach to performing the work

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

- The project is well designed and focused on overcoming barriers.
- This project's focus and progress to date on a "materials-based solution" to improve catalyst performance and durability will enable the simplification of fuel cell control and operation.
- The approach of this project is unique to currently funded DOE Fuel Cell Technologies Office projects—to develop a material approach to limit the degradation due to SU/SD and cell reversals by modification of the anode (versus the cathode), thus suppressing the oxygen reduction reaction (ORR) activity on the anode catalyst.
- The materials approach to protect the cathode during SU/SD or cell reversal and use relatively low-PGM catalyst loading is a great approach because it is always "on." No monitoring or controls are needed, as in a system approach. The key is that catalyst durability is improved and the cost of the catalyst is kept low in order to achieve DOE cost targets.
- 3M has developed an innovative approach to try to address fuel cell start-stop degradation and fuel starvation. It is a materials-based approach that does not depend on system mitigation. 3M has applied the inclusion of high oxygen evolution reaction (OER) catalysts on the cathode and low ORR catalysts on the anode with nanostructured thin film (NSTF) electrodes. The approach would prove more universally valuable if also applied on non-corrosion-resistant electrodes such as dispersed catalysts on carbon. The 3M approach includes testing at relevant start-stop conditions and H<sub>2</sub> starvation conditions, as well as stack-level testing.
- The project features a good balance of fundamental studies and testing under real-world conditions. Utilizing the Automotive Fuel Cell Cooperation (AFCC) to provide gas switching under real-world conditions allowed for the discovery of issues at low OER catalyst loadings that were not observable under simulated conditions. Fundamental studies of Ru-Ir-Perylene interactions should provide insight into differences observed between the laboratory's potential studies and AFCC's gas switching studies.
- The approach is sound; however, using catalysts that enhance the OER rates for the anode reaction is relatively known in the field. The durability of these catalysts in start-stop test conditions has always been

a concern. Further, while reduction in Pt loading for the anode is directionally correct, the impact of fuel cell contamination is a concern and was not evaluated.

- Although this project does address the serious durability issue of start–stop decay, it attempts to do so in a manner that has very limited decay-mitigation potential. In other words, even if the project is technically successful, the decay will still be greater than acceptable, and other mitigations will be required to meet the durability targets. Because these other (system-level) mitigations can enable the targets to be exceeded without this technology, the value of this technology is questionable. This approach may have merit in applications where only minimal mitigation of decay is required. It would appear that the researchers at UTC Power (who first reported on this decay mechanism) agree—UTC patented this approach some time ago, but there is no evidence that UTC attempted to reduce it to practice; please see Bett, et. al., in U.S. Patent 6,855,453 (2005).

## Question 2: Accomplishments and progress toward overall project and U.S. Department of Energy (DOE) goals

This project was rated **3.4** for its accomplishments and progress.

- Excellent progress has been made toward DOE goals.
- The project developed and demonstrated catalysts with improved resistance to OER and ORR conditions.
- The team has done an excellent job of implementing this secondary strategy and demonstrating the results in a complete stack at AFCC. As expected, the decay rate is still unacceptably high (>100 mV with only 2,000 cycles). Additionally, the team has not provided a good baseline for comparisons; although the team claimed that three stacks at AFCC have been built, the cyclic decay results for only one are presented herein. A “40% to 50%” improvement is claimed, but no data were provided to support this improvement on a stack level.
- In 2013, 3M and the team have done an excellent job of optimizing their electrodes to maximize mitigation effectiveness while minimizing the effect on performance during normal operating conditions. It is hard to truly assess the viability of the mitigation because details of the durability protocols were not provided. The gas switching and original equipment manufacturer (OEM) cycling protocols would be especially important to disclose. There is also no comparative benchmark for the AFCC short stack cycling results. 3M also showed that membrane additives can inhibit OERs at high voltages, yet the significance of this during actual start–stop testing is unclear. It would be nice to know if 3M’s OER catalysts are subject to degradation during conventional (0.6–1.0) voltage cycling, which could limit its ultimate effectiveness.
- The project has met all of its initial milestones. 3M has demonstrated stability over 5,000 start-up cycles with <0.1 mg PGM/cm<sup>2</sup> on the cathode. 3M has demonstrated considerable durability improvements over current commercial catalysts. The project has progressed to the state that two separate OEMs are evaluating this technology. Testing at AFCC indicates that more work needs to be done but that the technology has the potential to meet automotive durability requirements under real-world conditions.
- Significant accomplishments and progress seem to have been made toward objectives and overcoming the durability barriers. The researchers have demonstrated that relatively low catalyst loading (29 ug/cm<sup>2</sup>) can inhibit ORR activity on the anode, and the ORR inhibition has been verified in stack testing. They have shown improved cathode protection of 40% to 50% over the baseline OER catalyst during SU/SD and that the OER catalyst did not impact the overall fuel cell performance. They have also shown some work toward the understanding of cell reversal on Pt, Ir, and Ru loss and where they end up, as well as the effect of low catalyst loading on the catalyst structure and morphology. However, how or why this happens is not yet understood. More work toward this would be useful in developing a more durable catalyst. It is unclear how the SU/SD protocol affects the OER catalyst. Understanding the mechanism of this would be useful toward developing more durable catalysts (slide 7). It is unclear what “modified” means and whether the same “modification” is done for all “modified” catalysts. It is unclear why the modified catalyst suppresses ORR on the anode more significantly than the unmodified one at the same catalyst loading of 29 ug/cm<sup>2</sup>.
- The project has made modest progress towards accomplishing the goals of cost reduction. The researchers have achieved reduction in anode catalyst loading and improved the end voltage for reversal. However, the durability of the same catalyst in simulated start–stop conditions is not meeting expectations. Further, the progress compared to the 2012 DOE Hydrogen and Fuel Cells Program Annual Merit Review seems rather small.

- The researchers developed and tested a low-PGM modified anode with IrRu showing ORR suppression, yet had a hydrogen oxidation reaction (HOR) performance that should not be limiting. Approximately 50% cathode protection was observed (over the baseline). To determine how good this improvement is, the baseline cathode material and carbon material need to be known. It appears to be a relatively high loading of 0.4 mg/cm<sup>2</sup>. More information on the testing protocols, especially the stack testing protocols, would be helpful to other projects. While anode modifications are shown to be valuable, there still seems to be a relatively large decay over 2,000 SU/SD cycles, which is beyond the commercialization targets. More definitive results on what degradation mechanisms are at play would be useful.

### Question 3: Collaboration and coordination with other institutions

This project was rated **3.8** for its collaboration and coordination.

- This project features very close collaboration between industry and academic institutions.
- This project seems to be well integrated with its partners. Materials development, materials characterization, and materials testing all seem to be well integrated.
- The assembled team is excellent. It features a university partner that can do catalyst synthesis and basic characterization, national laboratory partners that can do advanced characterization, and industry partners that can do independent evaluation and short stack testing. The coordination and integration of the collaborators in the project are also excellent.
- This project shows effective collaboration between a materials developer (3M), a university, national laboratories, and an OEM. Without the full range of fundamental studies, applied research, and real-world testing employed, the project would not be as advanced as it is.
- 3M has put together an outstanding team with members that all seem to make valuable contributions. The fuel cell testing at AFCC has been essential to validation of the concept on OEM conditions. Dalhausie and Oak Ridge National Laboratory have been essential in verifying that they have in fact made the catalysts they were trying to make and determining how the catalyst structure changes during voltage excursions.
- The project has a reasonable amount of collaborations. The final task of short stack evaluation by the subcontractor has not been completed with the latest iteration of the catalyst to show improvement in “real-world” conditions.
- The addition of AFCC to the team to demonstrate the technology developed on a stack level is excellent. However, the stack results reported by AFCC are far less than expected.
- This project would benefit from adding an additional subcontractor to evaluate membrane electrode assemblies (MEAs) with the improved catalysts; this would accelerate evaluation and commercialization of this work.

### Question 4: Relevance/potential impact on advancing progress toward DOE research, development, and demonstration (RD&D) goals

This project was rated **3.1** for its relevance/potential impact.

- The project is very important to the DOE Hydrogen and Fuel Cells Program and has the potential to advance commercialization of PEM fuel cells.
- This is a potential material solution to some degradation effects due to certain transient conditions.
- The project addresses the major durability and performance issues associated with catalyst composition and structure.
- The project aims to develop catalysts that favor oxidation of water over the dissolution of Pt and C during transient periods of fuel starvation. This helps DOE achieve targets for catalyst performance, PGM loading, and durability. Therefore, the project is highly relevant to the Program and has the potential to have a big impact on DOE RD&D objectives. The cost of the catalyst may be an issue.
- Materials-based solutions to start-stop and H<sub>2</sub>-starvation-driven degradation may prove valuable for automotive fuel cell applications, even though system-based solutions have also proven to be quite effective without adding significant cost. The project’s value is limited by researchers’ only proving its viability on NSTF electrodes that (a) would experience less damage than conventional electrodes during

voltage excursion and (b) have other issues that may limit their viability, such as water management challenges and low mass activity.

- This project addresses durability during start–stop and cell reversal conditions that have been identified as major contributors to cell degradation. Addressing cell reversal is believed to be critical for OEMs to meet automotive application durability.
- This project appears to have successfully demonstrated a technology that can reduce start–stop decay, but the reduction is not sufficient to meet DOE targets.
- The project is not highly relevant towards cost reduction; while fuel starvation is a known issue, parts of the solutions shown by the project are already being applied in some real-world cases. Further, the frequency and magnitude of fuel starvation can be mitigated with known system strategies. The output of this project will only make modest gains over the state of the art, even though the project is showing significant improvement over the chosen baseline.

### Question 5: Proposed future work

This project was rated **2.8** for its proposed future work.

- The plans are built on careful analysis of what has been accomplished in the past.
- The future work addresses the needs of the project and will move the technology toward real-world application.
- The proposed future work is relevant to close out the project, even though the impact could be low.
- It would be good to see a comparison of other cathode catalysts, including lower loadings and different carbon support materials, to fully understand the impact of these anode modifications.
- This project’s future work plan is well focused, but additional stack testing with a second subcontractor would be appropriate to utilize the benefits of the improved catalysts—assuming that the improved catalysts are commercially viable and the MEAs are ready for manufacture.
- The proposed future work focuses on evaluating the OER catalysts in short stacks for “real-life” automotive applications, improving the durability of the catalyst, and understanding the impact of OER catalysts on other MEA components. The proposed work involves the relevant areas for focus in the last few months of the project. However, it is unclear whether much fundamental work can be done in the short time left. It would be good to see some work toward the fundamental understanding of the mechanism by which SU/SD degrades the OER catalyst.
- The details of the future work are not provided. More stack testing in real-world conditions is all well and good. Hopefully the protocols will be provided. It is not clear how the fundamental engineering studies will be done. These catalysts cannot be “ready for real life” until NSTF is ready for real life. Therefore, some proof of concept of the high-OER cathode/low-ORR anode on carbon-supported catalysts would be very interesting.
- It is not clear that the proposed future work will actually result in any substantial additional improvements; instead, it appears to be just some “tweaking” or optimization of an approach that still requires substantial improvements to be deemed extremely valuable. It is unclear why an all-NSTF MEA is not on the path forward. One would think that a carbon-free MEA with these OER catalysts would provide much greater durability. Presumably, this type of MEA is not being pursued because an all-NSTF MEA presents too many other issues, such as unacceptably high sensitivity to temperature and impurities.

### Project strengths:

- This project features a strong team that has made reasonable progress since the beginning of the project.
- This project benefits from strong technical leadership and the team’s ability to exploit unique technology.
- The project has a strong team that can address the fundamentals of stack testing. The results are of high quality and address the barriers.
- This is a sound, creative approach based on electrochemical fundamentals. Testing is done at an OEM at supposedly relevant test conditions. The team is strong.
- Strengths of this project include the collaboration with AFCC and the inclusion of start–stop and cell reversal testing under real-world gas switching conditions.

- This project's strengths include using cutting-edge microscopic and spectroscopic characterization tools to understand the behavior of the IrRu additives, and the team's good grasp of materials (both catalysts and membranes).
- The NSTF catalyst provides a nice architecture to implement this alternative-anode strategy. The principal investigator has done a lot of good work to fundamentally understand what catalysts can provide decay mitigation without having too much negative impact on the cell performance. Another strength is having fuel cell OEMs on the team to assess technology at the stack level.

#### **Project weaknesses:**

- The project is focused on 3M materials only (membranes and NSTF catalyst layers).
- The project needs to define an "optimized candidate" (adjust the Pt loading as needed for the overall benefit) so the industry can take advantage of the accomplishments.
- Weaknesses include the dependency of the concept on NSTF electrodes and the lack of disclosure of protocol details.
- This project is not a high-impact project and only provides a marginal improvement over the state of the art.
- There is no apparent route to developing an MEA that is sufficiently resistant to start–stop decay, which means that other strategies (e.g., system-level mitigations) are still required, and therefore the impact of this project is severely limited.
- The presentation was hard to follow. The information is somewhat cryptic because a lot of data are jammed into a short presentation. The oral presentation did not provide clarity and was difficult to understand. Consequently, the reviewers' work was difficult and time-consuming because they needed to spend a lot of time figuring out the data.

#### **Recommendations for additions/deletions to project scope:**

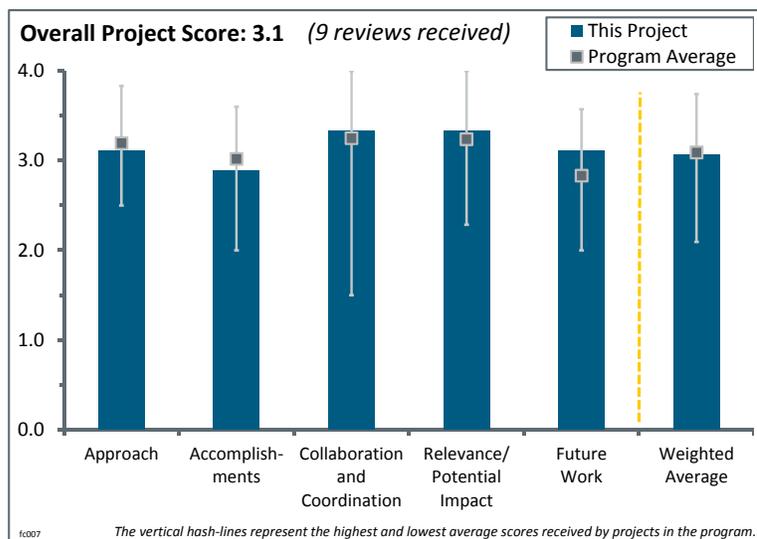
- The researchers should finish the existing scope of the short stack testing.
- The project should continue the focus on catalyst improvements, but a new project should be established devoted to membrane additives.
- The project team should include testing under non-excursion durability conditions and then run the excursion tests. The researchers should also apply the concept to carbon-supported catalysts.
- In situ EXAFS or XANES studies of the gas switching experiments may help elucidate what is happening with the RuIr (if the sensitivity is high enough to detect these low loadings).
- It would be good to see some work done toward understanding the mechanism by which SU/SD degrades the OER catalyst. Furthermore, it is unclear whether the Ru dissolves and crosses over from the anode to the cathode and, if so, how much crosses over. The team should use CO stripping as a method to detect the presence of Ru because this technique is very sensitive. If no Ru is detected on the cathode side, then it is unclear what is happening to the Ru.
- It would be good to see this anode protection applied to the SU/SD protocol with low-loaded cathodes, where the cathode support material can be discussed. In addition, a comparison between high surface area C, Vulcan, and graphitized carbons would be really valuable to see the effect of the anode protection. The start-up events should also be measured at low temperatures (such as 25°C) and with higher relative humidity contents. Related information of the stability of the Ru in the anode catalyst should also be measured—information such as stability to liquid water, which may happen upon SU/SD. Initial characterization of the materials is presented; post-characterization should also be completed.

## Project # FC-007: Extended, Continuous Platinum Nanostructures in Thick, Dispersed Electrodes

Bryan Pivovar; National Renewable Energy Laboratory

### Brief Summary of Project:

This project aims to synthesize and characterize novel extended thin-film electrocatalyst structures (ETF ECS) with increased activity and durability and to incorporate ETF ECS with the highest potential to meet U.S. Department of Energy (DOE) targets into membrane electrode assemblies (MEAs) for fuel cell testing of performance and durability. Work is focused on overcoming the cost, performance, and durability barriers for fuel cell commercialization by increasing platinum (Pt) mass activity. Extended surface Pt catalysts were developed for their high mass activity and durability, and these structures were incorporated into robust, high-efficiency MEAs.



### Question 1: Approach to performing the work

This project was rated **3.1** for its approach.

- The project's approach was both thorough and productive, quantitatively identifying each candidate's strengths and weaknesses.
- It was a good idea to incorporate 2020 targets in the last stages of the project.
- The project is highly focused on the key barrier of catalyst activity and durability. The "all metal" approach of unsupported catalysts is a good solution to the carbon corrosion problem. There is good balance between synthesis and making electrodes/MEAs. It is good to see the team take a "new slant" and pursue relatively low-surface-area materials but high utilization. It was brave to eliminate some less-than-promising catalyst approaches to focus on the best-in-class approaches to date.
- The use of the structures is interesting, and the work with MEAs is good. It is unclear how the MEAs are optimized. The comment on the short stack not being done is disingenuous.
- The extended electrode structures represent a promising approach, but it is not clear that they will deliver the performance that is expected.
- The guiding rationale behind the project—obtaining high-catalytic area-specific activities typical of extended surfaces, while also achieving high mass activities by using thin continuous layers/coatings of the catalytically active metal—is a sound approach and has been demonstrated to be valid by 3M with its nanostructured thin-film (NSTF) catalysts. The unique aspect of this project's approach was to incorporate these extended thin-film catalysts into a thick dispersed electrode architecture to enable mitigation of the issues that arise with the very thin electrodes of the 3M architecture. The project has, however, struggled with obtaining uniform and pinhole-free extended thin films that are thin enough to achieve high mass activities. The researchers should be commended for establishing strict go/no-go decision points for the various catalyst synthesis approaches and for following through on the down-selection of approaches in this last year of the project.
- This project addresses key barriers—the cost and stability of the catalyst—in a manner that is promising and apparently not being pursued significantly enough by others. The thin-film catalyst approach has shown great promise toward meeting the catalyst activity targets and has an inherent stability advantage over conventional dispersed catalysts. Although 3M originally introduced the thin-film catalyst architecture, the company appears to be either unwilling or unable to bring this promising concept to

commercialization. Specifically, the 3M NSTF MEAs are too sensitive to temperature and impurities to be considered commercially viable. This project appears willing to address these issues by exploring alternative thin-film catalysts and MEA compositions.

- The initial design of this project was excellent: grow and characterize extended continuous Pt nanostructures that could harvest the durability and specific activity advantages of 3M's NSTF while allowing flexibility of electrode design that could overcome some of the weaknesses of NSTF, such as cold start and stability during load transient, that arise largely from the thinness of the NSTF electrodes. While the initial design of the project was excellent, difficulties in growing real continuous layers (rather than aggregates of Pt nanoparticles) and in achieving the mass activity target have led the project into down-selects that make the remaining efforts essentially an investigation of Pt blacks, either unsupported (Pt/CoNW) or supported on a corrodible metal (Pt/NiNW), with limited structural control of the active Pt particle layer. Given the frustrating results with the other preparatory methods used, the down-selects were probably appropriate, but they constitute a major deviation from the original aim of the project.
- The use of extensive surfaces for new catalysts holds tremendous potential for value. Higher coordination of Pt has been associated with higher specific activity and better durability. If extended surfaces can be fabricated into high-surface-area catalyst layers with sufficient ability to reject product water, the decrease in precious metal loading could have a significant impact on cost status. A no-go decision was made on synthesis routes that were used in association with more intrinsically stable supports, such as metal oxides and graphitized carbon species. On the surface, the decision appears logical; catalysts that surpassed the mass activity target were studied further, and those that were lower than the target were not studied further. However, those that passed were based on the deposition of Pt onto base metals (Co, Ni, Cu, and Ag) capable of leaching in a fuel cell environment. Other projects from Argonne National Laboratory and General Motors are already studying PtNi and PtCo alloys but in ways that minimize the amount of Ni or Co, which is unlike the approach taken with the PtNi nanowires. The project may have benefited from an approach that first emphasized stability, followed by activity.

## Question 2: Accomplishments and progress toward overall project and U.S. Department of Energy (DOE) goals

This project was rated **2.9** for its accomplishments and progress.

- The project team thoroughly evaluated the ETFECS candidates, providing valuable insight to this class of supported catalysts.
- It is good to finally see some MEA results. The atom probe characterization seems like a good tool.
- The investigators have made very good progress and are incorporating the materials in MEAs. The oxide appears to cause durability issues.
- Great progress has been made toward exceeding the DOE 2020 targets for performance using galvanic displacement (slide 6). The switch from Ag to Co and Ni allows the possibility of spontaneous alloying to improve catalytic activity. The oxide film issue and the differences between Ni and Co are interesting, and the principal investigator has a good approach to understanding and using these issues to benefit the project.
- The researchers have identified catalyst systems that meet DOE activity benchmarks. The oxide states and characterization are important because this feature may lead to numerous routes with respect to activity and stability; however, precise control as an intermediate may be difficult. More electrode structure/incorporation work was expected by this stage in the project.
- This team has made excellent progress in developing new methods to fabricate ETFECS. This provides additional options that may actually be more commercially viable than the 3M synthesis. However, progress in MEA performance is disappointing; additional work is definitely still required in this area, yet the project is 80% complete. It is doubtful that the MEA performance targets can be met unless this project is extended.
- Significant progress has been achieved in obtaining high specific and mass activities in the rotating disk electrode (RDE) environment; however, this project has shown quite well that this is not directly translatable to high activity in the MEA, which is the true test of the potential of the materials to overcome the cost, activity, and durability barriers. The project team should be commended for down-selecting the most promising catalyst synthesis approaches this year and for fabricating and testing the down-

selected catalysts in MEAs. This down-selection should have been done sooner, though, as this year's report has shown that the MEA environment causes degradation and performance issues not observed in the RDE environment. In retrospect, a simple screening method of processing the catalysts as if they were being fabricated into an MEA to look for materials degradation via analytical characterization techniques would have been useful and could be useful to elucidate issues that will arise with the materials stability prior to optimization of the electrode composition and structure for utilization optimization. With so little time left in the project, it will be difficult to tackle all of the issues related to achieving high performance in an MEA, so the project should look for quick screening methods to determine the optimum electrode composition and fabrication procedure for the down-selected catalysts.

- The project has generated some novel catalytic materials with good specific and mass activities that challenge current hypotheses about the origins of high specific activities. NSTF was thought to achieve its high specific activity by taking advantage of the higher specific activity seen for flat Pt surfaces versus nanoparticles, likely due to the suppression of oxygen reduction reaction-slowing OH groups adsorbed on Pt defect sites. This project has generated catalysts with high specific and mass activities—sometimes containing very little alloying element—that have nanoparticle-like, small Pt grain sizes, yet achieve specific activities expected for flat surfaces of Pt or its alloys. These results show that higher specific activities can be achieved with Pt nanoparticles than had been anticipated. If continuing work in this project could explain the origin of these high activities, it could open up new rational pathways for catalyst development that could avoid the concerns about durability that arise whenever a non-noble element must remain present in the catalyst to maintain high activities during operation. The project has led to some further development of the rotating disk electrode technique as a means of screening the activity of catalysts of diverse structures. This is good as long as it does not divert DOE projects from the absolute necessity of testing catalysts in MEAs before decisions about relative merits of different materials are made. In other aspects, the progress of this project is disappointing. Real continuous layers, rather than clusters of nanoparticles, have not been achieved. Some of the structural control of the substrate that was achieved with the crystallographically defined Ag and Cu substrates has been lost in the shift to the less-well-defined commercial Ni and Co nanowires. Only a modest start has been made in learning how to make effective MEA electrodes with catalysts other than the standard Pt/C or Pt alloy/C materials.
- Most techniques for synthesis have not provided tenable catalysts. Even of those that passed the mass activity criteria, PtAg and PtCu were undesirable due to concerns about anode plating. For the PtNi and PtCo nanowires, the highest mass activities were achieved only at Pt weight percentages below 20%. The low Pt weight percentages may lead to thick electrodes and increased mass transport losses. This may have explained some of the low fuel cell performance. Failure analysis has not yet been thoroughly provided from fuel cell testing. It would be interesting to know whether Co or Ni entered into the membrane. The difference in Co and Ni behavior is somewhat puzzling. The Ni nanowires appeared to passivate, while Co leached out. In principle, it would seem that both metals should behave similarly. Some investigation should be made into whether the materials could be further engineered to provide Pt/base metal segregations that are best for activity and stability.

### Question 3: Collaboration and coordination with other institutions

This project was rated **3.3** for its collaboration and coordination.

- The project has assembled a strong and competent team of collaborators. Suggested additions would include industrial partners with expertise in catalyst ink formulations and application.
- This project features great coordination and management of a large and diverse team.
- The investigators have shown a high degree of collaboration with the partners, demonstrating excellent leveraging of resources.
- This project featured a good team, but everyone's role, input, and productivity were unclear.
- The number and quality of the collaborators were impressive, but it is unclear from the presentation what the contributions of each of the collaborators were to the progress presented.
- The involvement of original equipment manufacturers (OEMs) and catalyst suppliers is a rare accomplishment.
- At least 11 different organizations participated in the project, which was a considerable number. Only 4 organizations (the National Renewable Energy Laboratory, the University of Delaware, Oak Ridge

National Laboratory, and the Colorado School of Mines) appeared to remain involved in the base metal nanowire work that continued after the no-go decisions. The same four organizations were mentioned in the future work section. It was not clear from the slides whether Nissan remained involved.

- This project features a large and diverse team that includes all of the resources necessary to develop these new catalyst architectures. However, it is not evident that the team has the required expertise to fabricate and diagnose MEAs with these catalysts. Insufficient data on MEA performance is provided here, so it is unclear what is being done to understand the root cause of poor MEA performance.
- This project has drawn on the diverse talents of some of the best people available for the different preparation approaches. While the results have often been disappointing, this is not the result of incorrect choices of collaborators or inadequate efforts—the original subject matter of this project was very, very difficult. The project has resulted in a reasonable number of good published papers from multiple institutions. It might have been good to draw 3M more closely into the project to carry NSTF forward as a baseline continuous-layer system for comparison with the novel approaches.

#### **Question 4: Relevance/potential impact on advancing progress toward DOE research, development, and demonstration (RD&D) goals**

This project was rated **3.3** for its relevance/potential impact.

- Durable high-activity catalysts are critical to DOE automotive goals.
- The ETFECS approach is an exciting extension of the NSTF idea without the drawbacks of an organic substrate. The durability and performance possibilities are of great interest.
- The project explored in detail a unique class of catalyst supports, providing an excellent evaluation protocol for future extended surface Pt catalyst candidates.
- This type of catalyst structure appears to have the most promise toward meeting DOE's goals on catalyst loading, stability, and performance. However, much work is still required to develop a high-performance MEA that is not unacceptably sensitive to temperature or impurities (e.g., 3M's NSTF MEAs). This project has enabled new thin-film catalyst options and appears willing to try alternative MEA architectures as well, which is what is required to develop a complete and commercially viable thin-film MEA.
- Cost and durability are the two major barriers to fuel cell commercialization. Developing a catalyst that addresses both cost and durability is the most relevant activity in fuel cell research. This project achieves relevance by attempting to develop an electrocatalyst that can achieve lower cost and better durability by using the principles already validated through research on other extensive catalytic surfaces. The role of extensive surfaces in increasing area-specific activity, while also decreasing the tendency of Pt to dissolve, has already been substantiated. What this project attempts to add is the means to develop such surfaces in the context of a high-surface-area catalyst structure, as well as in the context of a catalyst layer that can provide sufficient rejection of product water.
- The impact could be good, but the project team also needs to understand some of the work that has been done with NSTF and modified electrodes, such as what General Motors has done.
- The work is promising, but there are significant technical challenges to making these materials commercially relevant.
- Unless the significant barriers to achieving performance improvements in an MEA can be surmounted with the relatively little time remaining in the project, the project will have had little impact on the DOE RD&D objectives beyond the more fundamental studies on optimizing activities in RDE measurements.
- The original plan of this project would have had outstanding relevance because it could have helped address some of the shortcomings of the NSTF catalysts that have been developed with substantial DOE support. As the project has evolved toward advanced Pt and Pt alloy blacks, the relevance has been diluted because the potential advantages over standard Pt/C and Pt alloy/C catalysts have been reduced largely to suppression of support corrosion (if decent electrodes, less subject to start-up and transient problems than NSTF, could in fact be made with these materials). Surprisingly good electrodes with moderately low loadings have been made with Pt blacks in the past, but they remained inferior, overall, to the carbon-supported electrodes. In the final months of this project and in the final report, the participants should spend some effort communicating the advantages of their catalysts over advanced versions of conventional-supported Pt nanoparticles because the final catalysts from the project are quite different from those originally proposed.

### Question 5: Proposed future work

This project was rated **3.1** for its proposed future work.

- The project identified an important issue—the difficulty of converting unique catalyst structures into electrodes—and it should focus on this issue.
- It is time to focus on “best in class” and develop the high-utilization structures that are part of the original approach. Limiting work to galvanic displacement and Pt:Co and/or Pt:Ni makes sense.
- The proposed future work is outstanding because it concentrates on the most important issue of obtaining high performance in the MEA environment through better catalyst synthetic and pre-treatment procedures prior to fabrication and improved MEA fabrication procedures.
- The plan going forward is a good one. There should be a focus on the oxide passivating layer on the Ni; it is unclear if it is a good thing (explaining the durability) or a bad thing (eliminating alloying and reducing performance). It is also unclear if it can be produced on the Co nanowires. There should be a big effort to get the fuel cell performance up. The structure of the catalyst layer needs to be fully addressed. It is possible that existing ink coating technologies are not going to work with these materials. This is a much longer-term activity that should perhaps be considered for a second phase of funding.
- Only a few months remain in the project, and the project team is doing what it can in the remaining time with materials derived from galvanic displacement. It would be good if one of the bullet points described efforts to improve mass activity for higher Pt weight percent samples, particularly with respect to PtCo.
- There appear to be many issues with fabricating MEAs, and it appears that the team has some near-term plans to address some of these fabrication issues; however, it is not clear if there will be sufficient time to overcome even these issues. More importantly, it is not clear if the team understands what the inherent challenges are that must be overcome to construct an MEA with ETFECS that will perform well under all operating conditions.
- The project is nearly over, so the future plans are not as important as they were earlier. The emphasis placed on trying to make electrodes that perform well at both low and high current density with improved versions of the down-selected catalysts is appropriate. More emphasis should be placed on understanding the origin of the very high specific activity achieved from some of these materials, which are aggregates of Pt nanoparticles and often contain very little if any alloying element.
- The future work with MEAs is good. It is unclear how the MEAs will be optimized, especially under different conditions such as saturated humidity, where there might be problems with flooding.
- The investigators have addressed concerns from previous years, but much more progress needs to be made on the materials synthesis.

### Project strengths:

- This project features good planning and direction. The industrial collaborators are a great asset.
- This project features a good concept and diagnostics.
- The project’s rationale and underlying premise are valid—that is the underlying strength of the project. The team is also outstanding.
- This project features a novel approach to improving the mass activity of Pt electrocatalysts.
- The project team demonstrated excellent capabilities to screen and down-select ETFECS candidates that meet the required performance goals.
- The “shotgun” approach to catalyst making has worked well, and the result is a good base set of materials to further develop. The team and partners are well positioned to capitalize on their knowledge and analytical base to develop electrode structures and MEAs using these novel “non-carbon” materials.
- The project team has successfully developed new thin-film catalyst options with high performance. This is an excellent team for catalyst development. The team is open to alternative MEA composition and fabrication methods with thin-film catalysts.
- This is a wide-ranging effort to synthesize continuous Pt layers on a range of nonstandard supports. The project has achieved improved reliability of RDE activity testing, although it is not clear whether the full range of surprising results from this technique has been communicated. The team has also achieved down-selects to the materials giving best mass activities in RDE, as well as the exclusion of Ag and Cu systems that can poison the fuel cell anode. A start has been made on MEA testing.

- The original premise is strong—deriving stable, high-specific-activity catalysts from extensive surfaces. The investigators were able to assemble a large number of organizations to assist with the project. Analytical techniques have been able to accurately show material deficiencies, whether such deficiencies are related to electrochemical activity or material structure.

#### **Project weaknesses:**

- The ETFECS technology may be difficult to implement from a manufacturing perspective.
- The project features too much work on RDE studies.
- It is a concern that the industrial collaborators are not as engaged as they might be with regard to scale-up and optimization of the catalyst layer.
- The MEA performance is still unacceptable. It is not clear that the team has the MEA performance diagnostic expertise required to successfully meet performance targets.
- A weakness for this project (and other catalyst evaluation projects) is the inability to convert supported catalyst candidates into catalyst coatings and electrode structures for MEAs. Each candidate has its own unique challenges, and catalyst ink formulations and application techniques can be difficult to resolve.
- Porosity control with all metal structures can be problematic. This problem may be further complicated when the inks are not stable and structures with poor uniformity are created. While mixing corrosion-resistant carbon materials in with the all-metal catalysts is a logical solution to the porosity issue, it seems to be an automatic dilution of the catalysts and thus leads to some loss of activity. If an oxide intermediate is critical, it may be difficult to control uniformly in production.
- The project's weakness has been its difficulty in finding a synthetic approach to obtaining a catalyst with the desired composition and structure. This challenge has consumed most of the effort and duration of the project, when the focus should have been on proving the concept and optimizing the catalyst performance in an MEA by utilizing an existing catalyst or catalyst synthesis procedure (e.g., 3M's NSTF).
- One weakness is the team's inability to grow true continuous Pt layers (this is, in fact, very challenging). Another weakness is the lack of comparisons of all measurements to NSTF, the established continuous-layer catalyst (which may start out as original crystallites but smoothes out closer to a true continuous layer during breaking and operation). Down-selects removed some pathways that may have a better chance to produce real continuous layers—the original goal of the project—than the retained Pt/NiNW and Pt/CoNW paths that produce aggregated Pt blacks.
- The no-go decision against more intrinsically stable supports was perhaps not the right decision. Granted, the activity was higher for materials derived from galvanic displacement, but the galvanic displacement technique allows vulnerability to in situ leaching of base metals. There are also other projects that may be able to address Pt/base metal nanowires while also adding considerable experience with acid leaching and annealing steps. Results yielded high mass activity at a low Pt weight percentage. It will be difficult to transfer the best technology to a practical fuel cell MEA without encountering mass transport issues. Catalysts might be limited to lower current density applications, such as stationary applications or MHEs.

#### **Recommendations for additions/deletions to project scope:**

- The team might want to consider trying to use NSTF and their inclusions in this framework.
- The team should demonstrate the performance of ETFECS in working devices.
- Now that the proof-of-concept stage has been successful, it would be good to see the OEMs and suppliers get more involved in the scale-up and optimization of the catalyst layer/coating processes.
- The project team should add at least one sub-scale cell test and diagnostics partner to the team, preferably one with good modeling capabilities, if this project is continued.
- This project (and other catalyst development projects) might benefit from additional resources within the national laboratories and industrial collaborators that can help with the conversion of promising catalyst candidates into electrode structures.
- The project has already deleted numerous research routes. No further deletions are necessary. The project may want to add some explicit investigation into increasing mass activity at higher Pt weight percentage, or at least make sure that steps related to ridding passivation layers from Ni or annealing are directly related to this topic.

- The project is nearly over, so major revisions are not feasible. To the extent possible, the researchers should try to emphasize the need to engineer electrodes that behave well at high current density on air (under a variety of operating conditions) as well as in the kinetic region under O<sub>2</sub>. They should take into account the possible role of high specific surface area in reducing local current densities (A/cm<sup>2</sup> of Pt), and thus in mitigating possible interfacial mass transport effects.
- The project should transition into electrode making because the initial approach is to build high-utilization structures. The team should develop methods and metrics for porosity characterization with the partners and then compare them to benchmarked traditional carbon structures to understand the difference. The team should also pursue porosity adjustment strategies. Although corrosion-resistant carbon additives could be considered a potential weakness, this avenue should be pursued fully to see if indeed the team can recover some of the activity lost when going to electrodes. It may be interesting to also mix all-metal catalysts of a different morphology to create the desired porosity. The researchers should consider developing a structure–function relationship around ink-making variables, the morphology of all-metal catalysts, and performance.

## Project # FC-008: Nanosegregated Cathode Catalysts with Ultra-Low Platinum Loading

Nenad Markovic; Argonne National Laboratory

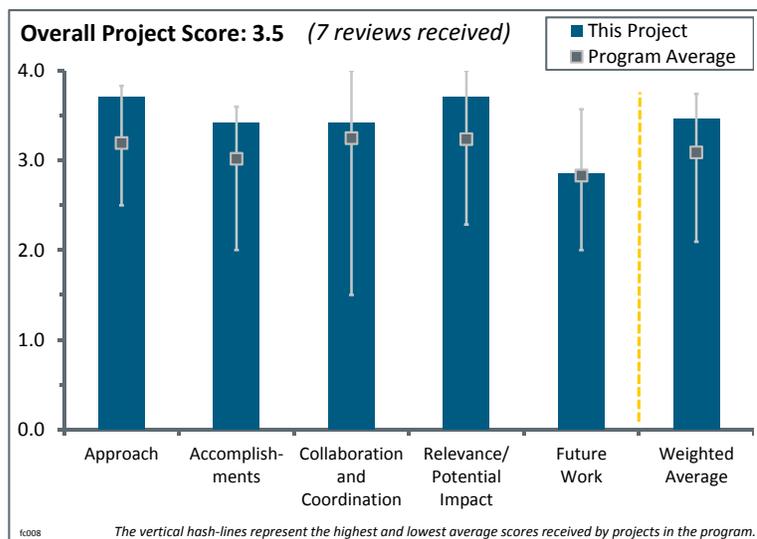
### Brief Summary of Project:

The main focus of this project is on developing a fundamental understanding of the oxygen reduction reaction (ORR) on multimetallic systems of PtMN alloys that will lead to the development of highly efficient and durable real-world nanosegregated platinum (Pt)-skin catalysts with low Pt content. The project has established a methodology to form and determine the nanosegregated Pt-skin surfaces for a different class of electrocatalysts, as well as established scalable synthetic protocols to produce large amounts of materials.

### Question 1: Approach to performing the work

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

- The approach is sharply focused on achieving U.S. Department of Energy (DOE) goals on catalyst activity and durability.
- This approach toward creating nanostructured alloys for enhanced O<sub>2</sub> reduction is aimed at ultimately lowering the MEA costs in terms of platinum group metal (PGM) loading. The approach is based on forming core shell materials and incorporating them as nanowires. Using a combination of ligand and strain effects, differences in both mass and specific activities are observed. Some additional benefits of durability are also observed. The approach utilizes a synthetic strategy that combines surfactants, long chain precursors, and metal salts including carbonyl compounds to engender relatively uniform core shell materials to be synthesized. The approach is based on a wealth of prior art from well-known reports, such as those from Bonnemann. While the results are certainly good in terms of ORR activity, scaling up such synthetic approaches is always challenging.
- The general approach is good, although it does seem somewhat more fundamental than what the DOE Office of Energy Efficiency and Renewable Energy (EERE) usually funds. The approach focuses on improving the catalyst activity and durability via fundamental understanding, synthesis and characterization, and MEA fabrication and testing. It leverages the previous accomplishments on nanosegregated Pt alloy catalysts with superior ORR performance.
- To date, the technical work has been very thorough. The challenge now is deciding whether there is something significant in which to invest all of the future efforts in scale-up. A comprehensive test of concept is needed.
- This project is sticking to the original goal of achieving theoretical Pt<sub>3</sub>Ni(111) activity and bulk character, and it is taking a systematic approach (Pt multimetallic skin surface and segregated structure).
- The researchers have conducted very careful work in a very disciplined manner, focusing on the fundamental aspect of making high activity and durable catalysts, although it is unclear if these findings would transfer to a real fuel cell.
- This project is focused on the key barrier of maintenance of activity at low loadings of Pt. Whereas some are concerned as to whether this project leads to scalable catalyst layers on MEAs, the strength of this project's approach is in developing the underpinning knowledge of catalyst structure and how it relates to durability and minimizing the cost of the catalyst. In other words, the focus is on developing the appropriate structure–function relationships in multimetallic nanoparticle catalysts, for example, the



“design principles” of Pt on multimetallic surfaces (films, particles). This is a very valid approach that will find its payoff in supporting the global community’s ability to design scalable, durable catalysts for MEA fabrication. The community needs a set of breakout ideas, not incremental ideas, and this team’s approach has a good chance of providing such a breakout set of design principles for thrifting Pt while maintaining durability. Perhaps this may be one such potential breakout, if the researchers can ferret out what is going on with the “mesostructured” catalysts. The principal investigator’s (PI’s) capabilities and approach lie in detailing the underpinning fundamentals, not the area of membrane electrode assembly (MEA) fabrication, and the researchers should focus on their strengths to drive the whole community forward. Others more skilled in the fabrication methods will adopt the design principles as they are further developed and if they can be proven with time. This is an excellent approach.

## Question 2: Accomplishments and progress toward overall project and U.S. Department of Energy (DOE) goals

This project was rated **3.4** for its accomplishments and progress.

- The project team has made excellent progress toward DOE goals. All 2015 DOE targets with respect to the catalysts’ activities and durability have been met (regarding rotating disk electrode [RDE] characterization) or exceeded.
- The synthesis and characterization of multimetallic core shell nanoparticles and Pt-alloy nanowires are outstanding. The work related to tuning the nanostructured thin-film (NSTF) surface structure is also good. The protocol for durability evaluation was not specified, making it difficult to determine if the durability test used was relevant. It is unclear if the electrochemical areas changed (slide 13). Impressive ORR activities and durability are shown in electrochemistry experiments. The ultimate test is how and whether this performance will be translated to MEAs; this should always be a part of the project. Results from only one set of MEA tests were shown. Much still needs to be done before the project ends. There is slight concern over whether MEA testing (50 cm<sup>2</sup>) of optimized catalysts and scale-up of catalyst fabrication will be done on time because these tasks are only about 50% complete.
- Good accomplishments have been made in terms of activity enhancements. DOE metrics have been met in terms of the activity rubric. In terms of progress on understanding the nature of such activity enhancement, the progress is incremental. Model systems, for example, do not account for changes with potential. No clear metrics were given in terms of durability towards carbon corrosion. In addition, the durability metrics for catalyst stability were in the range of 0.6 to 0.9/0.95 V. As apparent from the comparison of the cyclic voltammograms, the onset of oxide formation, and hence the associated place exchange with subsurface oxides, is shifted positive for these ternary alloys. As a result, the alloys’ higher durability would be predicted when compared to Pt, which has a more negative electrical potential to form such subsurface oxide formation. A true test would be to subject these materials to a higher potential, such as 1.1 V versus RHE. Under those conditions, large changes would be expected for such thin-film-coated nanostructures. Considering the fact that such potential excursions could occur on some cells in a stack, they should be included in such comparisons.
- Argonne National Laboratory (ANL) is making more than adequate progress in a difficult area of performing careful scientific work on difficult-to-characterize multimetallic structures, where the structure-function properties are just being defined—mostly by the team. DOE should be proud of the rate of accomplishments in this project. If there is an area of criticism, it would be the rate at which the milestones relate to the scale-up to MEAs. Because this is not the core technical strength of this team and the researchers appear to be relying heavily on the 3M collaboration, the perhaps slower-than-optimal progress is understandable. But this is a minor complaint. This team has a very respectable rate of publication in high-impact journals. While this is not necessarily an EERE metric, it endows this team with a good deal of credibility that its science is well reviewed and respected.
- There has been quite a stable of catalyst inventions from the work. There is a lack of real assessments of durability and performance.
- The approach to the mesostructured thin-film (MSTF) Pt–Ni catalyst is systematic, and MSTF shows significantly higher performance than NSTF. There are still a couple of remaining questions about (1) the stability of the preferred single crystal alloy surface (crystal orientation and segregation) after the cycle test,

and (2) whether there are any water management problems similar to 3M's NSTF, assuming the ANL team uses a similar whisker substrate to 3M's NSTF.

- The accomplishments over the last year appear to be the work in the areas of the Au sublayer, Pt alloy nanowires, and annealed NSTF. Although some work lacks originality, some valuable scientific achievements were generated. Demonstrated progress was shown using RDEs, but that does not necessarily correlate with MEAs. Syntheses were done in very small quantities; therefore, scale-up work is required prior to the much-needed MEA evaluation.

### Question 3: Collaboration and coordination with other institutions

This project was rated **3.4** for its collaboration and coordination.

- There is good collaboration between ANL, Brown University, and 3M. The roles of the Jet Propulsion Laboratory (JPL) and the University of Pittsburgh were not very clear.
- Overall, the collaboration and coordination of the project is excellent. It is unclear what JPL's role is in the project.
- This project leverages multiple national laboratories and universities to enhance its capability of analysis. It also uses an industry partner for fabrication of the catalyst.
- Good collaborations seem to be in place for this project. However, Brown University's role in this effort is not clear; perhaps it provided the synthetic approach. In addition, it is unclear if 3M was a materials supplier or whether it provided some other function. A clearer delineation of partners' efforts would help.
- The impact of the collaborations on the overall project is good; clearly Karren More is engaged, and the 3M collaboration appears to be okay. It is not clear what the others (JPL, Brown University, and University of Pittsburgh) are doing to support the project.
- It appears that many of the collaborators have been involved. The participation of General Motors (GM) needs to be strengthened.

### Question 4: Relevance/potential impact on advancing progress toward DOE research, development, and demonstration (RD&D) goals

This project was rated **3.7** for its relevance/potential impact.

- The project has the potential to significantly advance the commercialization of fuel cells by using catalysts with ultra-low Pt loading.
- The quantum leap of mass activity improvement is critically necessary to reduce PGM loading.
- The development of high-performing and durable catalysts is relevant and has a high impact on DOE Hydrogen and Fuel Cells Program (the Program) research and development goals and objectives. The impact would be more significant if the high catalyst activity and durability could be translated to MEAs and fuel cells.
- The project addresses fundamental understanding of Pt skin, which is very valuable for designing good durable catalysts. Prior work by the PI has shown important implications for real-life catalysts developed under other projects.
- This project, which is largely focused on developing the underlying design principles of multimetallic nanoscale structures as applied to fuel cell catalysis, is highly relevant to providing the Program with potential non-incremental "breakout" approaches to improving the activity and durability of "thrifty" Pt catalysts. If this project's approach continues to demonstrate progress, these results will be adopted by others in the community that are more skilled in the application of these materials/catalyst approaches to scaled-up MEAs. This is a very relevant approach that can lead to a decrease in the cost of future electrocatalysts.
- This project has the potential to lower the cost of a PEM fuel cell MEA to below \$30/kW, providing an important impetus to its commercial success. In this context, the project's meeting and exceeding of the DOE activity metric of 720  $\mu\text{A}/\text{cm}^2$  at 0.9 V versus RHE (iR-free) and 0.44 A/mg PGM (same conditions) are well received and acknowledged. The potential impact, however, should also reside on some of these nanostructured alloys in sustaining such activities at higher current densities. The PI assumes that such activity enhancement would be scalable; however, most of the ternary materials prepared in this effort

show the expected shift of the onset of oxide formation to higher potentials, and thereby have a relatively lower coverage of oxides at the comparative point of 0.9 V. This would, however, change when Pt oxide coverage changes at lower potentials. A higher current density (lower potential) comparison such as at 0.7 V (iR-free) would be more revealing. The potential impact is also based on the ultimate cost of these catalysts; typically, such nanostructured materials have remained an academic curiosity and have not translated well as commercial materials. Some work on scalability would be an important component in determining the potential impact.

- Until the durability is determined, the relevance/potential impact regarding DOE RD&D goals is open to some question.

### Question 5: Proposed future work

This project was rated **2.9** for its proposed future work.

- The future work is well balanced between RDE and MEA work, with the focus on MEA testing.
- The proposed future work is adequately addressed.
- All efforts should first be directed at deciding the real status of this catalyst. If this means making a series of laboratory-scale preparations for durability testing, then that is what should be done.
- The proposed future work is reasonable, with scaling up of catalyst synthesis and MEA optimization. It is unclear which of the approaches, or whether all of the catalyst approaches, will be brought to the MEA fabrication and testing.
- At this stage of the project, a higher priority should be placed on demonstrating the activity and durability of the most promising catalysts in MEAs.
- Regarding MSTF, questions still remain and future work should cover (1) the stability of the preferred single crystal alloy surface (crystal orientation and segregation) after a cycle test, and (2) whether there is a water management problem similar to 3M's NSTF, assuming ANL uses a similar whisker substrate to NSTF.
- The proposed future work follows the path of scale-up to address the milestones more geared to application in the last term of the project. No mention was made of what effort was going to be directed at the new and interesting "mesostructured" catalysts. The PI also mentioned in his talk that the influence of lattice mismatch was important to the tuning of electrocatalyst activity, and that the subsurface "core" metal atoms are affecting Pt dissolution, reordering, etc. It was surprising that there was no mention of (a) what studies supported those claims and (b) what modeling was ongoing or proposed to substantiate those claims. This comment may be related to the state of collaboration in this project, which is not well defined, at best.

### Project strengths:

- ANL has excellent material synthesis and analysis capabilities.
- This project's strengths include the team's ability to generate and characterize laboratory-scale catalysts and then show some desirable properties.
- The team has very good synthetic capabilities. The team's knowledge of underlying principles of the ORR electrocatalysis allows it to generate new concepts for catalyst design in a timely manner. New mesoporous thin-film catalysts look very promising both from activity and durability points of view.
- Catalyst synthesis, material characterization, and electrochemical characterization are all strengths of this project.
- This project's strength is its theoretical background to achieve higher mass activity (beyond the DOE target).
- This project details the preparation of nanostructured Pt alloys for higher activity and durability. Both fundamental understanding of the underlying principles leading to higher activity and preparative techniques are addressed in this effort.
- This project features an exacting, detailed approach to get at the underlying "design principles" or structure–function relationships of multimetallic nanoscale catalysts. It also features a good team that is taking a knowledge-based approach to catalyst activity and durability.

**Project weaknesses:**

- There is a lack of MEA and fuel cell data at this stage.
- These catalysts will be extremely difficult to scale up. Serious thought should be given to the decision of whether the optimization and scale-up are truly warranted.
- The project is pretty close to the end, but it is still focused on RDE testing (both for activity and durability). Considering that catalyst coated membranes will need to be optimized, the focus should be shifted to fuel cell testing.
- Scalability and the cost of the catalyst have not been adequately addressed to date, though they are on the list of future activities. A simple check on the cost of the precursor materials shows that the end product with lower loading would cost more than the typical Pt/C with conventional loading. This issue must be addressed clearly.
- An approach needs to be developed to transfer the knowledge gained to additional team members that are better suited to address issues such as scale-up of particle syntheses, incorporation into MEAs, etc., without affecting the rate of progress being made on new, more highly active, durable catalysts.

**Recommendations for additions/deletions to project scope:**

- There should be a stage gate with product durability and performance durability testing on a meaningful scale.
- Fe-containing catalysts may need to be excluded from consideration because of potential Fe leaching into the membrane.
- A clear mass and specific activity comparison with conventional Pt/C should be done between 0.95 and 0.7 V (iR-free). In addition, some OEM testing, such as in GM laboratories, should be a part of this effort.
- The influence of lattice mismatch on catalyst activity and durability effects would appear to be crying out for more theory to help guide the experimental effort and hopefully further increase the rate of progress.

## Project # FC-009: Contiguous Platinum Monolayer Oxygen Reduction Electrocatalysts on High-Stability, Low-Cost Supports

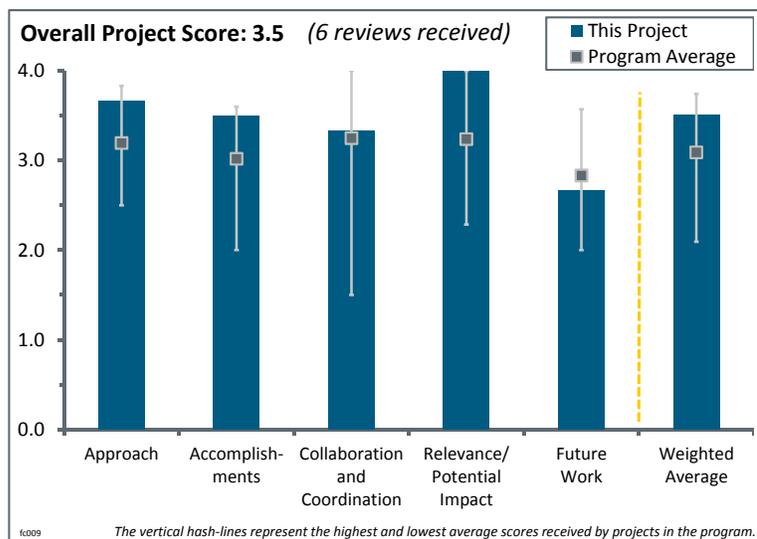
Radoslav Adzic; Brookhaven National Laboratory

### Brief Summary of Project:

The primary objective of this project is to synthesize a high-performance Pt monolayer (ML) on stable, inexpensive metal or alloy nanostructure fuel cell electrocatalysts for the oxygen reduction reaction. Another objective is to increase the activity and stability of the Pt ML shell and the stability of the supporting cores while reducing noble metal content.

### Question 1: Approach to performing the work

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



- The approach is sound and strong.
- This project aims at producing a stable catalyst with 100% Pt utilization and thus greatly improved mass and specific activities. The use of core-shell interaction to improve Pt ML properties appears to be quite successful. Employing refractory metal alloys as cores allows for further reduction of platinum group metal (PGM) content.
- The approach to demonstrating novel ways to reduce precious metal loading while maintaining or improving catalyst activity is very good. One or two of the paths will be less likely to succeed in the long term from manufacturability and throughput perspectives—namely the electrodeposition and atomic layer deposition (ALD) techniques. However, it is good to include them for completeness of approach. The other aspect of the approach is the involvement of industry collaborators as independent evaluators of the technology developed; this has been very good.
- The methodology originally developed by the principal investigator (PI) is well established and well aligned with U.S. Department of Energy (DOE) catalyst goals of low-PGM/high-activity catalysts. It was very good to see the move to scale up the results to large-format membrane electrode assemblies (MEAs). There are some concerns about the practicality of using electrodeposition of the catalyst on the gas diffusion layer (GDL) and/or membrane.
- Brookhaven National Laboratory (BNL) is working on very promising catalyst materials, as evidenced by the licensing and scale-up of the core-shell catalysts by N.E. CHEMCAT (NECC). Both the Pt nanospheres and the Pt on PdAu nanowires are promising concepts to get to high mass activity. The electrodeposition directly onto GDLs is also a creative, promising approach to increase Pt utilization, although how much the utilization could theoretically be improved by this method should be considered before investing too much in scale-up of the concept.
- Routes using Pd are subject to the possibility of Pd loss with any loss of Pt ML shell. However, to the project's credit, efforts have been made to reduce low-coordination-number Pt atoms and to investigate stable cores (e.g., refractory metals). The very thin catalyst layers from growth on GDLs could possibly face the same water management challenges experienced by 3M's nanostructured thin-film catalyst. There is also some possibility of degradation from dissolution of either W or Ni. A very interesting part of the approach is the aspect involving Pt hollow nanoparticles, which still need further reduction in the Pt shell thickness.

**Question 2: Accomplishments and progress toward overall project and U.S. Department of Energy (DOE) goals**

This project was rated **3.5** for its accomplishments and progress.

- The presented Pt ML catalyst performance is very impressive. Based on the mass and specific activities given on slide 10, the electrochemically active surface area turns out to be 236 m<sup>2</sup>/g of Pt compared to 240 m<sup>2</sup>/g of Pt for a true ML catalyst.
- It is truly exceptional that so much data have been gathered on such a wide variety of catalyst options. The team's ability to demonstrate stability to voltage cycling is also very encouraging. The DOE targets have clearly been met for a number of different options, and technologies identified in 2012 have now been scaled up with help from partner organizations. The ability to innovate and then implement is the measure of success for any catalyst development effort.
- This project features outstanding activity and stability of a licensed catalyst. Improvements in mass transport, and noted by the presenter, are needed to truly realize the potential of these materials. "Pt hollows" is a great approach to eliminate carbon corrosion, but it will need substantial electrode development to realize its potential.
- Overall, BNL has made good progress. There is a need for more work with MEAs and understanding the implications of ionomers with the catalysts.
- The activity results on MEAs in O<sub>2</sub> are encouraging for all concepts except for the PdAu nanowires. However, these measurements were made at much higher pressures than the prescribed method (350 versus 150 kPa), so it is difficult to know whether these materials actually meet the DOE mass activity target of 0.44 A/mg-PGM. The PI is also encouraged to include the loading of Au as well as PGM in his analysis. Encouraging durability results were shown for ML/Pd<sub>9</sub>Au<sub>1</sub>/GDL MEAs after 2,000 cycles. Tests should be run for the prescribed 30,000 cycles using the DOE-recommended protocols. For most concepts, the H<sub>2</sub>/air performance is very poor; BNL should work closely with its partners that have MEA development experience to try to optimize these electrodes to minimize mass transport losses.
- Impressive activities have been shown on a per-PGM basis for most catalysts, particularly for monolayers of Pt on hollow Pd (530 A/g PGM), Pt/Pd from ethanol (400 A/g PGM), Pt/Pd nanowires (500 A/g PGM), and Pt/PdAu (500 A/g PGM). Some indication of stability was shown for Pt on hollow Pd, although the true test will be in a fuel cell under realistic load cycling. The Pt monolayers on the PdAu core concept will have to be developed further to improve activity per mass of precious metal. So far, stress tests on catalysts with WN<sub>i</sub> cores supported on GDLs have not shown degradation in activity, but they have instead shown an increase with 0.6–1.0 V cycles. Failure analysis on these MEAs would be good to see to understand how the durability was maintained. Fuel cell data in air (or activity data in O<sub>2</sub>) will be needed to evaluate the usefulness of the ALD materials.

**Question 3: Collaboration and coordination with other institutions**

This project was rated **3.3** for its collaboration and coordination.

- BNL has excellent collaborations with universities (for fundamental characterization/calculation) and industry (for material processing and MEA testing).
- It was a great achievement to give a license to NECC. Team members 3M and Johnson-Matthey Fuel Cells, Inc. (JMFC) were important to the electrode structure development.
- This project features good technology transfer and partners, but the project team needs to identify a cell tester.
- The collaboration with partners has been very good. One consideration is the consistency in measurement across the different options of 2,000, 5,000, 10,000, and 15,000 potential cycles—it appears as though there is a need to standardize the approach across the different groups.
- It is unclear what the Massachusetts Institute of Technology did, and the JMFC fibrous support work seems out of place with the rest of the project. It was good to see BNL engaging 3M and General Motors (GM) to get cell and stack data after UTC Power left the project. The fact that the researchers have been able to commercialize the Pt ML/Pd/C catalyst at NECC shows strong industrial collaboration.

- Unlike other projects, this project is not in substantial need of collaboration at the material synthesis level. That said, JMFC has been used for collaboration on more novel catalysts. BNL has recognized that further collaboration is needed for both material scale-up and fuel cell testing. NECC has entered the project for the former and 3M for the latter.

#### Question 4: Relevance/potential impact on advancing progress toward DOE research, development, and demonstration (RD&D) goals

This project was rated **4.0** for its relevance/potential impact.

- This is a very critical component of the overall Fuel Cells program effort.
- This project addresses DOE automotive targets for catalyst activity and durability.
- The development of stable, high-activity catalysts is one of the most important challenges facing the commercialization of automotive fuel cell systems.
- The ability to reduce precious metal loading and maintain performance and durability is paramount to the successful cost reduction of fuel cells. This project clearly has all of these elements in mind, as well as the equally important technology implementation piece.
- Performance, cost, and durability are major barriers for H<sub>2</sub>-powered fuel cell vehicles to be commercially viable. This project addresses all of them. The presented results look promising for automotive applications.
- Cost and durability are the major barriers to fuel cell commercialization. The new cathode catalysts provide the possibility of addressing both barriers. The catalysts developed in this project seek to address both cost and durability.

#### Question 5: Proposed future work

This project was rated **2.7** for its proposed future work.

- The proposed future work is in the right direction to a low Pt-loaded catalyst enabling competitive fuel cell vehicles. However, the observed poor air performance needs to be addressed.
- The desire to do further work on electrodeposition is understood; however, perhaps this would be at the expense of other areas in the project, given the timing (i.e., perhaps it would be possible to make more progress in other areas if electrodeposition were dropped). If it is for fundamental understanding, and this is the only way to approach the core design at the moment, then this is acceptable.
- There are still many materials options being developed. BNL should prioritize one or two concepts based on activity and durability testing at DOE conditions and cost projections of the scaled-up process (e.g., it is unclear if electrodeposition is cost-effectively scalable), and then focus on electrode optimization and ultimately scale-up for stack testing of these down-selected concepts. The future work should also include thorough post mortem analysis of voltage-cycled catalysts. The 3M durability results are particularly surprising, and it would be good to know what is happening at the catalyst, particle, and molecular levels. Particle size and composition before and after cycling should be reported. For the electrodeposition work, microscopy should be done to make sure that BNL is actually getting only the proposed structure of accessible Pt.
- Electrodeposition for catalysts has been tried often throughout the years. However, commercialization is rife with difficulties because one needs precise control of the electric field to alleviate non-homogenous depositions, and this issue grows with size. While there are commercial high-speed electrodeposition processes, such as wire galvanization, the goal here is to create impermeable thick films, which is the opposite for fuel cell materials. The plan to focus on electrode structures to optimize utilization of these high-potential catalysts is well aligned with DOE goals.
- Much of the fiscal year (FY) 2013 future work focuses on synthesis optimization of Pd-containing catalysts. However, more interesting topics might include (1) using the new U.S. DRIVE Partnership Roadmap ([http://www1.eere.energy.gov/vehiclesandfuels/pdfs/program/fctt\\_roadmap\\_june2013.pdf](http://www1.eere.energy.gov/vehiclesandfuels/pdfs/program/fctt_roadmap_june2013.pdf)) to substantiate durability of the Pd-containing catalysts, especially the Pt/Pd/W/Ni catalyst; (2) exploring the low-temperature performance of catalysts directly deposited on the GDL in order to explore water

management; and (3) continuing to decrease the shell thickness of hollow Pt nanoparticles (the latter should be moved up from FY 2014).

- There seems to be a lot of work left to do including making enough catalyst and testing it in MEAs within fuel cell stacks, as well as continued optimization, without much time left. It is unclear whether the FY 2014 plans makes sense because the project is set to end this year.

#### Project strengths:

- This project features a good approach and progress.
- This project's strengths include its outstanding development of high-activity, stable catalysts and its "top flight" catalyst development team and PI, who have a proven track record endorsed by industry.
- The team has synthesized a wide range of catalyst materials and has moved quickly to MEA testing. Materials have been made that can be scaled up by suppliers.
- BNL has been able to leverage wet chemical deposition techniques to provide a variety of new catalysts. The leadership of the project has enormous depth and experience in the field. The project is able to reach out to suppliers for scale-up of catalyst concepts. The project has shown the ability to reach out to stack and MEA manufacturers for testing support.
- This project features a high "bench strength" with industry partners that can evaluate the technology and provide good input. It also has a solid technology pipeline, starting with the monolayer approach and then going forward with subsequent improvements. The use of multiple manufacturing methods to achieve the desired PGM target is a strength.

#### Project weaknesses:

- This project features too much work with H<sub>2</sub>/O<sub>2</sub>; it needs some MEA development.
- This project's weaknesses include the use of electrodeposition for catalysts and electrode development/structures for high utilization.
- This project has inconsistencies in the format of voltage cycling tests. It also uses multiple manufacturing methods to achieve the desired PGM target—this is a weakness.
- This project's weaknesses include a lack of data at DOE-recommended operating conditions, especially activity at 150 kPa. More postmortem analyses would be nice, too. Except for the Pt ML/Pd/C catalysts, the model structures are not supported by HAADF and Pd-EELS analyses. The team needs to focus on optimizing the most promising concepts.
- After developing a catalyst and measuring good beginning-of-life activity, the PI should move quickly toward performing durability measurements in a fuel cell. This should be prioritized over catalyst optimization. The PI should place a greater emphasis on core stability. This emphasis should translate to the scale-up of stable cores and immediate testing to validate the stability of cores. The project materials are often premised on the advantages offered by precious metals, such as Pd and Au.

#### Recommendations for additions/deletions to project scope:

- It would be good to see more work on H<sub>2</sub>/air as well as on the possible impacts of contaminants and water management, transport, and ionomer aspects with these new catalysts.
- The project team should narrow the focus to wet-based methods for catalyst preparation (the team should leave electrodeposition and ALD out unless there is a plan to be more aggressive in each of these areas).
- The project team should test activity and durability using DOE-recommended protocols. It should also conduct beginning-of-life and post mortem transmission electron microscopy analysis on all concepts. In addition, it should engage 3M, GM, and JMFC on electrode design of the most promising concepts to resolve the H<sub>2</sub>/air performance issues.
- While excellent performance was demonstrated in H<sub>2</sub>/O<sub>2</sub> measurements, mediocre performance was observed in H<sub>2</sub>/air operation, which is more relevant to automotive application. The root cause of such poor performance should be investigated in this project, rather than simply stating that it is a mass transport issue.
- Prior to further electrodeposition work, the team should perform a more thorough cost-benefit analysis to compare material throughput rates, cost of equipment, and envisioned configuration, and then compare this

to traditional bulk catalyst synthesis, ink making, and coating. The metrics for uniformity of the electrical field that would be needed should be defined as well as the cost to achieve this. The team should increase the involvement of ink-making and electrode structure development partners.

- The project is fairly late in its timetable, so there are no suggested additions. BNL should increase efforts to validate catalyst durability (especially in a fuel cell) for both prescribed stress tests and durability cycles. BNL should increase the priority for scale-up of Pd hollow nanoparticles, as well as durability testing for them in a fuel cell.

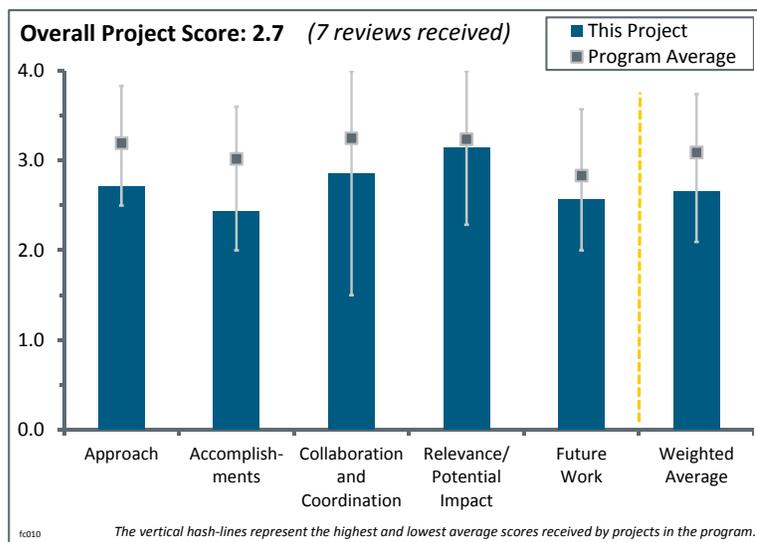
## Project # FC-010: The Science and Engineering of Durable Ultra-Low PGM Catalysts

Mahlon Wilson; Los Alamos National Laboratory

### Brief Summary of Project:

The objectives of this project are (1) development of durable, high-mass-activity platinum group metal (PGM) cathode catalysts, enabling lower-cost fuel cells; (2) elucidation of the fundamental relationships between PGM catalyst shape, particle size, and activity, allowing for better catalyst design; (3) optimization of the cathode electrode layer to maximize the performance of PGM catalysts, improving fuel cell performance and lowering cost; (4) understanding the performance degradation mechanisms of high-mass-activity cathode catalysts to provide insights to better catalyst design; and (5) development and testing of fuel cells

using ultra-low-loading, high-activity PGM catalysts. This project will help lower the cost and the precious metal loading of polymer electrolyte membrane (PEM) fuel cells and improve catalyst durability.



### Question 1: Approach to performing the work

This project was rated **2.7** for its approach.

- The project is focused on key barriers and approaches to each issue. It appears to be sound and is yielding results.
- The project is focused on U.S. Department of Energy (DOE) targets for PEM fuel cell durability and activity.
- This project has included good work in general, although the proportion of performance evaluation and low precious metals studies should be increased. A lot of characterization and modeling has taken place.
- The approach is fair and may be able to overcome the barriers addressed; some of the methods proposed in the approach are already being used to prepare state-of-the-art membrane electrode assemblies (MEAs).
- The approach seems to bundle together as much material as possible. The most important part is the focus on pyrolyzed polypyrrole (PPPy) structures as supports for low-loading catalysts that will work. The rest is largely padding.
- The approach of this project is good, but more material should be down-selected. The approach is well designed and combines the theoretical modeling and experimental work. The ultra-low PGM target for 2017 is 0.125 mg/cm<sup>2</sup>, so modeling and microstructural simulations should be focused on low or ultra-low PGM loadings. Using ceria as an additive is an interesting concept, but it is not clear how this will help for ultra-low PGM catalyst design. Durability advantages with this approach are shown, but it was not clearly explained how this will help ultra-low PGM design.
- This project consists of several disconnected activities without a clear path to how the various approaches will be combined to address key technical barriers. The modeling work does not seem to tie in with the synthesis work. The ceria work is more focused on membrane stability and has little to do with “Durable Ultralow PGM Catalysts.” The extended X-ray absorption fine structure (EXAFS) of the polyol catalyzation does not tie in with the other parts of the project, either. Only the Pt-PPPy nanowire catalysts—which include synthesis, characterization, electrochemical analysis, and fuel cell testing—seem to be a comprehensive study.

## Question 2: Accomplishments and progress toward overall project and U.S. Department of Energy (DOE) goals

This project was rated **2.4** for its accomplishments and progress.

- The project team has made good progress in all areas of focus. Especially notable is the progress in making high-performance MEAs with ultra-low PGM loadings and good performance stability. Because the issue with these types of MEAs is often performance sensitivity with different operating conditions (e.g., 3M nanostructured thin-film MEA performance at 25°C), the team should also report performance at room temperature. If the performance of these nanowire-based MEAs is not particularly temperature-sensitive, then this would be an important result that should be shared with others developing similar catalysts (e.g., 3M and the National Renewable Energy Laboratory [NREL]). Los Alamos National Laboratory's (LANL's) catalyst layer compositions are presumably quite different from 3M's MEAs (i.e., LANL's contain ionomer in the catalyst layer) and may be significantly different from NREL's thin-film catalyst MEAs as well.
- There has been significant progress towards the stated objectives.
- Progress has been adequate. A performance evaluation is a critical need.
- The team is on track to meet DOE targets, but the progress has not been very fast.
- The progress with ceria as an additive is interesting, but ceria's role in designing an ultra-low PGM catalyst is unclear. The Pt-PPPy nanowire catalyst work is very interesting, but performance is below the carbon-based baseline catalyst. Also, durability should be evaluated under the U.S. DRIVE Fuel Cell Tech Team's suggested automotive-relevant accelerated stress tests (ASTs). Many PPPy nanostructures with various templates were generated, but most of them were not tested.
- Pt-PPPy nanowire catalysts need more work to approach DOE performance and durability targets. Activity measurements (either in rotating disk electrode or MEA) are not reported. Thus, it is unclear whether materials development, electrode optimization, or both are required. It is unclear how the density functional theory (DFT) modeling, the catalyst layer microstructural simulations, or the polyol catalyzed synthesis will help to meet any DOE goals.
- The progress toward the objective has been miniscule. The principal investigators seem to be trying too many different things and not making a concerted effort in advancing the technology towards the barriers. The claim about ceria addition improving the durability of membranes has been reported in the literature previously.

## Question 3: Collaboration and coordination with other institutions

This project was rated **2.9** for its collaboration and coordination.

- This project has good collaboration with strong teams between national laboratories, universities, and industries, with clear task assignments among the partners based on their competencies.
- LANL has assembled a strong team with broad expertise from national laboratories, academia, and industry.
- This project features a decent balance between original equipment manufacturers, national laboratories, and universities.
- It appears that many entities are collaborating. There could be some different order imposed based on the criticality of needs.
- There is good collaboration between the industry, national laboratories, and universities. The role of the University of Delaware is not very clear, as it is not mentioned on slide 17.
- The collaboration is reasonable, and the modeling work by Ballard seems to make reasonable progress.
- It would be good to see more interaction with other teams that are developing ultra-low PGM MEAs based on thin-film catalysts (e.g., 3M and NREL). Ideally, this project should have a viable MEA supplier on the team to ensure that the technology developed here can be readily incorporated into commercial MEAs.

**Question 4: Relevance/potential impact on advancing progress toward DOE research, development, and demonstration (RD&D) goals**

This project was rated **3.1** for its relevance/potential impact.

- This project is definitely well aligned with the DOE goals, and the focus of the project is on key barriers.
- The project is relevant to DOE goals and the potential impact is high, considering the significant modeling effort.
- The project has the potential to advance progress towards the goals.
- The relevance of the project with the overall DOE goal for ultra-low PGM is very good, and the project features a very good team comprising national laboratories, universities, and industries. One of the objectives is the development of a durable, high-mass-activity PGM cathode catalyst to reduce the cost by utilizing ultra-low PGM loadings; however, no significant improvement in mass activity with ultra-low loadings has been shown so far. Optimization of the cathode electrode layer is limited to catalyst structure, and efforts should be put into understanding the ionomer effect in the catalyst layer, as well as its relation to durability.
- This project, if it is successful at lowering precious metal content with excellent performance, will be highly relevant.
- The stated objectives are relevant.
- Developing durable ultra-low PGM catalysts is one of the most important challenges that must be addressed to enable widespread fuel cell commercialization. Unfortunately, with the way that this project is currently structured, the work from this project is unlikely to promote that.

**Question 5: Proposed future work**

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

- The modeling should focus on the nanotube/wire morphology both in DFT and catalyst layer models.
- Performance assessment is key at this stage. Then there should be a stage gate approach to defining the critical aspects required for success. The work plan should be adjusted accordingly.
- Plans need to be more focused on overcoming barriers. The modeling effort is not complemented by experimental model validation.
- It is difficult to understand the actual path forward to achieve the objective with the proposed future work. More experimental work is needed with material similar to what was used in modeling to validate the model. Also, the catalyst structure design should focus on understanding the effect of low loadings on mass transport and durability.
- Only the Pt-PPPy nanowire catalyst future work shows the potential to enable ultra-low PGM durable catalysts, but electrochemical characterization and durability testing should be included. The DFT modeling and catalyst layer microstructural characterization work needs an experimental validation component to provide value. The CeO<sub>2</sub> stabilization work is not related to the project goals and should be stopped.
- The proposed future work does not seem relevant towards the barriers addressed. The modeling work seems fine; however, it is unclear how the degradation kinetics will be covered by the model.

**Project strengths:**

- This project features excellent bench-scale talents and capabilities.
- The project includes a balance of modeling, synthesis, materials characterization, and fuel cell testing.
- The modeling is a strength of this project.
- This project is focused on key barriers.
- This project features good management and good science.
- This project's strengths include its strong team, very good collaboration among the partners, and very good modeling efforts.

- There is a strong theoretical component in this project that can provide guidance for the design of better low-loaded catalysts and catalyst layers. This project features a very good set of characterization techniques.

#### Project weaknesses:

- There are too many non-relevant pathways.
- There is no commercial MEA supplier on the team.
- The value of the approach is not well addressed yet. A rigorous performance test and stage gate review should be undertaken.
- So far, the links between the outcome and the objective of the project are not very clear. An ultra-low PGM catalyst with high mass activity has not yet been demonstrated.
- The modeling is not supported by experimental validation. The performance of the MEAs with Pt–ceria catalysts needs to be compared to the performance of MEAs with a ceria-modified membrane. If ceria additives lead to a gain in durability but also result in performance loss, the point of using them is unclear. If nanowire supports are used, it seems like it would be beneficial to use thin films of Pt instead of Pt nanoparticles.
- The project should focus on the PPPy supports and drop the ceria work, which is in the literature and does not need to be done again. Perhaps LANL is doing too much. There is no link between the different parts of the project. It is unclear when ceria is going to be added to the PPPy-supported catalyst. It is also unclear when DFT is going to be applied as a design tool rather than modeling what is already known.
- The various project work streams are not coordinated to best address technical barriers.

#### Recommendations for additions/deletions to project scope:

- The Pt–ceria catalysts do not look very promising.
- There should be more interaction with MEA developers.
- The researchers should focus on the PPPy support with experimental work and modeling work. The team should stop the ceria work.
- The team should focus on Pt-PPPy nanowire catalysts. It should measure and report ECSA and mass and specific activity values. It should also conduct DOE-recommended ASTs on promising materials. The team should make sure any modeling and characterization work is directly tied to materials development efforts.

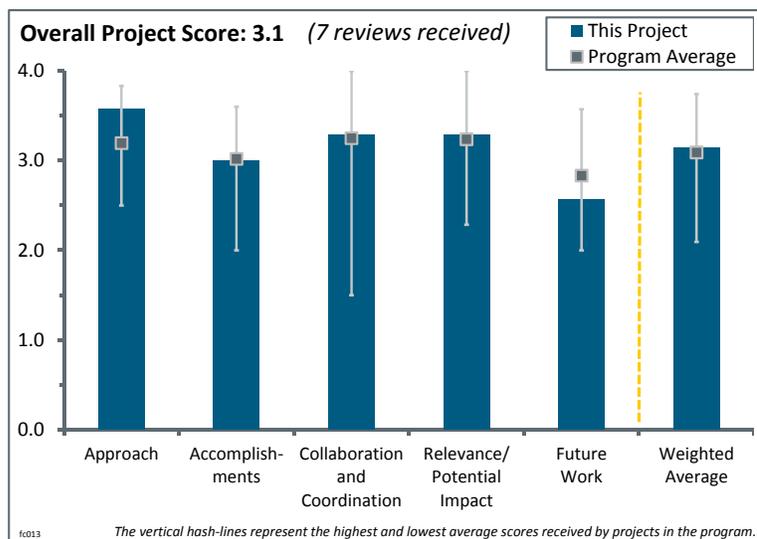
## Project # FC-013: Durability Improvements through Degradation Mechanism Studies

Rod Borup; Los Alamos National Laboratory

### Brief Summary of Project:

The objectives of this project are to identify and quantify the components and component interactions and operating conditions leading to degradation in fuel cells, understand electrode structure impact on durability and performance, and develop models relating components and operation to fuel cell durability or degradation. Through this analysis, methods to mitigate degradation of components in fuel cells, increase fuel cell durability, and maintain component costs at a reasonable level are explored.

### Question 1: Approach to performing the work



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

- The project is sharply focused on the key areas of fuel cell degradation mechanisms.
- The approach covers all of the components of the fuel cell and the most degrading modes of operation.
- This is a very broad-based approach that seems to be well managed and productive.
- Understanding the degradation mechanism of catalysts is a prerequisite for addressing the durability problem. This is a well-defined, comprehensive approach addressing the degradation of Pt, carbons, membranes, and bipolar plates.
- Because durability is a key barrier to commercialization, this project is very important, and the approach of obtaining a better understanding of all of the degradation mechanisms is worthwhile. Additionally, the team uses a variety of good experiments to ensure that root causes are fully understood.
- The team members and capabilities are solid. There has been little done related to “real-life” testing or to compare the team’s results with others. The fluoride emission rate (FER) has been studied, but only for a short time; this takes hundreds of hours to equilibrate. At low relative humidity, many investigators have shown the FER to increase rapidly with time as end groups are generated. One of the stated goals is to propose mitigation routes and offer solutions—these were not presented. The most important work the researchers have demonstrated is the difference in catalyst dispersion solvents. It would have been good to see a lot more work on this.
- Many of the data are similar to those that developers have already collected. Examples include (1) electrochemical surface area (ECSA) versus carbon loss; (2) evolution of surface oxides versus potential; (3) increased graphitic character of support carbon after cycling, as well as catalyst layer thinning; (4) performance degradation for various carbon types; and (5) fluoride emission rates (FER) from perfluorosulfonic acid (PFSA) membranes under various conditions. The project team needs to ask whether it can go deeper than just these data. If the assertion is made that corroded electrode layers are being compacted, then the porosity should somehow be measured. Changes in surface energies should be studied. It may be more useful for the project to focus on one component and examine it at a deeper level. The project is presently focused on the catalyst, the catalyst support, the catalyst layer, the membrane, and bipolar plates, which is quite broad. The electrode work was able to relate the role of electrode characteristics and processing (Pt%, ionomer/carbon [I/C], solvent type) to types of degradation in an empirical sense. However, most developers already have their own internal findings regarding these types of phenomena. Again, the project needs either to go deeper to discern the meaning in these data or to eliminate the task.

## Question 2: Accomplishments and progress toward overall project and U.S. Department of Energy (DOE) goals

This project was rated **3.0** for its accomplishments and progress.

- This project team has achieved a much greater understanding of fuel cell degradation.
- The project team has made good, steady progress on all tasks. There is a nice summary of key conclusions to date.
- The project team has made very good progress toward some fundamental, non-overreaching models for the durability of individual fuel cell components.
- This multi-laboratory, multi-team project achieved several useful results and developed models for membrane electrode assembly (MEA) components that help in understanding their degradation, the stability of various carbon supports, types of catalysts, and their loading.
- This project team has made good progress in understanding the electrode and membrane degradation, but it has achieved much less understanding of superimposing factors, specifically how the degradation of one component accelerates the degradation of other components.
- For the tasks that the team set out to do, there is a considerable volume of data. While there may be questions about the approach and which data add value to the community, it is without question that the project has diligently accumulated a voluminous database on all tasks. Interesting EA + E results show decreased thinning of the electrode. The models for catalyst layer degradation, membrane/ionomer degradation, and plate corrosion appear to have received a steady stream of inputs from experimentation and are still in progress. While the data collection has been excellent, the project does need to begin probing the utility of the data to developers. In many ways, a qualitative understanding has been developed of different phenomena, and a quantitative understanding is to be expected later through modeling. But the team needs to be aware of whether results can be extrapolated to more contemporary material sets. For example, there is question as to whether membranes with radical-scavenging or peroxide-scavenging additives would defeat the utility of the membrane model.
- There is far too much emphasis on carbon corrosion. Automotive original equipment manufacturers (OEMs) have low-cost options to avoid carbon corrosion. In addition, a lot of work has been done in this area, and not much light is added here. There have been some interesting results with the types of carbons, but the researchers have not done any work on generating their own supports to help prove their conclusions. The conclusion that decreasing performance is due to catalyst ionomer changes and ECSA, rather than the loss of catalyst surface area under some conditions, is certainly interesting and important. Some very easy experiments could be done to prove this. The cell could be flooded with an H<sub>2</sub>SO<sub>4</sub> solution to see if the surface area is there but has just lost ionomer contact. Ex situ absorption could also do this.

## Question 3: Collaboration and coordination with other institutions

This project was rated **3.3** for its collaboration and coordination.

- This project features excellent collaborations in key areas.
- This project features a good team that appears to be well managed and is also well coordinated with other relevant DOE-supported projects.
- Good coordination of such a large number of teams was necessary to obtain the results presented.
- The collaboration and coordination were very good; the project features an apparently well-selected team that is also apparently well coordinated.
- The collaboration effort is very substantial; many qualified parties are involved. It would be nice to see more coordination between Oak Ridge National Laboratory and Los Alamos National Laboratory (LANL) in concluding carbon balance between thinning from scanning electron microscopy (SEM) findings and directly measured CO<sub>2</sub>.
- In a sense, this is the most collaborative project in the Hydrogen and Fuel Cells Program. Eight organizations are listed, besides those involved in the other durability projects. The collaboration has been strong this past year and in prior years with respect to data gathering. The other national laboratories and University of New Mexico appear to have a strong collaborative network. Collaboration could be improved by contact with suppliers and stack developers to understand where the project could adjust to truly meet

application needs. While it is true that the team is tasked by DOE to carry out particular tasks, the team could benefit from obtaining feedback from developers to find out if its tasks are adding value or not, and then working with DOE to adjust to that feedback. LANL has a fantastic amount of scientific horsepower, but it could go wasted if a project such as this mostly reproduces data that developers already either have or have a notion of from their own findings.

- This project has too many collaborators working on different things with not enough to tie them together. There are 11 institutions at different locations, and only rarely is there coordination between them.

#### **Question 4: Relevance/potential impact on advancing progress toward DOE research, development, and demonstration (RD&D) goals**

This project was rated **3.3** for its relevance/potential impact.

- This project is highly relevant to the commercial success of fuel cell systems.
- This type of project is key to meeting the DOE Hydrogen and Fuel Cells Program's durability targets. LANL has demonstrated that it can continuously deliver good insights.
- Degradation prevention would make some fuel cells applicable tomorrow.
- A project probing individual component degradation could be of extraordinary value to developers. Durability is one of the barriers preventing wider fuel cell commercialization for some significant applications. The project addressed polymer electrolyte membrane fuel cells at low temperature, which is a relevant technology for automotive, material handling equipment, backup power, and other applications.
- Most aspects align with the objectives; however, the real impact to the industry could be less significant.
- Durability models are at the component level; more system-level durability would be more relevant, but this is an important first step.
- A lot of this work is repetitive and has been done without searching for solutions or finding solutions, which is a stated goal. A large effort is being put forth on carbon corrosion, but just in the area of characterization, and a lot of this is already known.

#### **Question 5: Proposed future work**

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

- There is a good plan for future work.
- The project is almost complete. One assumes that a comprehensive final report summarizing the key findings of the project will be issued.
- The proposed future work is good and appropriate in light of the budget remaining. This team apparently has not yet worked much on the thin-film type of catalyst architectures (e.g., 3M's NSTF), which DOE appears to hope is the future for meeting both cost and durability targets. There may be a gap in addressing potential durability issues that arise with these types of MEAs versus the more conventional dispersed catalysts on carbon supports, which has been the primary focus.
- Because contemporary material sets may differ, it may be good to reduce the work on membranes and bipolar plates. The ability of the team to gather data is established. The team would do well in the future work to include consultations with industry to understand if there are deeper directions to investigate with respect to catalyst-related components.
- It is not clear what priorities would be assigned to which aspects of the project, because a lot of modeling remains unfinished for the short time left in the project.
- Most of the emphasis is still on carbon corrosion, with the entire emphasis on characterization. The researchers have done a great job in showing how carbon corrodes the catalyst and where the catalyst corrosion occurs; it is difficult to see what benefit can come from modeling a corroded catalyst.

#### **Project strengths:**

- This project features a strong team and good coordination.
- A strength of this project is its in-depth determination of fuel cell degradation mechanisms and processes.

- Work on the effect of the solvent on catalyst dispersion casting is very interesting and can have an impact on many players; more work on understanding this would be most welcome.
- Discovery of the weak characteristics of the electrode structure under high potentials and mitigation of degradation by mixing different supports into one electrode is worth noting.
- This project features a large, well-coordinated team that is making systematic progress toward understanding fundamental durability issues in fuel cells. Another strength is the good use of LANL's expertise.
- This team has an extraordinary ability to collect a lot of data. It has leveraged the abilities of the national laboratories very well. The team has access to an extraordinary scope of characterization and analytical techniques. The leadership of the project has a deep understanding of degradation phenomena.

#### **Project weaknesses:**

- The project is unlikely to wrap up by September 2013.
- There should be more avenues and routes suggested for the mitigation of degradation mechanisms.
- The membrane degradation work is very superficial; no insight was given into the mechanism or changes with time. There is too much emphasis on carbon corrosion.
- The team needs to become more involved in understanding and blazing trails beyond what developers already know. The project is fairly spread out among a number of topics, rather than finding a particular focus where it can go deep and produce previously unknown results.
- The effect of open circuit voltage (OCV) degradation is described insufficiently. Stating that Pt deposition in the membrane is promoting H<sub>2</sub> crossover is not supported by the data. At the same time, potential cycling polarization curves are plotted with the same OCV during aging. It is not clear whether OCV degradation is studied only under OCV conditions or also during catalyst cycle tests, and whether and to what extent Pt loading affects OCV degradation. Mitigation recommendations are very minimal. More substantial recommendations are expected from LANL. Mixing of stable cathode supports into a single electrode is good, though it is not very novel and already utilized in the industry.

#### **Recommendations for additions/deletions to project scope:**

- The project team needs to figure out how to wrap up and publish work by the end of the project—or award an extension.
- The project team should prioritize modeling work of critical components and show at least one superimposing phenomena.
- A large effort to obtain bipolar plates from as many manufacturers and OEMs as possible would be helpful. Modeling transport in a carbon-corroded diffusion medium is of little value; work should focus on mitigating carbon corrosion. The prediction activities (i.e., predicting how long catalysts will last under different shutdown scenarios) should also continue.
- The project team should delete most of the membrane and bipolar plate work if there is no way to extrapolate it from materials under study to materials that will be used in a future commercialized fuel cell system. An automotive stack OEM (e.g., General Motors, Nissan, and Automotive Fuel Cell Cooperation) should be added to the project to provide development context.

## Project # FC-014: Durability of Low-Platinum Fuel Cells Operating at High Power Density

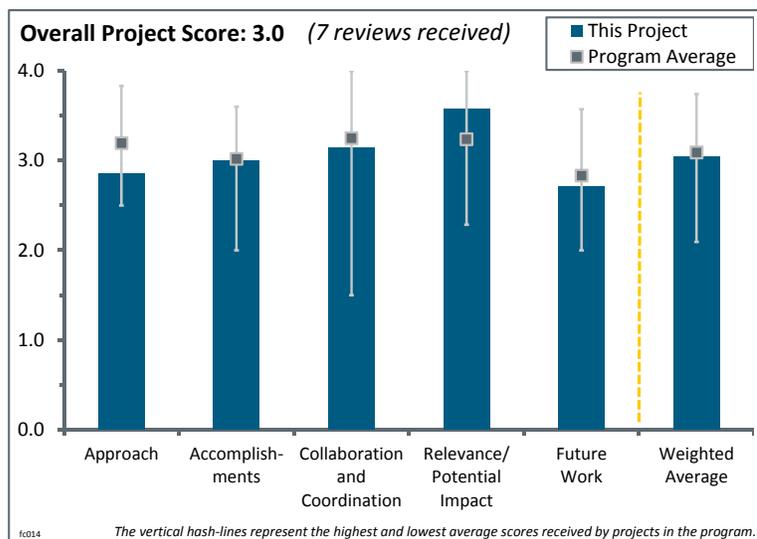
Scott Blanchet; Nuvera Fuel Cells

### Brief Summary of Project:

The objective of this project is to identify and model polymer electrolyte membrane (PEM) fuel cell durability factors associated with low-platinum membrane electrode assemblies (MEAs) operating at high power density. The key deliverable of the project is a durability model that is validated experimentally over a range of fuel cell stack technologies operating at high power.

### Question 1: Approach to performing the work

This project was rated **2.9** for its approach.



- The approach is good. The conditions of experimental validation and modeling focus on low Pt loading and high-power-density operation.
- The approaches to collecting data and developing models for describing durability dependence on operating parameters and platinum group metal (PGM) content are well organized and systematic. The results for this activity are outstanding. The initiation of the stack durability tests with automotive cycling appears to be a little behind schedule if the project is going to achieve 5,000 hours. There was no obvious approach to defining the stack cost. The provided presentation did not contain a reference to this barrier. If this barrier will not be addressed until the future, it should be stated; however, under the proposed future work, there was no indication that this work will be done. If it was done in the past, the presentation should say so. Because of the lack of information on stack cost, the approach deserved a rating of “good,” rather than “outstanding.”
- Both land-channel and open flow field designs are being evaluated. High current density and power operation are being used to address cost. The comparison of decay rates as a function of Pt loading is instructive.
- The project combines the use of modeling and experiments. The use of accelerated stress tests (ASTs) and their linkage to fuel cell or stack data are a valuable part of the approach. The model approach is not entirely clear, because the specific aspects related to phenomena experienced at high currents and the role related to the expected effect on the degradation mechanisms were not fully discussed or linked to the observations seen in the experiments.
- The approach was full of data and charts, but it was hard to interpret the conclusions. Without fully understanding the technology, one would not be able to easily decipher the impact of the plots shown.
- The technical approach is very systematic. Comparing Pt dissolution using ASTs and drive cycle performance in various single cell hardware configurations is very valuable; however, an understanding of shutdown/start-up degradation is necessary to understand performance degradation in the field. Thus, voltage excursions to beyond 1.0 V upper potential limit should be investigated.
- The overall objective of this work—to develop a universal predictor model for catalyst degradation—seems a bit far-fetched, considering the empirical basis from which the entire fuel cell community is presently operating (i.e., it is questionable that one test can be a fair predictor of all of the different materials being used, systems controls, and operational conditions of all fuel cells). While it is a nice thought that one might be able to just sit down in front of a computer, input some parameters, and then see how long a fuel cell is going to last, that seems a bit too simplistic. The use of the General Motors (GM)/Rochester Institute of Technology (RIT) flow field for comparison was also not clearly defined. It is unclear what the GM/RIT

flow field is, but it is well known that GM does not publish what it is really doing, and it is hard to predict why GM worked with RIT on the flow field or its true purpose. The implication is that the Nuvera technology is more stable than the GM technology; this seems like a big step, considering that most companies have many system-level controls in place to prevent degradation, and such conditions would be difficult to implement in the Nuvera (or any) model.

### Question 2: Accomplishments and progress toward overall project and U.S. Department of Energy (DOE) goals

This project was rated **3.0** for its accomplishments and progress.

- The researchers have made good progress towards their stated goals.
- Nuvera has quantified decay rates as a function of Pt loading. A durability model is nearing completion for dissemination.
- The work is demonstrating the capability to reach the existing cost/durability targets. In particular, there is no acceleration of the degradation mechanisms due to operation at high power density. This conclusion is valuable and useful for the rest of the industry.
- The project has made good progress. Of concern is the large scattering in voltage loss at the high loading in comparison to the low-loading results. Furthermore, the thickness changes with cycling indicate that there is substantial cathode catalyst corrosion, which is quite surprising given that the AST and simulated driving cycle did not exceed an upper potential limit of 1.0 V. Voltage loss breakdown analysis would provide a better understanding of the results.
- The technical progress is steady. The remarkable point of this project is the study for high-power-density operation, as shown in the objective. Surely the conditions of experimental validation and modeling are related to low Pt and high power density, but what researchers study in the project and the description of the outcome should focus more on properties and key factors specific for high-current-density operation, which is more helpful for stack downsizing and thus future costs.
- Excellent progress has been made towards the development of durability models. The information regarding the impact of PGM loading is surprising, but the data appear to be reasonably obtained. The project appears to have a long way to go to get to the 5,000-hour durability target with cycling. If the project ends on September 30, 2013, it is not clear whether the researchers will reach 5,000 operating hours. The third-party data in chart 8 appears to state that the researchers have reached the durability with a short stack; it is unclear if the short stack data meet the objective. Perhaps the presenter said so in the talk. The presentation did not state that the short stack data was acceptable.
- The accomplishments seemed to be the accumulation of the data of the whole 3.5 years, so it was hard to isolate just the past year. If that is incorrect and all of the data presented were just during the last period, then the rating would be higher, but the presenter's talk seemed to cover more than one year.

### Question 3: Collaboration and coordination with other institutions

This project was rated **3.1** for its collaboration and coordination.

- Collaboration was impressive and well noted.
- This project features a strong team; the collaborative efforts are well coordinated.
- The project demonstrates a strong interaction with both academic institutions and national laboratories.
- The project has a high level of competent collaborators. The modeling activity and the post-test characterization of the Pt in the membrane are both very good. It is unclear if the stack durability testing is a problem at LANL or Nuvera.
- More effective and interactive collaboration can be done (e.g., analysis results from one site can be transferred to another site for modeling).
- The speaker mentioned that the model was available to everyone and was published, but no one can seem to find it. A better collaborative approach would be to truly make the model available for use/criticism/improvement prior to the completion of the project.
- There is no automotive fuel cell systems integrator on the team.

**Question 4: Relevance/potential impact on advancing progress toward DOE research, development, and demonstration (RD&D) goals**

This project was rated **3.6** for its relevance/potential impact.

- The project addresses stack durability and cost—the top two DOE priorities. A durability model will be disseminated.
- The project supports and advances progress toward DOE Hydrogen and Fuel Cells Program goals and objectives. The data developed to date expand the overall understanding of fuel cell stack durability. A successful stack durability model that is independent of flow field design would be very beneficial.
- Reducing cost and increasing durability of fuel cells are key DOE goals. This project is well aligned with those objectives because it addresses the performance and degradation of low-loaded MEAs and stack architectures that facilitate high-power operation, enabling cell count reduction.
- The project clearly supports the need to improve the durability of PEM fuel cells; in particular, the project's focus on understanding the effect of going to high power is of specific relevance to automotive applications.
- The study on high-power operation is valuable for potential cost reduction of the stack.
- The subject is clearly relevant to lowering the cost of fuel cells; it is just hard to interpret the conclusions.
- It is doubtful that the model developed has any real relevance beyond the Nuvera system, but it is hard to tell.

**Question 5: Proposed future work**

This project was rated **2.7** for its proposed future work.

- The plan and expected achievement should focus on specific factors and properties for high-power-density operation with low Pt. The project is wrapping up. Hopefully the researchers will make their model available.
- The project is coming to an end, and the durability model is well worth completing. It is hard to judge how relevant it will be for all Pt cases because of the complexity of the variables.
- The proposed future work is adequate, considering that the project ends in December.
- The proposed future work addresses the durability model and understanding the degradation of the stacks. The future work does not address stack cost.
- The project ends in 4 to 5 months, so the future work is mostly wrap-up and reporting. Dissemination of the durability model to industry is particularly important, although it is not entirely clear how applicable the model will be to other cell/stack configurations.
- There were deviations in the results of the tests done by each of the participants. Further, there were also issues with the post-analysis test regarding the cathode thickness. Both of these aspects could substantially affect the applicability of the information from the project. Neither of these issues was highlighted in the proposed future work, yet they seem important to address in order to firm up the conclusions and results.

**Project strengths:**

- The project has a strong and experienced team.
- This project's strengths include its theme and value.
- This project is a very relevant topic that is of interest to a broad audience. The model could be useful as long as the user understands how to calibrate the variables. The project generates lots of useful, detailed data and an experimental design protocol for catalyst developers.
- The project's greatest strength is the collaboration team. The project successfully builds on the strengths of each of the collaborators. The systematic evaluation of durability with operating parameters is very good work. The comparison of stack architecture is interesting, but it probably needs more explanation. The degradation model information is very good.
- The project has strong interaction between collaborators and a combined model/experimental approach that facilitates both real data and theoretical understanding contributing to the outcome and achievements of the project. The use of different cycles—from voltage, load, and drive cycles—is very valuable in establishing

the linkage between ASTs and the real-world linkage to stacks in the field. The accomplishment of the model verification using an EIS-based parameter determination approach in order to simulate the AST/performance of the various cell configurations is also commendable because it provides insight into key measurement approaches and parameter determinations that can be used to obtain model inputs.

#### **Project weaknesses:**

- Although an enormous amount of data was generated, the conclusions and impacts were not clearly defined.
- No information was given regarding MEA components such as catalyst support. The observed corrosion at an upper potential limit of  $<1.0$  V is a concern.
- The presentation appeared to emphasize the validity of the open flow field design. It is unclear if this is a sub-issue for Nuvera. Hopefully the project was not undertaken just to prove that the design was valid.
- The objective of developing a universal model for stack degradation using contractor technology as the core technology is questionable. While a universal model sounds good, it is probably not realistic. It also seems that a not-for-profit contractor would be a better location for such work.
- There is clearly an unconsidered mechanism or potential carbon corrosion that is affecting the cathode catalyst thickness during the course of the testing. This effect could affect the outcome of the results of the project; in particular, the model does not consider carbon corrosion, only Pt dissolution. No analysis is discussed as to what impact this omission has on the model verification or fitting parameters. The discrepancy in the tests between the RIT cell and the SCOF also should be addressed; there is clearly some local condition that is affecting the results. In particular, given the focus of the project on high-current-density operation, some discussion of liquid water, running water content, the role of liquid water in the degradation mechanisms that are proceeding, and the manner in which the model describes and includes the effect of liquid water should be discussed or considered in light of these discrepancies.

#### **Recommendations for additions/deletions to project scope:**

- The project should end as scheduled.
- Resolution is needed regarding when stack cost work will be done.
- The project team should conduct voltage loss breakdown analysis to better understand the impact of catalyst layer changes on performance loss.
- This project can bring potential value and insight for durability and cost/downsizing. Therefore, if the project focuses more on what is more specific for high-power operation with low Pt, it should be accelerated more.
- The project is ending, so there are no recommended changes on this project. However, there is a question regarding whether DOE should pay for-profit companies to develop models that favor their technology.

## Project # FC-016: Accelerated Testing Validation

Rangachary Mukundan; Los Alamos National Laboratory

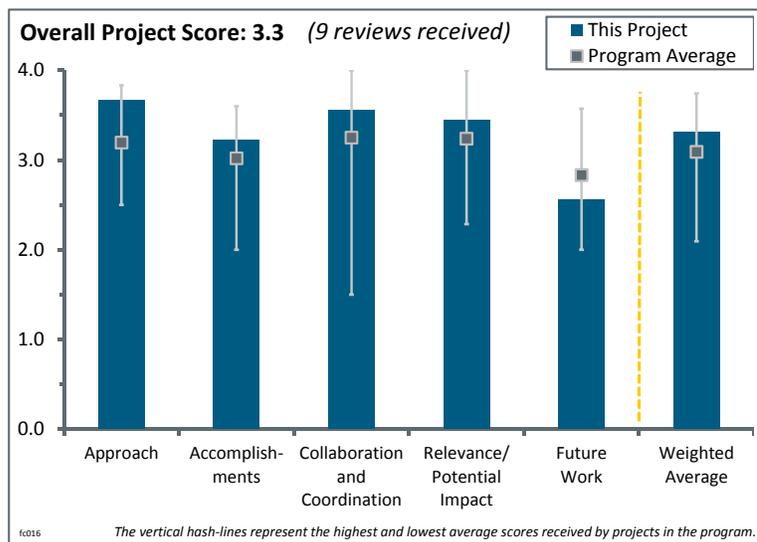
### Brief Summary of Project:

The objectives of this project are to correlate component lifetimes measured in an accelerated stress test (AST) with real-world behavior of each component; validate existing ASTs for catalyst layers and membranes; and develop new ASTs for gas diffusion layers (GDLs), bipolar plates, and interfaces. The AST is important in that it allows faster evaluation of new materials, provides a standardized test to benchmark existing materials, and accelerates development to meet cost and durability targets.

### Question 1: Approach to performing the work

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

- The approach is very good/outstanding. The key is correlating the AST methods to the bus data.
- Durability is a key barrier, and having good AST protocols is very valuable to the fuel cell community with respect to developing more stable materials.
- The approach to achieving the durability technical target is sound and well designed. Durability is a critical barrier to reaching commercial fuel cell viability. Accelerated stress testing is one way to meet durability targets using a much-reduced time frame. Comparing accelerated test failure mechanisms with actual data from demonstration projects can provide useful and validated test procedures. Identifying specific tests that achieve a targeted failure mechanism is difficult to improve on.
- This work on ASTs is systematic, comprehensive, and sharply focused on overcoming the durability barrier. This kind of work, getting knowledge on degradation out into the public domain, is important so that component manufacturers—which are generally smaller companies, at least compared to car manufacturers—get access to knowledge on degradation mechanisms. It is not enough if the car industry has this knowledge available and holds it confidential. This work is also valid for the stationary sector, in which generally smaller companies are active.
- The principal investigators (PIs) are conducting valuable research on the durability of fuel cells that may contribute to understanding and addressing the degradation issues in fuel cell stacks. The approach integrates modeling and fuel cell stacks in operation. In some ways, this approach is systematic; however, it could be potentially improved if it was capable of pointing out what should be done to prevent decay in performance.
- The project has a well-defined structure focused on achieving the technical barriers. The approach identifies the probable failure modes and systematically evaluates these failure modes under controlled conditions. The approach incorporates expertise from industry and other national laboratories. It is somewhat a concern that the stationary 40,000-hour target does not include purposefully degrading the performance of the stationary system. While this technical target is established by the DOE Hydrogen and Fuel Cells Program (the Program), there was no discussion regarding the conditions at which 40,000 hours would be attained.
- The approach is good. The PIs are using available data from the field to establish the correlation factors for the AST protocols. However, the materials of choice are of old vintage; therefore, the failure rate and correlation factors may not be relevant for newer materials.
- Using the data that are currently available (which are somewhat outdated), the approach of this project will be its legacy. The approach is well organized, and the group has sought the input of key collaborators. The



researchers have adjusted and brought in the right expertise where necessary. The accelerated testing and validation results will serve future work mainly in terms of approach, rather than the actual results.

- The project has focused on ASTs for key components (e.g., the catalyst, catalyst support, GDL, and membrane) and analysis and correlation of test results.

### Question 2: Accomplishments and progress toward overall project and U.S. Department of Energy (DOE) goals

This project was rated **3.2** for its accomplishments and progress.

- The team has made good progress with respect to refining current ASTs and proposing new ASTs.
- The project team has made excellent progress toward its objectives. Specifically, identifying how many cycles of accelerated testing correlate to hours of operation of various applications is a great step. Updating AST profiles as new data become available, specifically from demonstration vehicles, is also a great step.
- Reasonable progress has been made to understand the failure mechanisms for the various ASTs. Further, the PIs have used industry-recommended protocols and compared these with other protocols. Tests were conducted with drive cycle durability to understand the correlation between field data and ASTs. Overall, a lot of progress has been made.
- The researchers have made good progress on the development of ASTs for the catalyst, membrane, and GDL, but it appears that there are no ASTs for bipolar plates.
- The project team has made strong progress in demonstrating the ASTs.
- The researchers have generated lots of data. It will be interesting to see if they can wrap the whole project up in three months.
- The AST results could be correlated with the U.S. DRIVE cycle. Further acceleration in performance degradation is necessary. Different test procedures have been identified for the different degradation mechanisms. The work went very much into the details of degradation mechanisms. This is necessary, but the focus of AST should be kept. The results are very good.
- The PI presented a fair amount of progress in the last fiscal year. Even though the project is related to validation and testing, the outcome should be a valuable set of plausible solutions that may prevent current state of performance loss. As of now, the PIs are focused mainly on conclusions that are already known.
- The drive cycle testing does not appear to be completely focused. The PI identifies test conditions, but the explanation and discussion for the drive cycle testing is inferior to the other accomplishment discussions. The U.S. drive cycle testing correlates well with the AST for potential cycling; this work needs a better explanation. Carbon corrosion at low potentials is reported to be significant at 0.9 V; it is unclear if the researchers quantified the value. It is also unclear if there is a dependence on the type or manufacturer of the carbon. It is unclear how LBNL confirms the “collapse of cathode structure” and whether the collapse is gradual or occurs at some catastrophic condition. For the voltage loss breakdown analysis, it is unclear what simultaneous fitting of air and  $\text{H}_2\text{O}_2$  data at different current densities means. It is also unclear whether the work was done or whether this is a statement of future activity.

### Question 3: Collaboration and coordination with other institutions

This project was rated **3.6** for its collaboration and coordination.

- This project features an excellent selection of team members and data sources.
- The collaboration is outstanding and features a proper division of responsibilities.
- The PIs demonstrated a well-coordinated effort between the participants.
- This project features close collaboration with W.L. Gore, Ballard, and now Ion Power.
- There is good collaboration among the various partners. The segmented cell study to understand the impact of start–stop degradation is useful for the community.
- This project leverages industry partners, demonstration fleet performance information, drive cycles and testing protocols from the U.S. DRIVE Partnership’s Fuel Cell Tech Team [see [http://www1.eere.energy.gov/vehiclesandfuels/pdfs/program/fctt\\_roadmap\\_june2013.pdf](http://www1.eere.energy.gov/vehiclesandfuels/pdfs/program/fctt_roadmap_june2013.pdf)] and other DOE national laboratories. Coordination with experts in the AST field provides useful data on what parameters the specific end users are looking for and how the experts are currently conducting these tests.

- This project is well coordinated with other DOE-supported projects. There is also good coordination within the project team. It would also be good to include real-world results from other fuel cell original equipment manufacturers (OEMs).
- The collaboration encompasses three national laboratories and four companies, two of which are materials suppliers. All of them are notable players in fuel cells. Moreover, a European university was included—the University of Nancy.

#### **Question 4: Relevance/potential impact on advancing progress toward DOE research, development, and demonstration (RD&D) goals**

This project was rated **3.4** for its relevance/potential impact.

- The project fully supports the objectives of the Program.
- This is a very good step in the right direction to validate membrane electrode assembly (MEA) degradation with actual performance data.
- This is an extremely important project that is providing a database that will be valuable for some time. The results generated will significantly advance the progress toward DOE research and development goals and objectives.
- Establishing relevant, validated, and universally accepted AST protocols is critical to meeting durability targets.
- This project is helping to identify AST cycles designed to induce failure of certain components of the fuel cell stack and correlate the number of cycles to a number of hours of normal operation. This correlation will allow rapid testing to obtain data that would normally require thousands of hours. Rapid testing saves time and money for OEMs and users. This project plays a significant role in advancing progress toward meeting DOE durability goals.
- This project has the potential to improve current knowledge about what is causing fluctuations in fuel cell performance over time, and for that reason it is relevant to the Program. It would be important not only to list what is degrading over time but also to propose how degradation can be minimized.
- The project is relevant because it helps to address the barriers listed. The impact of these ASTs on new materials sets may be limited due to correlations to the limited field data. Further, the field data of the older design might be irrelevant in light of improvements in system design to eliminate or reduce some of these failures so that the systems can meet the targets for commercialization.
- In some cases, the ASTs are oversimplified to be of use to fuel cell developers.
- The project targets the major barrier for transportation—durability. The project digs very much into mechanisms of degradation, which is necessary to prevent creating wrong testing procedures in accelerating testing. Nonetheless, an AST project should clearly target an acceleration factor for a whole—even if synthetic—life cycle of a car. The diversity of different acceleration coefficients is physically correct and acceptable. Technically, one acceleration factor can be set for a known (or defined) life cycle of a car by putting the respective mechanism-driven acceptance test procedures together. The impact of the project will be high. Considering the approach, it will be easier to get it into the engineering domain.

#### **Question 5: Proposed future work**

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

- The project is ending in this fiscal year, and the proposed future work is in line with ongoing efforts.
- This team has a plan for future work and builds on the work done in a logical manner. The plan will contribute to further push the durability testing and get closer to meeting the end durability goals. Independent validation of stack-level tests should be considered.
- The plan to update the test protocols (based on the results obtained to date) is recommended. It is unclear if there is a plan for ASTs for bipolar plates.
- Putting the data online sets a great precedent in the Program and will certainly force rigor.
- The proposed future work is appropriate for the funding that remains, but it is not clear how additional work that remains to be done will continue beyond this project.

- The proposed future work is sound; however, it would have been nice to study the failure mode with a newer class of catalysts. The AST related to GDL aging is less important for field failure. The dissemination of information through publications is adequate for failure modes. The models developed under this project should be made available for use by others within the field.
- It seems like the researchers are going to run out of time before they can wrap up their work.
- The focus should be kept on vehicles. The scientific depth in degradation mechanisms is appreciated and fully understood as being necessary as long as the final goal of accelerated testing is also pursued in an engineering way. For certain driving cycles, the different mechanisms of degradation should be quantitatively allocated and combined in a way that the accelerated test represents the particular driving cycle. The existing work is very good, but some engineering perspective should be added to make it really useful.
- The future work is a list of activities to be performed with no discussion of their benefits. Perhaps the researchers assume everyone is so familiar with the technology that no explanation of benefits is needed.

#### Project strengths:

- Recommending relevant ASTs for material development is a strength of this project.
- The well-designed testing approaches on key fuel cell components are a strength of this project.
- The technical capability of the team members is extremely high. The results reflect the quality of the team.
- This project features a very good team that is solving real-world problems with MEAs and doing meaningful validation of ASTs versus in-field durability tests.
- This project features a systematic approach in accelerated testing and a strong team that relies on expertise in modeling and fuel cell stack testing.
- Strengths of this project include the very qualified partners and getting ASTs outside of the car manufacturers' domain.
- This project's methods are an area of strength. This project represents the most comprehensive effort for fuel cell ASTs. Its successes and failures will certainly serve to improve the lifetime analyses of those who choose to study the work done.

#### Project weaknesses:

- An area of weakness is the impact of system design and material changes on correlation factors.
- Correlation with automotive drive data is recommended to demonstrate the relevancy/validity of the ASTs. The materials are an area of weakness. The materials used in most of the validation work are not state of the art; however, it must be understood that state-of-the-art materials are not generally available with >5,000 hours of service, especially for public disclosure of their performance. The LBNL modeling work seems redundant in light of all of the other projects the group contributes to.
- There is a lack of conclusions about how to prevent or slow down degradation in performance.
- The strongest weakness—the focus on bus data—has been amended. As for future work, there should not be a focus on bus data again.
- The team will not likely have time to finish the project and publish the results.
- The explanations of the accomplishments were in some (many) cases incomplete. The slides were not definitive and did not provide enough information to describe the benefits of some of the achievements. The future work slides did not provide any insight into the benefits of the work. It is recommended that future presentations provide more information on benefits attained and expected benefits of future work.

#### Recommendations for additions/deletions to project scope:

- The project team should study the impact of these ASTs on the state-of-the-art MEAs.
- The team should carefully document not only the successes of the project but also the shortcomings of the ASTs.
- Los Alamos National Laboratory needs some extra time/funding to publish the results.
- The different identified mechanisms and procedures for accelerated testing should be put together to form one test representing the life cycle of a car. Ideally, a routine would be developed that is in a position to identify and quantify the necessary modules to be applied for arbitrary life cycles. This routine should be in a position to emulate a given life cycle and create an appropriate AST program.

## Project # FC-017: Fuel Cells Systems Analysis

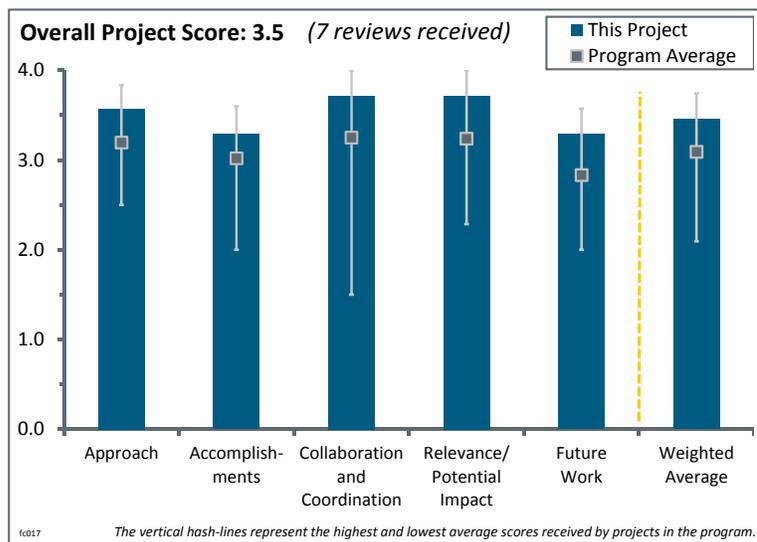
Rajesh Ahluwalia; Argonne National Laboratory

### Brief Summary of Project:

This project is focused on developing a validated system model to use for assessing the design-point, part-load, and dynamic performance of automotive and stationary fuel cell systems. The model will also be used to establish metrics for gauging the progress of research and development (R&D) projects and to provide data and specifications for cost estimates on high-volume manufacturing.

### Question 1: Approach to performing the work

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



- This is an excellent contribution to fuel cell technology. The approach is clear and has been well developed over the course of the project.
- This project features excellent continuation of the great work done in this field before.
- The approach to modeling goes down to a level of the science that governs fuel cell performance and behavior.
- The main objective is to develop a validated system model and use it to assess design-point, part-load, and dynamic performance of automotive and stationary fuel cell systems. The proposed approach is in agreement with the challenges to overcome, and its annual reorientation does a nice job of reflecting the issues to take into account better.
- These tasks are critically important to the Fuel Cells program. The engineering modeling provides understanding of the many elements that dictate reliability, performance, and cost of all fuel cell hardware. Moreover, these contributions serve to develop a vocabulary that makes it far easier for everyone in the program to communicate effectively. The result is a very clever integration of the research part of the DOE-sponsored work and the commercial part of the program. By using that vocabulary, the entire group of participants has the ability to communicate rapidly and effectively.
- The main technical approach is sound. The modeling is based on experimental validation, as it should be, and several partners contribute with experimental data that are used to validate the model. However, there are two main points for criticism: (1) the fuel cell data is based on 50 cm<sup>2</sup> work and should be expanded to stack systems, ideally full-size stack systems, and (2) the work in 2013 concentrated on one particular catalyst type from one particular supplier. While it is important to include nanostructured thin-film (NSTF) catalysts in the work, it would have been better if the work included other electrode layer structures and a comparison of these systems. This would have demonstrated the capability of the model as well as given some insight into a technology comparison of competing catalyst structures.
- The approach taken in this project is very good. The general approach is to develop and validate versatile system design and analysis tools. The collaboration with external organizations for validation of the model is highly appreciated. However, most of the design work is done at high pressure, and considering that cost is a challenge for fuel cell systems, the approach should be focused on low-pressure design and modeling that can reduce the system cost. The project team should look at other fuel cell models developed under other DOE projects while designing the system model under this project. It would be interesting to see system cost at low Pt content for lower volumes, although this may be out of the scope of this project.

## Question 2: Accomplishments and progress toward overall project and U.S. Department of Energy (DOE) goals

This project was rated **3.3** for its accomplishments and progress.

- The sophisticated model is well developed and addresses the details (e.g., mass transfer and Pt-loading issues). The model is validated using real test data and is in very good agreement with the data. The key issue of system cost is also addressed.
- The accomplishments are well documented, but in some cases they represent incremental advancements.
- The project has progressed well this year. Main areas of progress included extending the nanostructured fuel cell stack model operating point, introducing modeled Roots compressors and expanders, validating the humidifier model against data for a full-size unit, and extending and validating the model for H<sub>2</sub> ejectors. Unfortunately, only the 3M NSTF membrane electrode assembly (MEA) is investigated, even if its modeling is more detailed.
- The modeling effort and set of results are very good overall; however, the modeling effort aimed at stack-related performance/parameters needs to be verified with an actual stack system. Small-scale single-cell data are not sufficient to verify this model. It is unclear if and how the model is made accessible to the public.
- The progress made so far is significant, but it is not enough to understand the cost savings from different systems. The collaborative work on fuel management (Ford Motor Company), stack model validation (3M), and water management (W.L. Gore, Ford, dPoint) is commendable. The Artificial Neural Network model for cathode mass transport is a good approach, but other models developed under DOE projects related to cathode over-potential analysis need to be considered and cross-validated.
- These activities produce progress in a continuous and rewarding way. Moreover, this progress really covers a rather broad base and is obviously building upon itself—each new calculation uses results of previous ones. Questions are raised, and answers are quickly calculated. Moreover, results are published and made available to many in the community, while protecting the interests of those working to develop fuel cell markets.
- The barriers claimed to be addressed by the model include (a) Cost; (b) Performance; (c) System Thermal and Water Management; (d) Air Management; and (e) Start-Up and Shutdown Time, and Energy/Transient Operation. There is clear evidence that the project addresses barriers (b), (c), and (d). The linkage between this project and barriers (a) and (e) is more tenuous. Although cost results are in the backup slides, it would be good to see some of the major outcomes on cost produced by the model, for instance, a sensitivity study looking at several of the major drivers of cost, Pt loading, current density, and power.

## Question 3: Collaboration and coordination with other institutions

This project was rated **3.7** for its collaboration and coordination.

- The collaboration is extensive and appears to be very interactive.
- The collaboration is well balanced, and there is an important emphasis on industrial partners.
- The collaboration with external organizations is excellent, specifically with 3M, W.L. Gore, and Ford. Also, the collaboration with the component supplier for the compressor and expander (Root and Eaton) is very good. This project has strong and sufficient partners to accomplish what has been proposed.
- This project features a very good team of collaborating partners. The portfolio consists of a number of research laboratories; companies that create fuel cell system materials and/or balance-of-plant (BOP) components; and national and international working groups such as the tech team, the modeling working group, and the H<sub>2</sub> fuels purity-related working group. It is an impressive set of partners.
- The entire thrust of this work is collaboration. The information flow integrates R&D and provides DOE with excellent, timely information, making the management job less difficult. Perhaps this project is the best example of collaboration one could think of. It can be viewed sort of as the model—the one taught to explain what collaboration could be. It is also apparent that these timely results facilitate analysis of proposals for new activities in ways that promote intelligent program management.
- The coordination appears correct, and the quality of the results reflects it. New industrial collaboration is appreciated and enables links between different projects, such as the project with Eaton. Collaboration

between Argonne National Laboratory and the partners appears to be very good, but there is no indication that collaboration between the other partners of the project exists.

- The collaboration looks good; however, it would be good to see system-level validation of the model compared to an actual original equipment manufacturer (OEM) powertrain. That would demonstrate that the model is valid and could be applied to other system topologies. It would be good to have OEMs with more active fuel cell programs than Ford on the list of collaborators.

#### **Question 4: Relevance/potential impact on advancing progress toward DOE research, development, and demonstration (RD&D) goals**

This project was rated **3.7** for its relevance/potential impact.

- This is an excellent contribution to fuel cell technology.
- This project provides valuable modeling tools. It is of high value to industry partners.
- The relevance and impact of this project are very high because it will help OEMs that are designing relevant fuel cell systems according to DOE technical and economical targets.
- This project's relevance to the DOE Hydrogen and Fuel Cells Program is perfect. It is one of the most important studies to address system-level performance and cost barriers. The cost projections are correlated to Strategic Analysis, Inc. (SA) models, which makes more sense. The focus can be increased by featuring more actual stack-relevant system design and modeling than a 50 cm<sup>2</sup> cell.
- A comprehensive system model that can guide decision making for DOE as well as industry is a highly desirable tool. However, developing one is a very large challenge because system characteristics are OEM-dependent and the developed tool has to be very versatile to be applicable over a large range of system architectures.
- The extent to which the model is available to, and customizable by, automotive OEMs and other stakeholders is unclear. Making the model open will aid its relevance and usefulness. The model provides a very detailed look into system details as well as physics controlling performance and efficiency. Nothing like it is available in the public domain.
- The project is driven by DOE-derived targets that are somewhat achievable goals. The complicated and thorough analysis done in this project is all about addressing and meeting those targets—the how, when, and if.

#### **Question 5: Proposed future work**

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

- The project team should keep it up. The project is worthwhile and should be funded even further.
- The proposed future work is a natural continuation with convincing additions.
- The future work is to continue these ongoing calculations. There is no question that should happen. The rewards are apparent. It appears that this is money well spent.
- The future work item of most interest is “System analysis with durability considerations on drive cycles.” It would be interesting to see this in light of different degrees of hybridization with batteries/ $\mu$ Caps because most fuel cell electric vehicles will be deployed as hybrids.
- The proposed future work is good. The introduction (or at least the presentation, if it is already implemented) of the system control may complete the modeling. The actual durability of a stack will be highly influenced by the control strategy for the BOP components.
- The overall future work to support DOE development efforts at the system and component levels is very good. However, MEAs other than NSTF or de-alloyed NSTF should be considered. It seems that only NSTF was considered because 3M was the only stack validation partner. Other stack validation partners need to be approached, and other MEAs with Pt or a Pt alloy catalyst can increase the value of this project. So far, researchers have not demonstrated enough focus on significant cost reduction, other than the idea of reducing Pt loading in the catalyst. Suggestions for significant cost reductions in other systems would be a great add-on.
- The future work needs to include model verification with one or more stack systems.

**Project strengths:**

- This project is very comprehensive and thorough.
- This project is extremely well documented, and the detailed basic physics add up to a robust model.
- This project features a good modeling backbone, as well as good exchange and collaboration with partners.
- This project features a solid approach, very strong partners, and strong work with component suppliers. The team has made excellent progress.
- Certainly it would take a special person to do this, and this principal investigator is unique. Others might grow into such a role, but few could. This principal investigator is a key project strength.
- The project is running well and takes into account major parameters for stack and BOP components. Good links have been established with component suppliers and OEMs. The results are well presented. The collaboration with SA is important because it enables the team to establish a reciprocal critical review of the outcomes of pure technical and pure economical approaches. The maximum operating pressure proposed (3 atm) is a representative example.

**Project weaknesses:**

- No significant cost reduction at the system level has been proposed.
- Even if the presented goal is for either automotive or stationary systems, the presented results only concerned transportation. It is unclear if there are any results for stationary applications.
- These are not weaknesses of the project but of the presentation: (1) the slides contained too many abbreviations known only by insiders, and (2) the slides are far too busy—fewer but clearer ones would be desirable.
- It is hard to criticize what is going on in this project. Even so, there should be attention paid to fuel cell systems of alternative design. The MEA and essential cell fabrication have only been tweaked during the last decade. It would be good to look “outside the box” and see what organizations outside of the DOE family have been up to.
- There was no validation with stacks or real fuel cell systems. All stack performance data points are extrapolated from 50 cm<sup>2</sup> cells, which renders the results questionable in their usefulness.
- The project claims to address the barrier of Start-Up and Shutdown Time, Energy/Transient Operation, yet no dynamic model results or runs have been shown. The project lacks collaboration with an OEM on a system-level validation of the model.

**Recommendations for additions/deletions to project scope:**

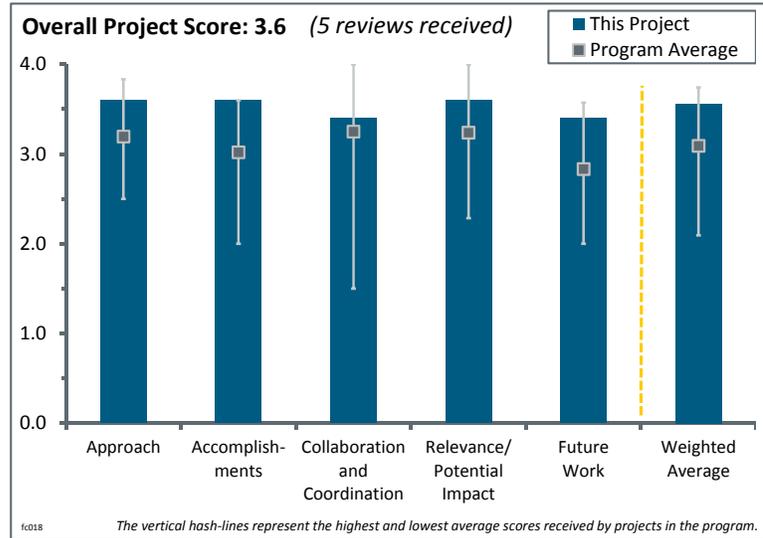
- It seems like all of the bases are covered.
- The project should be extended.
- The project team should pursue validation with full-size stacks, short stacks, and/or systems.
- The researchers should focus on incorporating durability considerations in system analysis.
- This project should produce model dynamic results relative to data from an integrated system. This will likely require tighter collaboration with an automotive OEM to allow comparison of its system to a version of the model tailored to its system.

## Project # FC-018: Fuel Cell Transportation Cost Analysis

Brian James; Strategic Analysis, Inc.

### Brief Summary of Project:

Cost analysis is used to assess the practicality of proposed power systems, determine key cost drivers, and provide insight for the direction of research and development priorities. This project is a continuation of previous years' cost analyses of automotive and business fuel cell systems, and it is exploring subsystems and alternative configurations of those systems. The 2012 analysis looked at a plate frame humidifier, looked at low-cost roll-to-roll membrane electrode assembly (MEA) manufacturing, and improved quality control techniques.



### Question 1: Approach to performing the work

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

- This is a well-established and great process for system evaluation.
- This project features appropriate cost estimation methodologies and well-defined assumptions.
- Independent cost analysis is very important for the U.S. Department of Energy (DOE) to gauge the state of development of fuel cell technology, both within the DOE Hydrogen and Fuel Cells Program (the Program) as well as outside the Program. Knowing the state of development enables DOE to set research targets that reflect a feasible stretch from the current technology. The automotive application has the most aggressive cost target and has received the most attention. However, other applications need similar attention if the Program is to be a success. Strategic Analysis, Inc. (SA) uses well-known cost estimating techniques that have wide industry acceptance. SA accounts for many smaller features and details in its system designs. The results have been vetted by original equipment manufacturers (OEMs). The approach is very good.
- This project features a detailed cost analysis that is identifying key contributors to cost and determining realistic process-based costs. The project also considers realistic production rates for buses. The production rates for MEAs and humidifiers are an order of magnitude higher than the production rates for buses; it is unclear if this is an apples-to-apples comparison. MEAs made by the new process are assumed to have the same performance as ones made by the old process. It is unclear if laboratory data are available to make this assumption.
- The project addresses the barriers of cost and thermal, air, and water management. The bus production rate for cost analysis of buses is set to 1,000 units per annum, which makes much sense for evaluating the market introduction phase. The catalyst loading was increased to a reasonably higher level for the sake of the longevity requirements for buses over vehicles. The procedure and the data used for the cost analysis are apt and up to date (compared to sensitivity analysis and Monte Carlo analysis). The W.L. Gore manufacturing process for vehicles applies very thick catalyst layers, which might not make a big difference in cost. The technology approach does not sound coherent because at the same time very high production speeds of >10 m per minute are assumed, which would result in very long dryers at that high speed. Other than that, the assumptions are sound, and the evaluation is at a cutting-edge level.

## Question 2: Accomplishments and progress toward overall project and U.S. Department of Energy (DOE) goals

This project was rated **3.6** for its accomplishments and progress.

- The progress to date is very good.
- The project team has done an excellent job of updating work.
- The presenter showed system optimization (slide 28), with selections for catalyst loading, air stoichiometry, and pressure. It is unclear if the model is sufficiently thorough to make conclusions. For example, electrochemistry is affected by air stoichiometry, including water management (high air flows improve voltage but also help remove water droplets in the stacks). The pressure of operation improves current density but induces auxiliary power. Catalyst loading balances performance and more importantly life/robustness. The relationships here can be very interactive. It would be good to know if the researchers' conclusions are in line with OEM views.
- The bus system cost analysis uses the same estimating methodology as the automotive application, which has resulted in cost estimates that align with industry projections. The same level of attention to detail is evident in the bus analysis. The balance of plant (BOP) in these systems remains a significant contributor to the cost estimate and could benefit from additional DOE research attention. The 2013 automotive cost analysis update looked at changes in operating conditions and in humidifier design that did not change the estimate substantially. The automotive analysis is based on the 3M NSTF catalyst system. It would be helpful to prepare the equivalent analysis using a dispersed Pt catalyst, as is the current practice. If the continued analysis of system modifications results in the cost estimate remaining relatively unchanged, then DOE needs to refocus its research efforts in areas likely to lead to more substantial cost reductions to meet the ultimate targets. It is good to see the attention paid to the quality control aspects of the manufacturing process.
- The 2013 data basically confirm the earlier results but on a much more detailed level, and new components were considered. The data seem to be pretty robust and reliable. The cost structure is well understood. The approach to investigate lower production volumes that are relevant for the market introduction is very useful. The investigation of the W.L. Gore process combined a relatively high production speed with very thick catalyst layers. This is not only a materials consumption issue but also creates a problem regarding drying these thick layers at that speed. This process might be looked into closer. This strongly contributes to the DOE goal of cost reduction.

## Question 3: Collaboration and coordination with other institutions

This project was rated **3.4** for its collaboration and coordination.

- Major national laboratories and major industry players are involved in crucial parts of the analysis.
- There is good collaboration with project partners.
- Formal collaboration occurs between SA, Argonne National Laboratory, and the National Renewable Energy Laboratory. Industry review of assumptions and cost projects is important to the project as a means of ensuring that the results are consistent with industry expectations. Without this interaction, the project would not be successful. SA has reached out to OEMs and the component suppliers to verify assumptions and methodology. Additional interaction with suppliers of BOP components would expand the opportunity for comparison of alternative technology.
- The input and feedback from collaborators are unclear.

## Question 4: Relevance/potential impact on advancing progress toward DOE research, development, and demonstration (RD&D) goals

This project was rated **3.6** for its relevance/potential impact.

- The project fully supports the objectives of the Program.
- The impact will be high because the project delivers unbiased data and makes these data publicly available, which is important for economic considerations and even decisions of the supply industry.

- The project is relevant to the Program. It provides an independent assessment of the manufacturing cost of fuel cells. In addition, the method used has been vetted by numerous OEMs and reviewers. While the results are not necessarily spot on, they give DOE a consistent picture of the trends in the manufacturing process from year to year.
- This is an independent validation of costs for fuel cell buses. The project does not present a cost market curve.

### Question 5: Proposed future work

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

- The proposed future work, especially the proposed continued vetting of the assumptions, is very appropriate for this project.
- Continued comparison of the bus system with the automotive system should provide additional insight into the differences between the two systems and an opportunity to take the “best components” and practices from one system and apply them to the other system to explore additional means of cost reduction.
- The future work proposed looks a little weak, considering that just 50% of the project has passed. The proposed work makes sense, though, and needs no changes in terms of the points proposed. It is suggested the project include different production quantities for vehicles as well (e.g., 1,000, 10,000 and 100,000 p.a.) in order to reflect the ramp-up, as was done for buses.
- Determining the sensitivity to annual production volume would be good.

### Project strengths:

- The project features excellent cost estimation and analysis approaches based on well-defined assumptions.
- The principal investigator’s team is extremely effective with this analysis. The team should keep doing exactly what they are doing—nothing should be changed.
- Strengths of this project include the creation of publicly available and unbiased cost data, and strong cooperation between a consulting company and national laboratories.
- The project features a good approach in calculating costs for realistic production rates at this time. In addition, the project team has considered ranges of values with upper and lower bounds.
- The collaboration with industry to vet the assumptions and methodology of the analysis is excellent and crucial to the determination of viable cost projections. The analysis is clear and methodical, which provides high confidence in the validity of the cost projects. In addition, the accumulated database also inspires confidence in the results.

### Project weaknesses:

- It is hard to cover all aspects of the bus and automotive analyses in such a short presentation.
- There is a lack of details on the input and feedback of the collaborators and fuel cell system and component developers.
- The individual components are costed at significantly higher production rates than the total system production rate. It is not clear if the new developments mentioned in the study are available for implementation.
- There are no notable weaknesses.

### Recommendations for additions/deletions to project scope:

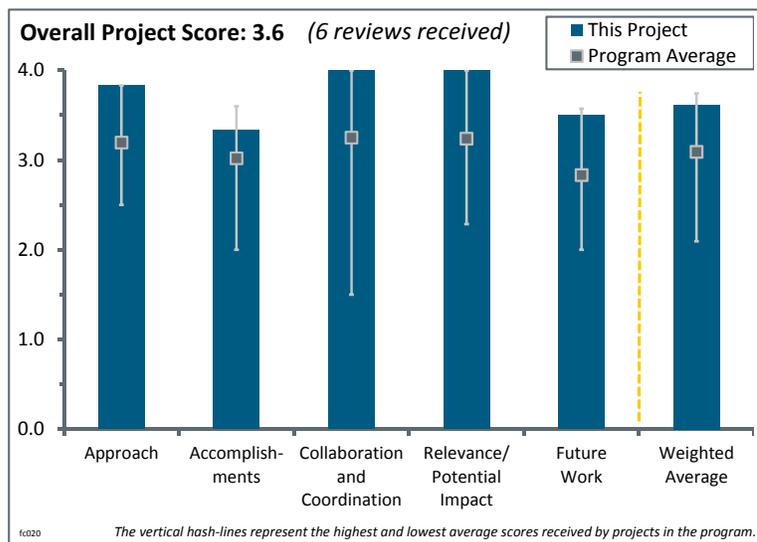
- The U.S. DRIVE Partnership is continually evaluating research targets in light of the most recent advances in the state of the technology. SA should strive to incorporate the latest information from the U.S. DRIVE Fuel Cell Tech Team into the analysis.
- It is suggested the project include different production quantities for vehicles as well (e.g., 1,000, 10,000 and 100,000 per year) in order to reflect the ramp-up, as was done for buses.
- The project team should consider adding a detailed cost study on high-impact BOP components—the sensors and air loop.

## Project # FC-020: Characterization of Fuel Cell Materials

Karren More; Oak Ridge National Laboratory

### Brief Summary of Project:

The objectives of this project are to (1) identify, develop, and optimize novel high-resolution imaging and compositional/chemical analysis techniques and unique specimen preparation methodologies for the micrometer-to-angstrom-scale characterization of material constituents composing fuel cells (catalyst, support, membrane); (2) understand fundamental relationships between the material constituents within fuel cell membrane electrode assemblies (MEAs) and correlate the relationship data with stability and performance; (3) integrate microstructural characterization within other U.S. Department of Energy (DOE) projects; and (4) apply advanced analytical and imaging techniques for the evaluation of microstructural and microchemical changes to elucidate microstructure-related degradation mechanisms contributing to fuel cell performance loss.



### Question 1: Approach to performing the work

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

- The project's focus on developing and perfecting the necessary tool and analytical competence needed for evaluating fuel cell materials, coupled with serving an extended group of collaborators, has enabled significant contributions to the DOE Hydrogen and Fuel Cells Program (the Program).
- This is a characterization project that supports the development of others to help understand the development of materials and devices. The principal investigator (PI) showed this is being done and more. The use of microscopy tools by the teams seems to have revealed an important failure mechanism; namely, that compression is a first step leading to local Pt-enriched sites promoting carbon corrosion.
- The approach adopted by this project—to be a center of excellence for nanoscale microscopy—is very valuable to the community. Based on the number of collaborations established, it is clear that the project is well integrated with other efforts.
- The imaging techniques applied are outstanding on a world level. The very inclusive approach makes the basic research contribute in an ideal way to technical development (e.g., the great number of partners, integration of microstructural characterization within other DOE projects, making capabilities available to researchers outside of Oak Ridge National Laboratory [ORNL]). The targeted components such as catalyst nanoparticles, polymers, catalyst support materials, MEAs, etc. are the most important ones for longevity and cost reduction. The research contributes to the most important targets: durability and performance.
- This project applies state-of-the-art electron microscopy to problems of interest in fuel cell design and durability studies. Access to these appropriate tools is only one aspect of the project. Another is that the project develops and maintains a core of experience in issues specific to fuel cells, providing a high level of added value. Having a common electron microscopy resource for many research projects capitalizes on the advantages that specialization offers, “leveraging” the knowledge gained in one research project for the benefit of many. In addition, the collaborative approach demonstrated by this project—for example, using problems suggested by the U.S. DRIVE Fuel Cell Tech Team to guide future work—contributes greatly to its value.

- This project features excellent, highly relevant work. This work provides significant contributions to understanding degradation mechanisms through detailed microstructural characterization. This project provides a focus on the characterization, which is critical to achieving an understanding of degradation mechanisms, which in turn is critical to improving the durability of fuel cell systems. However, the work is focused on the characterization techniques, as it should be, and depends heavily on results from others. This appears to result in some potential disconnects between the interpretation of the structural changes as a function of the degradation mechanism, and hence some potential errors in the hypothesis about mechanisms. It may be better to either limit observations to changes in structure without hypotheses on mechanisms (preferred), or work more closely on the mechanisms. In the former instance, the hypotheses should be made under the durability projects where the mechanisms are being studied. Some examples of potential issues include the following:
  - Validation and comparison to realistic operational conditions is very important; for example, corrosion under H<sub>2</sub>/N<sub>2</sub> instead of H<sub>2</sub>/air may affect the structures formed.
  - The amount of carbon corrosion (CO<sub>2</sub> production) was not shown, nor was it determined how this correlates with thinning, but conclusions were still drawn regarding this correlation.
  - It was not determined how the volume of carbon converted to CO<sub>2</sub> could result in a change in compaction and porosity of the catalyst layer; for example, an estimate based on a packing model may provide a rough comparison.

### Question 2: Accomplishments and progress toward overall project and U.S. Department of Energy (DOE) goals

This project was rated **3.3** for its accomplishments and progress.

- This project continues to provide the necessary characterizations to better understand failure modes and evaluate new approaches for improved durability and performance.
- Carbon thinning was perfectly proved by imaging. Carbon oxidation and graphite oxide formation were proved and quantified. This is great progress.
- The work to date is meaningful. It would deserve a rating of “outstanding,” but there are some delays, although the PI expects things to be back on track in about a month.
- The PI explained that at each Program Annual Merit Review, the project team focuses on a different area of its research and accomplishment (slide 7). This year, the presentation focused on quantifying cathode degradation, especially carbon corrosion. Slides 9–16, together with the PI’s oral explanation and the question and answer period at the end of the presentation, demonstrated a significant body of accomplishment in this area. The lack of presentation time precluded a similar discussion on accomplishments concerning measurements of ionomer films (slides 17–21), but there is little doubt that this project is highly productive nonetheless.
- The work provides significant contributions to understanding degradation mechanisms, which are critical to achieving DOE goals. There has been excellent progress on understanding changes in microstructure due to the carbon corrosion mechanism, but it has not been quantitatively linked to the corrosion/CO<sub>2</sub> production mechanism.
- The work conducted is very challenging. The ORNL team has made good progress. The results presented for the carbon corrosion effort were very interesting and support the broader fuel cell community. Hopefully in the remaining portions of this work, mechanisms that explain the loss of porosity in the cathode layer will be identified, along with a deeper understanding of the mechanisms by which localized graphite oxide regions are formed, in close proximity to coarsened Pt particles/clusters. The ionomer film studies are unique and could be valuable in determining the differences between traditional supported Pt catalysts and the catalyst-coated nanostructured thin film (NSTF), which apparently behave differently when using 3M versus Nafion ionomers. Hopefully in the next year more studies will be presented detailing the nanoscale microstructural degradation in the Ni<sub>7</sub>Pt<sub>3</sub>-NSTF nanoscale materials, which appear to have been adopted by the fuel cell community even though there is substantial loss of Ni during operation.

### Question 3: Collaboration and coordination with other institutions

This project was rated **4.0** for its collaboration and coordination.

- A very large number of collaborators are using the facilities for a multitude of characterizations.
- This project's success depends on collaboration in order to have access to material for analysis. The annual report of outstanding accomplishments highlights the synergy developed between ORNL and its partners.
- By virtue of the project team's strongly adhering to the project charter (approach), this is an area where the team has performed extremely well (i.e., by providing critical support to a number of funded efforts).
- This project is inherently collaborative because it provides an expert technical resource to non-ORNL collaborators. The presentation demonstrated an impressive list of university, industry, and government partners (e.g., slides 2 and 4).
- This project features extensive collaboration with a large number of partners. However, the work shown was focused on the efforts at ORNL, so it is difficult to tell the level of collaboration that actually occurs.

### Question 4: Relevance/potential impact on advancing progress toward DOE research, development, and demonstration (RD&D) goals

This project was rated **4.0** for its relevance/potential impact.

- The work targets the most important issue in longevity.
- The direct observation of preservation or failure of components is critical, and this team is serving that need.
- The project's investigation and analysis of the effect of carbon structure on carbon corrosion will guide improvements in catalyst development.
- The work is highly relevant, and the results achieved are advancing the supporting knowledge base to understand degradation mechanisms. Ionomer imaging is very important and may lead to the ability to design better catalyst layers to both improve performance and mitigate degradation mechanisms.
- This is a valuable, core project in the Hydrogen and Fuel Cells Program. It provides broad access to electron microscopy and relevant expertise for projects studying fuel cell materials (e.g., the MEA material constituents). Electron microscopy is relevant because it measures and diagnoses the microstructure and nanostructure of the functional materials within a fuel cell. Understanding this microstructure and nanostructure is key to understanding the performance and durability of a fuel cell.
- Given that 34% or more of the fuel cell costs are tied up in the catalysts and membranes, it is crucial that fundamental work such as this is performed. As the community moves to low-platinum-group-metal catalysts in order to meet performance requirements, this work will be key to the discovery and application of these new materials.

### Question 5: Proposed future work

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

- The future work proposed is in line with the barriers identified.
- The future work on ionomer imaging is very important. The correlation of the observations with real-world results is critical. There is some concern about the accelerated stress test used and the relevance to real fuel cell operation.
- The electrode structure (catalyst + ionomer) can be significantly different depending on formation (coating, spraying, etc.), and it may be necessary to examine the "as made," "pre-conditioned," and "used" MEAs to ascertain the structure as it exists during actual fuel cell operation.
- The project plans its future work in a logical manner by consulting with the Tech Team and other constituents (e.g., see slide 8.) The future plans described on slide 24 seem reasonable and appropriate, including the studies of ionomer films and the continued development of in situ electrochemical "liquid cell" transmission electron microscopy/scanning transmission electron microscopy (TEM/STEM).
- Besides continuing the very successful work, the researchers plan to correlate the knowledge to experimental data from fuel cell testing. This takes the work to a next, higher stage. As for the observed

compression of the catalyst layers, it is recommended the project put in effort regarding understanding the mechanism of densification in detail. This might open up new options of carbon modification other than the already-identified Pt on low surface area carbon (LSAC).

- The plans for use of the microscopy facilities are well thought out. The researchers should use some simple “sanity checks” to ensure this work is on track. Instead of relying on microscopy to find everything (such as compressive loss of porosity), the team should conduct simple weighing of samples before and after use to see if mass change and thickness change corresponds to densification expected for pore loss. Also, utilizing gas flow through electrodes on gas diffusion layers (GDLs) at constant pressure before and after applying pressure should help determine whether compression is the cause of electrode thinning as opposed to corrosion being the cause of electrode thinning.

#### **Project strengths:**

- This project’s strengths are clearly attributed to the ORNL team’s continuous efforts to improve its tools and analysis capabilities.
- This project features a skilled team as well as strong and numerous collaborators.
- This project features outstanding experimental proficiency in imaging and an openness to sharply focus on the requirements of fuel cell development. The inclusive approach to the fuel cell community is part of this.
- This project provides core technical competence and develops relevant experience in the field of electron microscopy for a broad range of projects within the Program.
- The team provides crucial characterization capability to the fuel cell community and DOE at large. Without fundamental work such as this, it is unlikely that the barriers facing the fuel cell community will be overcome. Therefore, it is critical that the Program continues to support this work.
- This project provides very detailed work with correlations to structure, for example, the carbon/graphitic structure. The project features an excellent number of collaborators and attempts to draw on the extensive research and industrial community. It also provides significant advances to microstructural characterization capability and features a very accomplished lead researcher. The new focus on ionomer imaging is very important and relevant.

#### **Project weaknesses:**

- The project could use additional staffing in order to make timely progress on the proposed activities for 2013 and beyond. There is a combined need to meet the demand for routine “expert analyses” as well as develop new tools and protocols for ionomer and electrochemical “liquid cell” projects.
- This project features rigid thinking. The researchers need to think “out of the box” a little more. Granted this is hard when one has to focus on handling precision tools, but taking a deep breath and rethinking what one is doing once in a while is a good thing.
- There is a very large number of collaborators, but it is not clear how much is actually done with each of them. The attempts to understand mechanisms based on studying microstructure may be based on inadequate links to the degradation conditions and quantitative analysis of the processes occurring (e.g., carbon corrosion). The corrosion study shown used H<sub>2</sub>/N<sub>2</sub>, which is not a realistic condition, and observations were made without taking that into account.
- There is nothing that could be identified as a “weakness.”
- There are no significant weaknesses.
- There are no obvious weaknesses.

#### **Recommendations for additions/deletions to project scope:**

- The project team should include research for understanding in detail the compression effect of the electrodes during operation.
- In addition to the ionomer study, the researchers might include the “interfacial aspects” between the electrode (catalyst + ionomer) and the membrane.
- The researchers should weigh the samples. They should also check the components of the MEA separately (check gas flow through the catalyst layer on the GDL before and after compressing, and check the image by microscopy before and after compressing).

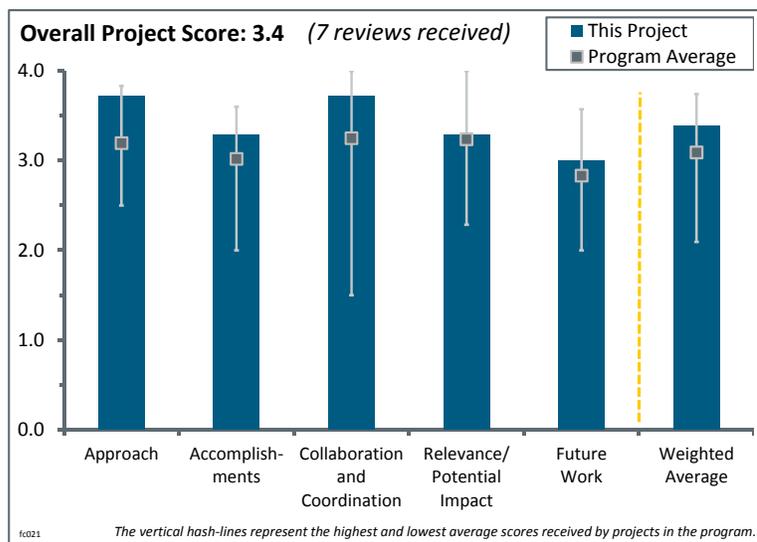
- The researchers should prioritize work to a few areas. They should also increase quantification of correlating data (e.g., correlation of CO<sub>2</sub> produced against changes in carbon volumes). It is not clear why thickness changes. It is also unclear how the new carbon volumes, when taking into account porosity changes, compare against CO<sub>2</sub> measurements. The researchers should do more comparisons of results to realistic operational conditions. It is unclear why bands are seen in the catalyst layer. They do not seem to be related to the initial high-density Pt regions, which were much more localized. The bands in the catalyst layer may be due to the use of N<sub>2</sub>, which does not allow the Pt to leave the catalyst layer, which may occur in H<sub>2</sub>/air conditions. Providing linkages to measures of surface oxidation for the corrosion studies would be worthwhile.
- The scope is fine as is.

## Project # FC-021: Neutron Imaging Study of Water Transport in Operating Fuel Cells

Muhammad Arif; National Institute of Standards and Technology

### Brief Summary of Project:

Neutron imaging allows for the study of a wide range of fuel-cell-related issues, such as water transport in the flow fields and manifolds, steady-state liquid water distribution anode versus cathode in diffusion media, steady-state liquid water distribution in the membrane, and catalyst degradation induced by liquid water. Objectives of this project include studying water transport in single cells and stacks, enabling the fuel cell community to use state-of-the-art neutron imaging capabilities to study water-transport-related issues, tailoring neutron imaging to the needs of the fuel cell community, and improving spatial resolution to study relevant-length scales such as catalyst layers.



### Question 1: Approach to performing the work

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

- This is a high-tech project to diagnose in situ the water transport in a working fuel cell. This high-resolution work provides a nice tool for fuel cell industries and will also give very good support for future material development. It is excellent work.
- The approach to making microscopic measurements of water transport is very good. No other imaging technique can provide real-time imaging during operation of a fuel cell.
- The project team features a great amount of expertise in neutron imaging of water locations inside of an operating fuel cell.
- The proposed approach is right—to improve the sensitivity of the measurements and the imaging to enhance the resolution and therefore ease identification of the roles in various components in water management. The team is also providing access to the fuel cell community by sharing the results. This approach is of huge importance to contribute to overcoming the performance and durability barriers on the basis of scientific criteria and not only financial criteria.
- The approach is indirectly focused on overcoming U.S. Department of Energy (DOE) barriers on durability and performance by improving water management in the fuel cells.
- The project is focused solely on enabling the visualization of liquid water in a running stack/cell. Recent work in polymer electrolyte membrane fuel cells (PEMFCs) has begun linking the running water content to the acceleration of degradation mechanisms, in addition to the usual linkages made to overall cell performance. As such, the ability to visualize total water content under operation is a highly valuable tool in correlating observed performance and durability effects to cell design. The project focus on increasing the resolution of the test is critical to ensuring that the method has the capability to resolve both water content of the membrane and catalyst layers, which are two key components for both performance and durability.
- The current resolution of the neutron imaging is approximately 10  $\mu\text{m}$ , which may allow determination of the water distribution in the flow field and around the manifold. It is crucial to know if the water content changes at different current densities and if the flow field and manifold design can manage the water. Regarding the water across the membrane electrode assembly (MEA) or along the plane of the MEA, the

water state (localized liquid water or water vapor) and whether the anode is drying out at high current density must be known. It is doubtful that the neutron imaging can determine these issues or help improve the resolution to below 10  $\mu\text{m}$ .

### Question 2: Accomplishments and progress toward overall project and U.S. Department of Energy (DOE) goals

This project was rated **3.3** for its accomplishments and progress.

- This is very good work. The data sets are good, and it is good to see a real working fuel cell with water transport.
- Significant progress has been made toward improving resolution for water imaging in fuel cells and evaluating the accuracy of water distribution measurements.
- Significant progress has been made on improving the neutron imaging techniques, and completion of the large-area high-resolution detector is very useful for large cell start-up/shutdown studies. Further, the analysis of the error and accuracy is extremely important in interpreting the results and discerning which changes are significant between samples.
- The use of the Gd/Si grating technology, plus the National Aeronautics and Space Administration (NASA) optics (from Chandra), clearly show that resolution on the  $\mu\text{m}$  scale is achievable, at least from the optics end.
- The presented results are of high quality and in accordance with the proposed milestones. Achieving the goal of a 10  $\mu\text{m}$  resolution enables users to image the water distribution in the MEA and the channels of bipolar plates. But working to enhance this resolution to 1  $\mu\text{m}$  will enable studies of flooding and liquid-water-related degradation in the catalyst layers of a fuel cell, which is a key point. The quality of the work relies on the use of either the theoretical or practical competences of different partners such as the National Institute of Standards and Technology (NIST), NASA, and the Massachusetts Institute of Technology. Potential artifacts have been investigated so that they could be taken into account for the fuel cell imaging.
- It would be nice if there was more progress on getting down to the 1  $\mu\text{m}$  resolution level. The accuracy of the water measurement analysis was excellent.
- NIST has made efforts to have the neutron imaging applicable to the fuel cell applications. The team should think about what valuable information can be gained by utilizing the technique and what the strengths and weaknesses of the technique are, as well how to provide such valuable results to assist researchers in improving the cell design and performance in a timely manner. This improvement also could give people confidence in the neutron imaging applications in the fuel cell field. Overall, it is a matter of priority determination.

### Question 3: Collaboration and coordination with other institutions

This project was rated **3.7** for its collaboration and coordination.

- There is close collaboration with NASA and users of the NIST facilities.
- The collaboration is good, and clearly the project supports a wide range of customers.
- The researchers are doing a lot of work with a variety of operational fuel cell systems.
- The achieved results have been possible because of close collaboration between partners. Moreover, the collaboration between NIST and many other partners has been highlighted and appreciated during several presentations at the DOE Hydrogen and Fuel Cells Program Annual Merit Review.
- This project features very good cooperation. It would be better if the principal investigator could explain more about which partner did what job.
- The use of the facility is largely user-driven—in particular, via either open research or closed, paid projects. The process by which projects are chosen and hours allotted could be made clearer, as well as the criteria by which projects in the open research area are selected. Further, pending projects in the open research area should be listed in the presentation to better appreciate the types of work for which the facility is being leveraged.
- A lot of research groups have been involved, although not very deeply.

**Question 4: Relevance/potential impact on advancing progress toward DOE research, development, and demonstration (RD&D) goals**

This project was rated **3.3** for its relevance/potential impact.

- The project is very important for the Program because it addresses water management issues in operating fuel cells.
- This is the project every fuel cell developer needs. It is a significant work for fuel cell development.
- The location of water inside operating PEMFCs is highly relevant to optimizing the performance of the fuel cells.
- Neutron imaging is a powerful method to help researchers understand a fuel cell or stack under operation by imaging a critical parameter for PEMFCs: the water. Therefore, enabling the visualization of this material has an important impact on the potential ways to improve the performance and durability of PEMFCs.
- Neutron imaging has the potential to make a significant impact in advancing knowledge of water transport at micron-length scales. However, to achieve less than 1  $\mu\text{m}$  resolution, improvements in detector resolution and imaging resolution are required. The team has identified a viable path forward for meeting these goals via collaboration with the Chandra team at NASA.
- Linking the imaging of water to the project objectives is largely left to the reviewer. The project presentation should generally recheck the project impacts against the use of the facility in achieving DOE RD&D goals. This rechecking, in part, could be done via the list of open research projects the technique is used for and some high-level accomplishments and findings. In particular, this rechecking would also help cast the need for increased resolution.
- It helps to publish some papers.

**Question 5: Proposed future work**

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

- The future work seems quite reasonable.
- The future work is a continuation of the proposed approach. The project team is encouraged to address the membrane swelling issues depending on the water content.
- The proposed work is focused on improving the resolution of water imaging in order to understand the regularities of water management in the catalyst layers.
- The future plan is correct, in particular the target to improve the resolution to the 1  $\mu\text{m}$  range. This improved resolution will be very useful to better investigate the MEA components individually. The lens optic work has to be continued to improve the resolution while keeping the record time in the minute range.
- The future plan is very good. If the project can detect which layer the water transport goes through, it would be even better. The project so far has obtained two-dimensional images. It would be good to know if there is any way to check three-dimensional pictures, and if there is any connection between the fuel/oxidant consumption versus water transport.
- The future work well identifies the plan to improve resolution using gratings and x-ray focusing techniques. No mention was made of efforts to increase resolution of a 9 x 9 cm MCP detector. This needs to be a focus area for even greater resolution required by the community.
- The development of the grating-based imaging is showing promise; however, it appears there are still significant technical challenges associated with the method that need to be overcome. In particular, the collection time necessary for the grating-based imaging is substantially long, which may in part limit the value of the technique in studying anything other than steady-state water content. The alternative path of using the neutron collecting lens seems to a degree like the optimal path; however, the timing and barriers related to this development are not clear, and largely this amounts to leveraging a technology that “may” reach fruition depending on the success of another organization. Clearly there is significant risk in the proposed path forward.

**Project strengths:**

- Neutron techniques are the best way to investigate water issues inside operating fuel cells.
- Applying neutron imaging to water content detection is a strength.
- NIST is bringing a powerful characterization tool to the fuel cell community. As resolution metrics are met, the results will enable a much-improved understanding of water transport.
- NIST features cutting-edge instrumentation for neutron imaging, strong collaboration with NASA, and a combination of modeling and experimental approaches.
- The project provides “eyes” to see the fuel cell water transport in a working mode. Thus, it provides useful information about fuel cell flow channel and manifold design as well as catalyst distributions.
- The main strengths of the project include its (1) effective collaboration between high-quality partners and bringing competences from different horizons (equipment, fuel cell) for a common target; (2) work to improve the measurement quality while increasing the spatial resolution for imaging the water in a fuel cell; and (3) free access for open research, enabling the contribution of any partner on based on scientific criteria.
- The industry use of the facility is strong, and the technique provides much-needed insight into the location and changes in liquid water during operation. The project is clearly focused on the needs of the user community in driving the technique to appropriate resolution for studying water content in membranes and catalyst layers. The project is also clearly leveraging advancements and techniques that are being developed in other organizations/applications, which demonstrates a high degree of collaboration.

**Project weaknesses:**

- It is difficult to get the one-micron resolution necessary to address catalyst issues.
- The membrane/catalyst layer and catalyst layer/gas diffusion layer interfaces are not distinguishable.
- It is unclear if the technology can be used for a stack diagnosis.
- There is considerable risk in the proposed path forward for the high-resolution detector. An analysis of the technique in comparison to other approaches (x-ray or nano-CT) should be included to cast the risk of the technique improvement compared to the current state of the art of this and other techniques.
- The imaging resolution limits its applications. Prioritization is needed as to how the imaging helps researchers to improve design and performance by utilizing a valuable result from the neutron imaging.
- Because the record time for a picture can be in the range from some seconds to some hours, the way to ensure the stability of the fuel cell should be made more precise. Actually, in a one-hour range, the water distribution in a fuel cell may evolve, in particular for high-area cells. A presentation of consecutive pictures under stationary conditions would be appreciated. Single-cell investigation is useful, but imaging short stacks would be of added value.

**Recommendations for additions/deletions to project scope:**

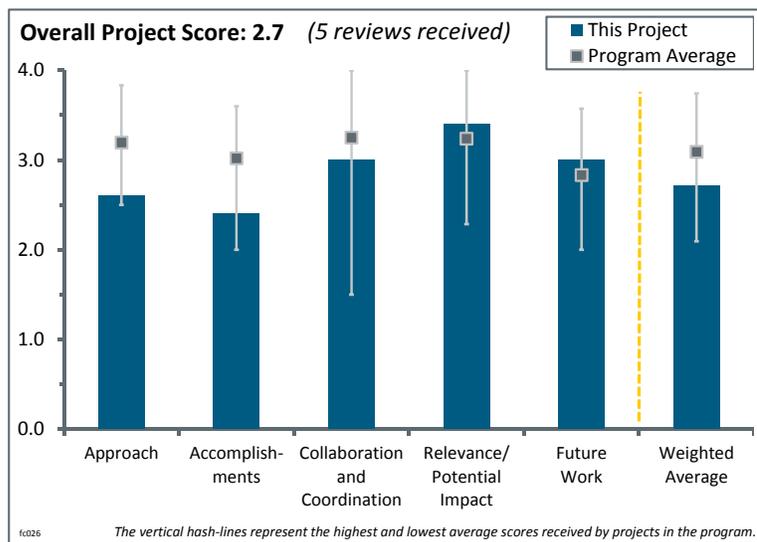
- The project team should move forward toward improving resolution.
- The project team should prioritize the fuel cell stack drying-out investigation.
- Any additional paths that may assist in mitigation of the risk related to the high-resolution detector development would be beneficial.
- The scope is fine.

## Project # FC-026: Fuel Cell Fundamentals at Low and Subzero Temperatures

Adam Weber; Lawrence Berkeley National Laboratory

### Brief Summary of Project:

One objective of this project is to gain a fundamental understanding of transport phenomena and water and thermal management at low and subzero temperatures using state-of-the-art materials. Water management with thin-film catalyst layers and water management and key fundamentals in the various fuel cell components are examined. The project seeks to enable the development of optimization strategies to overcome observed operational and material bottlenecks. This project also strives to elucidate the associated degradation mechanisms due to subzero operation and enable mitigation strategies to be developed.



### Question 1: Approach to performing the work

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

- The approach is good and systematic; it involves state-of-the-art materials, studying one of the critical weaknesses of these materials, substantial experimentation, and modeling efforts.
- The project seems to develop individual models to elucidate each single phenomenon. It is unclear if there is any approach to integrate them to develop a membrane electrode assembly (MEA) performance model. It may be effective to clarify which model platform could be proper—the stochastic pore-network model or the deterministic finite element analysis (FEA). Because the nanostructured thin film (NSTF) catalyst layer has a critical water management problem, it is good to add a conventional catalyst later to alternative materials to make the knowledge base more universal with respect to water management in cold temperatures (including subzero temperature start-up). The parallel flow field is widely used by stack original equipment manufacturers and is better (easier) for modeling.
- Although the approach is focused on overcoming U.S. Department of Energy (DOE) barriers on durability and degradation, it looks more like a basic science project.
- The project addresses water management issues. Low-temperature performance is critical to automotive fuel cells, and understanding water condensation and flooding at low temperatures is critical. The project includes NSTF, which has advantages in low platinum group metal (PGM) content and durability but also has water management issues at low temperatures. Solving the NSTF water management issues at low temperatures would be a big step forward. The gas diffusion layer (GDL) effective diffusivity work addresses program needs and is complementary to work from other transport projects. It is not clear what is new in the (bulk) membrane morphology studies. There have been extensive studies of Nafion® morphology, including numerous SAXS studies, TEM studies, AFM studies, conductive AFM studies, etc. It is not clear what is different here and what new information is being obtained. It also is not clear what new information is gained by using the Nafion morphology to model transport through bulk Nafion, or its relevance to low-temperature operation of fuel cells. This portion seems to be a basic sciences study embedded in an applied project, where the basic science study provides little to no added value. Studying the morphology of Nafion thin films on Au and Si provides no useful information for this project. Thin-film Nafion morphology on Pt and C may be useful, but the transport properties are more useful. Direct measurement of the transport properties would be more beneficial than calculated morphologies from a transport-morphological model.

- The overall approach aims at providing inputs from modeling to help industry and national laboratories resolve some of the typical fuel cell performance issues related to 3M, Los Alamos National Laboratory (LANL), and United Technologies Research Center (UTRC). Considering that these diverse sources of MEAs have different electrode structures and natures of catalysts, this effort is expected to provide relative metrics to their operation. In terms of the approach, most of the modeling aspects are not new or innovative; they are well established. Most of the results of this modeling work are, in general, what would be expected. An expected outcome of this effort in terms of modifying the approach would have been the ability to predict results of the various parametric contributions during transient conditions. Such time resolution would be an important step forward in predicting the effect of load variation, humidity, temperature, etc. In addition, modeling inputs such as impedance data are not used; this will be more important as compared to the imaging used to follow water at the interface.

### Question 2: Accomplishments and progress toward overall project and U.S. Department of Energy (DOE) goals

This project was rated **2.4** for its accomplishments and progress.

- The project team has developed a good understanding of the resistivity properties of thin films and narrowing operating windows. The effort should continue into describing areal gradients in order to prevent a voltage drop in the lower-temperature conditions. Critical milestones got delayed or changed in scope. The fundamental understanding of the anode GDL effect on flooding remains uncertain, and specific material factors were not quantified.
- The project team has made significant progress in modeling and understanding some fuel cell transport fundamentals, but it has made only modest progress toward eliminating the water flooding problem at the anode.
- The accomplishments here have been good. The lack of inputs such as impedance data and the lack of the modeling exercise in considering transients are important oversights. It is highly recommended that the researchers incorporate time resolution into these models.
- Good matching model and experiments can be seen; however, modeling information should be disclosed further (such as information on water saturation at low temperatures, what kind of model was developed, etc.). For the anode GDL study, the materials properties should be disclosed to explain why the MRC GDL showed better water management. It is necessary to explain the unmatched PTFE uptake model and experimental data. For membrane water uptake, SANS may be more useful than SAXS.
- The model has been able to reproduce the effect of temperature on NSTF performance. The model predicts that NSTF proton conductivity can have a strong influence on cell performance. Results for a transient MEA-level cold-start model have not been seen yet. A validated transient cold-start model is needed. The project is behind on meeting milestone M3 for the microporous layer (MPL) model in terms of predicting breakthrough pressure and capillary pressure-saturation behavior. The project is behind on milestone M4 for determining the impact of water balance on start-up performance for NSTF and low-loaded traditional MEAs. While milestone M5 has been changed (to adiabatic single-cell tests versus rainbow stack tests), it appears that the researchers are behind schedule for this milestone.

### Question 3: Collaboration and coordination with other institutions

This project was rated **3.0** for its collaboration and coordination.

- This project features good collaboration between industry and academia.
- The project is pursued with wide collaboration, including with industries.
- It is not clear how all of the studies are being tied together and brought into the final model. Coordination with other projects (3M MEA, LANL durability) is evident.
- The partners carry a significant scope of the experimental work for the project. The design of the experiments on the partner side lacks consistency or was not articulated enough in the presentation in order for reviewers to determine the value of the results obtained for modeling.
- This project features good collaboration; however, the exact role of 3M remains an issue. 3M still remains as the primary source of the materials in this effort. This makes the project heavily tilted toward performing

a systems optimization for a single company. More emphasis should be made on materials from other sources. Despite any proprietary considerations, it is important to link the different MEA design elements to the performance and outputs from the model.

#### **Question 4: Relevance/potential impact on advancing progress toward DOE research, development, and demonstration (RD&D) goals**

This project was rated **3.4** for its relevance/potential impact.

- The project is important for advancing DOE RD&D goals.
- Water management and operational robustness are very important for the stack development. High area-specific power density is required to reduce the total active area and enables significant reductions of the stack cost.
- The project addresses water management issues. Low-temperature performance is necessary in automotive fuel cells, and understanding water condensation and flooding at low temperatures is critical. The project includes NSTF, which has advantages in low-PGM content and durability but has water management issues at low temperatures. Solving the NSTF water management issues at low temperatures would be a big step forward.
- If the project demonstrates modeling and component solutions toward tolerating sub-freezing and low-temperature conditions with the respectful operating windows for thin-film electrodes, this may strategically impact the research and development layout of the Hydrogen and Fuel Cells Program.
- This modeling exercise provides important inputs to MEA- and system-level integrators for their respective designs. In this context, the lack of a system integrator approach and clearly defined queries from their perspective represents a glaring gap. Clearly defined inputs from a system integrator, typically an automotive company, would enhance the potential impact of this work.

#### **Question 5: Proposed future work**

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

- The proposed future component characterization work is relevant (excluding membrane morphology work). The planned transient testing and modeling of transients is of high importance.
- MPL is added in the proposed future work.
- The proposed future work is well delineated. However, incorporating transient models and inputs from an automotive company would be further recommended.
- The plans are substantial for each party on the team, which may be overwhelming considering there is less than a year left in the project.
- The proposed future work is still focused on understanding the water management problems; however, at this stage of the project, one would expect to have a solution.

#### **Project strengths:**

- The project team features strong modeling capabilities. There is good collaboration between industry and academia.
- The project features strong modeling capability.
- The approach and collaborations are strong, and the best experts in materials, testing, and modeling are involved in this project.
- Strengths of this project include the GDL characterization work and the neutron imaging studies.
- The project provides important input for system integrators and MEA designers for predicting results of variation in an operating environment. For this project, MEA and other inputs from 3M are considered as the principal materials provider. These are put in the context of more traditional MEA designs from LANL and UTRC. Most of the model outputs are important for this stated objective.

**Project weaknesses:**

- More explanation of model development in the project is needed.
- The project is focused on fundamental studies of different MEA components and their assemblies, while less effort is invested in problem solving.
- The correlations between the fundamental properties and component metrics are not well articulated, leaving questions about what component features become governing in tolerating low-temperature operation.

**Recommendations for additions/deletions to project scope:**

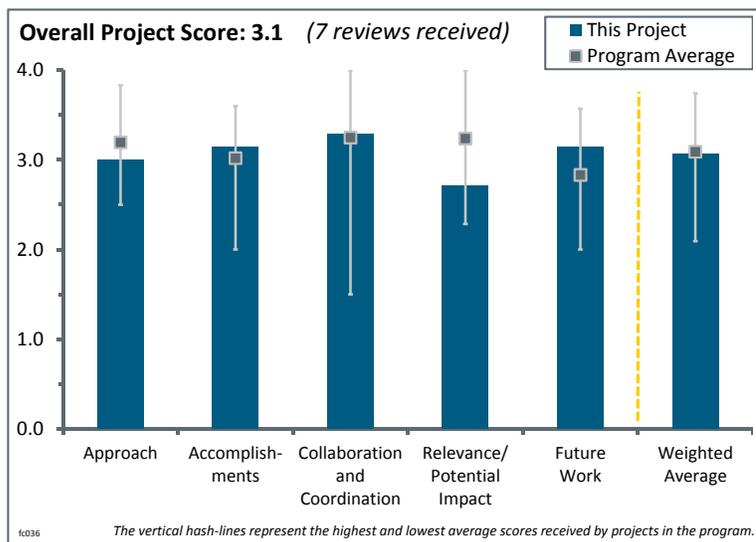
- The project team should continue the modeling work using degraded membranes to produce narratives on how the whole picture would change with time and how sensitivities would change with time.
- The membrane morphology work should be deleted from the project. It is not clear what new information is to be gained compared to the numerous morphological studies already in the literature. It is unclear what value the Nafion morphology study adds to the project and how any new information from these new studies is critical to low-temperature operation.

## Project # FC-036: Dimensionally Stable High Performance Membranes

Cortney Mittelsteadt; Giner, Inc./Giner Electrochemical Systems, LLC

### Brief Summary of Project:

Three viable pathways were investigated in this project for developing dimensionally stable membranes (DSM<sup>TM</sup>). Inversion casting, which was not pursued further, displayed too many problems with process control and the intrinsic properties of inversion cast films. Ultraviolet (UV) microreplication became a secondary pursuit despite having the lowest ultimate cost, achieving the desired material properties, and having straightforward scaling for the process. The mechanical pathway was the main focus of research because the best materials choices (thermoplastics) are available for this pathway; costs are not prohibitive; and when high (50%) porosity is reached, DSMs<sup>TM</sup> perform the best.



### Question 1: Approach to performing the work

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

- The team clearly focused on challenging aspects of the problem and screened a variety of options and materials before closing in on the most attractive option to spend the most time on.
- As long as Nafion® or any deformable membrane is used in a fuel cell, this approach will be valuable for meeting durability standards needed for automotive and other applications.
- The approach is clear and well articulated, though single-sided, addressing the mechanical reinforcement of the membrane without ionomer stability.
- DSMs<sup>TM</sup> are critical to extending the cell performance and life; however, the viable pathways need to be further developed.
- This project features a good approach that seems to address better stabilization but needs to show ionomer incorporation as well as stability and durability of the supports. Its cost impact and benefit compared to traditional supported membranes are not clear. It would be good to see some modeling to figure out the utilization of the catalyst layer, as well as to guide the membrane support design.
- A membrane support structure of 50% porosity may not be sufficient to reach the DOE membrane conductivity target. Fuel cell performance and durability testing using the accelerated stress tests (ASTs) as well as freeze/thaw cycling should be conducted before optimizing the support.

### Question 2: Accomplishments and progress toward overall project and U.S. Department of Energy (DOE) goals

This project was rated **3.1** for its accomplishments and progress.

- The team has met all goals and demonstrated meaningful results, such as 10,000 hours of high-performance operation when reinforcing webs are used. The team has optimized web structure and manufacturing process.
- Although there are still issues that need to be overcome, the advances that have been made are quite impressive, and the progress toward the well-defined objectives is what one hopes to see in these types of projects.

- The project has demonstrated good durability of the membrane on the process optimization. Because the project is still in the stage of pathway determination, the team should address the fundamental strength of the selected or prioritized pathway (mechanical).
- Goals for this year included fuel cell qualification of membranes, which was not presented. The team has made good progress in optimizing the UV-microreplication and mechanical DSM™ fabrication methods. Both processes are feasible for high-volume continuous roll-to-roll fabrication.
- The progress has not been that great, but it is good relative to the budget. Good metrics were shown, but too much focus was placed on previous efforts. The research team did nice work on determining the membrane support fabrication materials and methodologies.
- The research team claimed to have achieved the relative humidity (RH) cycling target in ex situ testing, but the team did not provide any data of crossover metrics throughout the types of the supports utilized in the testing. Polarization data from the beginning to the end of the RH cycle test or post-test images would be more credible to show the stability of the ionomer-support interface.

### Question 3: Collaboration and coordination with other institutions

This project was rated **3.3** for its collaboration and coordination.

- The team is small but effective, as seen by its excellent progress and meeting of goals.
- Solid collaborations are established both at the industrial and university levels.
- This team features strong interaction between project partners.
- This project features a good team, but it is unclear what is going forward in terms of the down-selects and partners. There should be discussion with ionomer suppliers.
- It is clear that collaboration is occurring, but it was not completely clear how the collaboration is coordinated or functions in terms of team meetings and other interactions. Overall, however, the advances are evidence of collaboration.
- Further collaboration may help the project team to accelerate the development in the pathway.

### Question 4: Relevance/potential impact on advancing progress toward DOE research, development, and demonstration (RD&D) goals

This project was rated **2.7** for its relevance/potential impact.

- The DSM™ may facilitate the cell and stack design, as well the control of the operation protocol.
- This technology has relevance to Nafion® and any deformable membrane, as seen by the fact that it may just be the final touch needed to make practical the membranes made by another DOE team, Fuel Cell Energy.
- The work could have a “good to outstanding” impact. The potential impact would have been rated “outstanding,” but it seems that there are still quite a few hurdles to overcome before it is clear what level of success and impact will be felt.
- Reducing membrane costs by introducing a dimensionally stable hydrocarbon reinforcement support is on the path toward reducing the cost of the membrane electrode assembly (MEA), and thus the project is relevant to the overall DOE objectives.
- Without addressing ionomer stability, this project partially supports the Hydrogen and Fuel Cells Program and DOE RD&D objectives.
- This could be an important project if the research team can use low equivalent weight (EW) and low-porous matrices, provided the cost is really less expensive and the adhesion and compatibility problems can be solved.

### Question 5: Proposed future work

This project was rated **3.1** for its proposed future work.

- The future work is highly relevant to proving fuel cell performance.
- The team is on track to meet all of its goals.

- Mechanical focus is the right way to go so that the membrane can be produced on a larger scale and in a cost-effective way.
- The focused plan that is proposed has benefited from the well-structured and disciplined approach. The proposed future work is a logical extension of the work done so far and the interpretation of the data that were outlined.
- The research team needs to show the performance gain before moving on for processing and manufacturing controls to show the benefits and what the costs need to be. The proposed future work looks acceptable.
- The future plan seems adequate.
- Cost analysis should be included in the future work.

#### **Project strengths:**

- This project features good partnering, a good plan, and a logical approach.
- The project has a strong and experienced team.
- The project has yielded good testing results in a practical way.
- The project is well focused. Reasonable progress has been demonstrated in screening the three viable pathways for making the porous support.
- This project features creative thinking about various ways to address a really challenging topic.
- This project features an interesting approach to reinforce membranes. The team has made good progress on making the membrane supports.
- The project explores alternative methods for mechanical reinforcement of the membrane. Establishing new manufacturing technologies in MEA processing is valuable and could be synergistic with other materials developments for the electrochemical power sources.

#### **Project weaknesses:**

- The project needs deeper stress analysis and swelling analysis.
- There are no weaknesses, except it would be nice to know more details of the process for making the web that is put in the membrane to stabilize the dimensions.
- High-volume cost predictions for the engineered supports seem viable for PFSA based membranes but too expensive for hydrocarbon membranes.
- There is question about the overall gain in cost. There is also question about the priority of this project, especially because Giner is already working on this in its existing technologies.
- The timeline and timing for the go/no-go decisions were not specified in the presentation. Judging by the starting time, the project should have passed the end of Year 2. However, the project has not demonstrated whether it passed the go/no-go for Year 2. The mechanical properties of 50% porosity support made by the mechanical deformation method are critical information and should be included in the presentation. One of the objectives of this project is to reduce the cost of the membrane down to  $< \$20/\text{m}^2$ . A target should be established for the porous support because it is the focus of the project. As noted by a reviewer last year, the cost target for the support probably should be  $< \$5/\text{m}^2$ . The cited cost numbers in the presentation are very high compared to this “target.” A more detailed cost analysis is needed to demonstrate the viability of the proposed approaches. More details about the mechanical deformation method are needed to understand the cost/performance aspect.
- This project potentially leads away from the more difficult developments of the higher temperature, conductivity, and stable ionomers, which are durable under fuel cell operating conditions.

#### **Recommendations for additions/deletions to project scope:**

- The researchers should pursue a patent so the Giner team can discuss the work more openly.
- The conclusions need to be backed up with solid data and analysis.
- The team should focus on demonstrating DSM™ performance and durability prior to further optimizing the support structure and fabrication processes.
- If the project continues to focus on solely mechanical durability, the project team should investigate the sensitivity of the resulting DSM™ to different flow fields and GDLs during fuel cell testing.

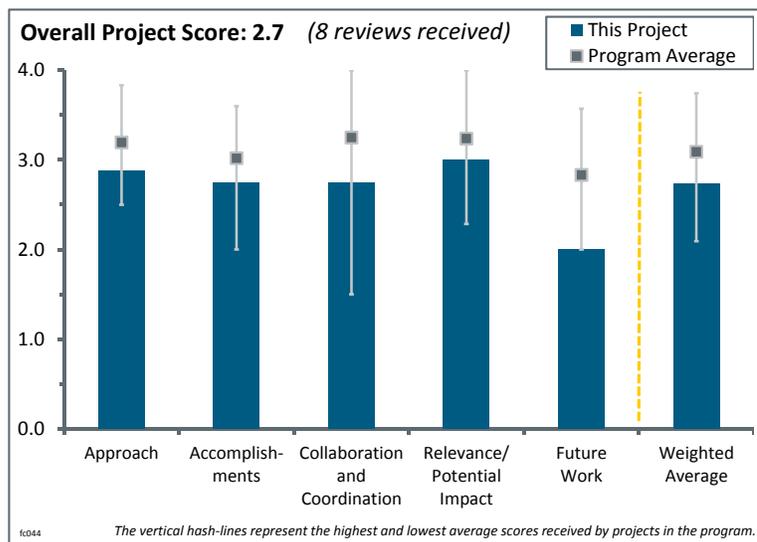
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- The project team should look at low EW ionomers and perhaps hydrocarbon ionomers as well to see if there is a more significant gain, but admittedly this is a support project and not a membrane one. The project team needs to think about adhesion of the catalyst layer to the support, especially under stressed conditions of humidity, freeze, etc. The team should also think about looking at accelerated stress tests for both just the support and when a membrane and catalyst layers are incorporated. The team should do some computational modeling to help guide the design of the structure and how it should behave under operation.

## Project # FC-044: Engineered Nano-Scale Ceramic Supports for PEM Fuel Cells

Eric Brosha; Los Alamos National Laboratory

### Brief Summary of Project:

The objective of this project is to develop a ceramic alternative to carbon material supports for a polymer electrolyte fuel cell cathode. Ceramic cathodes must have enhanced resistance to corrosion and platinum (Pt) coalescence; preserve positive attributes of carbon such as cost, surface area, and conductivity; and be compatible with present membrane electrode assembly (MEA) architecture and preparation methods. Materials properties must possess the required surface area, foster high Pt utilization, exhibit enhanced Pt-support interaction, provide adequate electronic conductivity, and exhibit resistance to corrosion. Materials used in ceramic cathodes should also be amenable to scale-up and have reasonable synthesis costs.



### Question 1: Approach to performing the work

This project was rated **2.9** for its approach.

- The approach of this project is much improved from last year. It is good to focus on Mo<sub>2</sub>N and Mo<sub>2</sub>C (excess carbon-free) from various materials and synthesis methodologies. From the technical standpoint, it is also valuable to clarify reasons why other materials and synthesis methodologies were dropped; for example, Mo<sub>2</sub>C (polymer-assisted deposition).
- The project is focused on non-carbon supports for Pt-based catalysts. The principal investigators (PIs) had a systematic approach to tackling challenging demands that support materials should meet, such as high conductivity, resistance to degradation, high surface area, and strong attachment to the catalyst particles. Study materials are systematically characterized, and detailed insight into structure function properties was possible to obtain.
- Exploring the possibilities of replacing carbon supports by providing more stability to oxidative degradation ceramic materials is a reasonable topic.
- This project started out with the somewhat vague idea that ceramic supports would be useful. The project ended up with Mo<sub>2</sub>C, Pt-embedded Mo<sub>2</sub>C, and Mo<sub>2</sub>N.
- Los Alamos National Laboratory (LANL) has identified a promising ceramic material based on molybdenum. However, the performance of this material needs further improvement.
- The approach is generally effective (involving many structural and spectroscopic probes), but it could be improved, in particular with regard to electrochemical characterization.
- Carbon supports have been necessary to keep Pt loadings low, but they suffer from corrosion and weak Pt binding. Alternatives with improved performance and durability would be preferred. The development of high-surface-area, electronically conductive, corrosion-resistant ceramics is a reasonable approach. The approach for the project was laid out much better in past U.S. Department of Energy (DOE) Hydrogen and Fuel Cells Program Annual Merit Review presentations, and milestones as presented are not clear in terms of time frame or how go/no-go decisions have been made.
- The project focuses on a few materials and relies heavily on the synthesis capability of The Materials Foundry and University of New Mexico (UNM). It is unclear if the team has sufficient resources and expertise. The elimination of all carbon should not be the goal of the project. A noticeable portion of the

effort was dedicated to investigating Pt-support interaction, rather than to developing the support to perform well in a fuel cell.

### Question 2: Accomplishments and progress toward overall project and U.S. Department of Energy (DOE) goals

This project was rated **2.8** for its accomplishments and progress.

- There is no denying the stability of the Mo<sub>2</sub>N supports. The Mo<sub>2</sub>C data are not as clear, although it is still better than the incumbent technology (carbon). There is clear progress here.
- The project demonstrates progress toward DOE goals. These materials show promise, but it is not clear that they can be scaled up to produce a cost-effective solution.
- The PIs presented good progress over the last fiscal year and were able to overcome demanding barriers for implementation of novel supports in fuel cells. The high performance has not yet been achieved, but this project serves as a source of valuable data for the future catalyst design.
- The demonstration of the “nanoraft” (NR) Mo<sub>2</sub>C materials is a significant step forward and offers some hope in improved performance and durability for the non-carbon supports investigated. These materials appear to have promise and merit further investigation, while the other materials investigated to date had shown little in terms of promise. It is somewhat difficult to fully evaluate the potential of the NR Mo<sub>2</sub>C materials because the durability (waterfall) charts presented are based on changes in electrochemically active surface area (ECA), and judging by the limited cyclic voltammograms (CVs) of these materials presented, it is not clear that the surface area or surface area changes reported are appropriate. The high mass activities of these materials are promising, but it is not clear what happens to mass activity after cycling or exactly which cycling protocols have been applied in all cases.
- The focus is narrow, mostly on one support for Pt–Mo<sub>2</sub>C and, alternatively, MoO<sub>3</sub>. The paper by Rossmeisl (*ChemCatChem* 2012) showing that NbO<sub>2</sub> is the best support for Pt should be a comparison.
- It is unclear if a clear specification for material selection was set. Few materials investigated have made it into fuel cell evaluation. The results that were shown demonstrated that this is a significant challenge.
- The PIs made minimal progress toward the objectives, especially if the results are compared to the most active Pt-based systems supported on carbon. The stability and conductivity of systems are still far from being realized. Therefore, there has been modest progress in overcoming barriers, but the rate of progress has been slow.
- The fuel cell performance and durability with Pt/Mo<sub>2</sub>C is very poor. It is good to distinguish oxygen reduction reaction (ORR) kinetics and H<sub>2</sub> crossover problems. It is necessary to investigate whether damage of the electrolyte membrane is critical to use ceramic support for the catalyst layer. Passivation of the Mo<sub>2</sub>C surface seems to be critical. It is interesting to see the effectiveness of the lattice mismatch of the Mo<sub>2</sub>C support and the catalyst activity of Pt (modeling work).

### Question 3: Collaboration and coordination with other institutions

This project was rated **2.8** for its collaboration and coordination.

- The PIs have demonstrated a strong team effort.
- Collaboration is very good, as seen by the structural characterization.
- LANL is making very good use of collaborators at multiple institutions.
- Although partners are well coordinated, some improvements are still desirable—especially with the experts for electrocatalysis.
- It would be good to add an industry collaborator to the project and leverage its influence regarding technical approach and fuel cell testing.
- The project has limited collaboration. It should look to expand if the few materials the researchers are currently investigating do not show promise.
- The project consists of modest collaboration, but it is also reasonably small in scope, so this is appropriate. It now contains an industrial partner owing to the spinoff from LANL for the Mo<sub>2</sub>C NR synthesis. The use of UNM and Oak Ridge National Laboratory in providing complementary characterization efforts is appropriate.

- There is not a clear path to scale-up. Perhaps it is time to engage a catalyst supplier. Original equipment manufacturer (OEM) fuel cell testing is needed to prove the concept.

#### **Question 4: Relevance/potential impact on advancing progress toward DOE research, development, and demonstration (RD&D) goals**

This project was rated **3.0** for its relevance/potential impact.

- The project aligns very well with the R&D goals of the DOE Hydrogen and Fuel Cells Program. The choice of proper high-surface-area support is critical for the future development of catalysts. The knowledge accumulated from this project can certainly serve in future considerations of catalyst supports, considering that the PIs have conducted a systematic structure function evaluation of materials.
- The impact on durability is very clear.
- This project is relevant, but elimination of all carbon is not necessary.
- This project only partially supports the Program.
- The corrosion of catalyst support is a critical issue for fuel cell durability. On the other hand, some mitigation strategies were proposed. If use of an alternative catalyst support would require sacrificing fuel cell performance, the relevancy is relatively lowered.
- The project has the potential to develop more robust and perhaps higher-performing catalysts that could help address cost, performance, and durability of fuel cell systems—the primary remaining technological barriers. The materials developed to date have not yet met DOE electrocatalyst activity targets and have remaining challenges regarding utilization in high-performance fuel cells. The very low fuel cell open circuit voltages and poor performance in MEAs reported on slide 21 are a concern along these lines.
- Finding a good replacement for carbon would have a great impact on fuel cell research and technology.
- Surface passivation, corrosion, and loss of performance are major technical issues that need to be addressed.

#### **Question 5: Proposed future work**

This project was rated **2.0** for its proposed future work.

- The investigators are making excellent progress in addressing the technical challenges.
- The focus should be made broader, and the Pt-support interaction should be addressed.
- The proposed future work aligns with the project outcomes but does not point clearly to whether ceramic supports are a real alternative for carbon supports. It seems that stability issues may prevent this class of materials from becoming a valuable candidate for high-surface-area supports.
- There is not enough time remaining because this project is supposed to end in September. Therefore, the project team should be focused on some critical areas. In addition to the completion of fuel cell tests (durability), it is important to clarify the cause of the MEA damage, model work for the possibility of performance enhancement, and address the criticality of the surface passivation of Mo<sub>2</sub>C.
- Few materials are investigated. It is not clear if the team has a good understanding of its materials and the properties needed to obtain good fuel cell performance.
- Owing to the length of the presentation (too many slides) and the presenter's running out of time at the end (in the oral presentation), the future work was not conveyed very well. The approach to future work presented on slide 29 is not compelling or clear; it consists of general statements without guidance to the approach or prioritization.
- The PI should drive toward a conclusion here by making something that works and engaging a supplier and a customer. The project team has something here; it should not waste the opportunity. It is unclear where the value proposition is.

#### **Project strengths:**

- This project features a good idea—a good synthesis that works.
- This project features a novel ceramic support that might provide enhanced properties.
- This project features the capability for various synthesis approaches.

- The project is relatively well organized and has a clear focus. The PIs are good scientists, and synthesis of new ceramic materials is based on understanding of the systems and not just testing of “new materials.”
- NR Mo<sub>2</sub>C has shown promise in rotating disk electrode performance at low Pt levels. Initial results suggest durability may be favorable, but more work is needed.
- Strengths of this project include its systematic approach, strong team effort, and fundamental insights into the structure-function properties of novel supports.

#### Project weaknesses:

- The lack of industry collaboration is a weakness.
- The material is likely not cheap—it is not easy to manufacture and its long-term stability is questionable.
- No suppliers or OEMs are involved. The project team should get focused. The team is not narrowing down to a conclusion. It should take one option to the next phase.
- The selection of new supports is rather narrow. Electrochemical characterization is almost nonexistent, and thus comparisons in activity of ORR on different materials are questionable.
- Weaknesses include the lack of vision for future work and a support of choice that can exhibit outstanding performance.
- Too little is known about the new synthesis route to understand how viable it is for further advances to occur. Significant data were presented, but most of the interesting work revolved only around NR Mo<sub>2</sub>C. Data that would have been useful were often not presented, while extraneous data with less value were presented.

#### Recommendations for additions/deletions to project scope:

- The project team should focus on scale-up to produce enough quantity of material to perform statistically meaningful tests.
- This project is almost completed, so there is little to be done in the end. The embedded Pt–Mo<sub>2</sub>C looks better than the Pt–Mo<sub>2</sub>N. It is unclear if this is really true, and it is important to know.
- Work should focus specifically on Mo<sub>2</sub>C NRs by the new novel synthesis route. These materials show some promise but lack sufficient data to make a strong statement about potential. CVs of these materials should be given, test conditions for cycling should be presented, CO stripping should be used to investigate ECA, and mass activities should be presented before and after cycling. The modeling studies provide no immediate leverage for the project and should be ceased. The fuel cell studies can be de-emphasized until the materials are better characterized and understood.

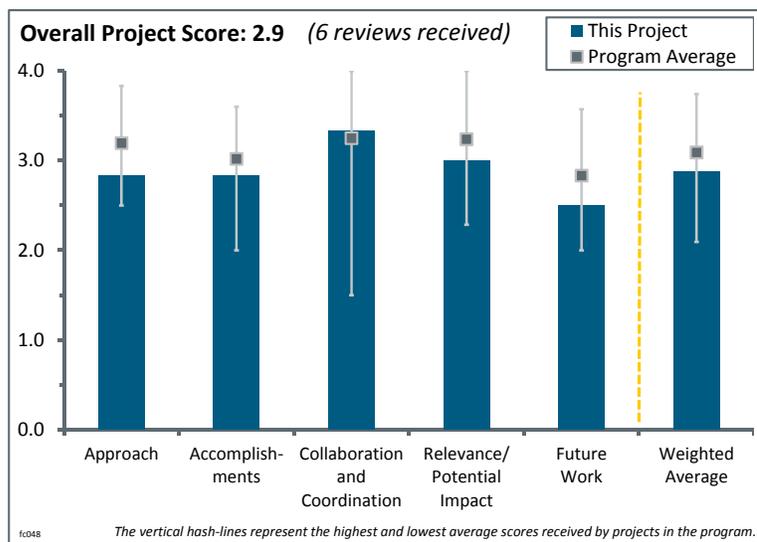
## Project # FC-048: Effect of System Contaminants on PEMFC Performance and Durability

Huyen Dinh; National Renewable Energy Laboratory

### Brief Summary of Project:

System contaminants have been shown to affect the durability and performance of fuel cell systems, thus prompting research to limit contamination-related losses. As fuel cell stack costs have decreased, the focus has shifted to addressing balance of plant (BOP) materials costs to further decrease overall fuel cell system costs. This project worked to identify poisoning mechanisms and recommend mitigation strategies, develop predictive modeling, and provide guidance on future material selection.

### Question 1: Approach to performing the work



This project was rated **2.9** for its approach.

- The project provides a very systematic approach to screening a large number of relevant contaminants, understanding key mechanisms, categorizing the contaminants into logical groups, and determining performance impacts and recovery behavior.
- From an engineering standpoint, the objective of this project is valuable for materials screening. From a technical standpoint (this factor is the most important for U.S. Department of Energy [DOE]-funded research and development [R&D] projects), without investigation of performance degradation mechanisms, outcomes cannot be fully applied to improve fuel cell durability. Looking at ORR kinetics and HFR is good in order to distinguish the type of degradation mechanism. It is questionable whether this database can be applicable for types (levels) of fuel cell materials. For in situ analysis, the fuel cell technology (e.g., catalyst and membrane materials) should be disclosed.
- The project is well worthwhile, but it is structurally overwhelming and complicated by too many sources of contaminants. The approach of using model compounds is logical and probably the best approach given the circumstances, but because the actual contaminants and their real-life concentrations are not really determined, the effects seen from model compounds show only potential effects and not real-time effects. Measurement of the macro effects of the functional interaction of the amine or hydroxyl functionality ion exchanging or the organic sorbing on the catalyst is very instructive in determining which mechanism has the most impact; that work is nicely done, but the biggest impact mechanism needs to be studied in actual un-doped cell operation to determine the relationship between model compounds and real operation. Also, no mention was made of mitigation routes.
- The approach has been systematic. It seeks to identify which systems contaminants exist, separate them into fundamental classes (for greater universality of results), and then identify which are most harmful. For such a project, the probability that identified contaminants will not be universal for all developers will always exist. The fact that only one developer has been highly involved in contaminant selection (General Motors [GM]) is a weakness. It does not appear that Ballard or Nuvera contributed highly in that regard.
- The team is quantifying voltage loss into fuel cells but only looking at constant current measurements. It is well known that there is a strong voltage dependence of many of the contaminants, and this dependence should be considered. Also, it is well known that pure organic compounds will oxidize at a Pt cathode in air at >0.6 V or so. A bigger problem is the additives. The team should work harder to study the individual constituents of the materials of interest to the automotive industry and identify the true bad actors.

- The contaminants selected are by-products of other BOP components. It is unclear how it was determined that all contaminants should be tested at 1,280 ppm, for example.

### Question 2: Accomplishments and progress toward overall project and U.S. Department of Energy (DOE) goals

This project was rated **2.8** for its accomplishments and progress.

- Many materials have been screened to determine their effect on the fuel cell. Some inconsistency exists in the number (55 in slide 6, 62 in slide 7) of materials studied. In addition to quantifying the performance loss, the project tries to identify the type of degradation.
- Lots of data and the big effects are nicely determined for model compounds, but it appears that the translation of the most powerful effects for real-time operation is missing.
- A large amount of data (materials and parametric analysis) enables researchers to identify a tendency of performance degradation. Deeper investigation of the degradation mechanism is expected for some possibly critical material problems, for example, the ORR effectiveness of organic contamination.
- The project had made good progress and already provides a useful tool for fuel cell designers. The website is a very useful tool. Some additional information on the types of mechanisms and recovery behavior would be useful on the website. There has been good characterization of a large number of contaminants to categorize and study in an efficient manner.
- For the contaminants identified and with the techniques identified, the project has generated considerable data and has identified mechanisms (e.g., membrane contamination for 2,6-DAT). It would be useful if some of the results were reproduced on a large cell or stack scale. The study of contaminant mixtures is useful and helped to address some questions with the project. The study did well to include the effect of catalyst loading on the results.

### Question 3: Collaboration and coordination with other institutions

This project was rated **3.3** for its collaboration and coordination.

- This project features excellent collaboration with very capable partners.
- The collaboration seems excellent; the materials information came from fuel cell original equipment manufacturers (OEMs).
- This project features good collaboration and coordination, particularly with GM. The researchers have also included additional industry partners to ensure that relevant materials are being studied.
- This project has a good-sized group of contributors. It is unclear if all of the experiments were conducted at the National Renewable Energy Laboratory (NREL). It is unclear which partner contributed to which results presented.
- A broadening of developer input would have been better for the project. Ballard and Nuvera appeared to have some input into the testing, but there is no evidence that either provided inputs for contaminant selection. The University of Hawaii has years of experience looking at fuel cell contamination, and it was a good addition to the team. GM made a substantial contribution toward defining the materials set.

### Question 4: Relevance/potential impact on advancing progress toward DOE research, development, and demonstration (RD&D) goals

This project was rated **3.0** for its relevance/potential impact.

- The relevance and potential impact are high, and the project objectives of determining the effects of contaminants are needed.
- The project addresses the effect of contaminants that can enter the fuel cell and degrade the performance. Identifying the potential contaminants and their effects is necessary to help maintain the desired performance and durability.
- There is value to developers in knowing about system-borne contaminants. The project risks relevance by going after particular compounds and even particular functional groups that may not be applicable to some

developers' designs. The project did well to enhance its relevance by considering lower Pt loading, as well as the role of water in either washing away or recovering from the effect of impurities.

- From an engineering standpoint, the objective of this project is valuable for materials screening. From a technical standpoint (which is the most important for DOE-funded R&D projects), without investigation of performance degradation mechanisms, outcomes cannot be fully applied to improve fuel cell durability.
- This work is very important for stack/system design. It is a common problem that materials used either in the stack itself or somewhere in the system design can have contamination effects. In a working fuel cell system, these effects can result in performance problems that take considerable efforts to diagnose. A tool that can be used during the design process is extremely relevant and will provide significant improvements to the design process. This tool will become more important as (1) designs become appropriate for commercial cost targets, requiring lowest-cost materials to be used; and (2) increased volumes of fuel cells are introduced into new applications, resulting in new system integrators without past knowledge of acceptable materials. This project is different from most of the funded projects in that it combines research activities with a highly practical and pragmatic approach.
- The research needs to make clearer which particular compounds to avoid and which ones are safe. There is no way to tell from how all of the data are rolled up.

### Question 5: Proposed future work

This project was rated **2.5** for its proposed future work.

- The proposed future work is appropriate.
- The plan could be a little more specific. It is unclear what “in-depth analysis” is.
- The project has only a short time left, and the researchers mention mitigation strategies, which would be very valuable. Hopefully they can find some that can be demonstrated in the short period of time left.
- This project is ending in September; therefore, there is not enough time to do a new task. It is questionable how valuable the modeling of parametric analysis with operating conditions is, or how it can be valuable to identify degradation mechanisms.
- The project is nearly over. All that appears left is to assemble and disseminate the model, which is appropriate. The only experimental activity that would be interesting to add would be to repeat one of the contamination experiments with a large-size (about 300–400 cm<sup>2</sup>) cell to see if the results scale.

### Project strengths:

- The team presented a lot of data this year.
- A large number of contaminants have been screened. Their effects have been quantified. The researchers have some insight into how the contaminants are affecting the performance. The research team is good.
- Strengths of this project include the amount of data and analysis, both ex situ and in situ, and the information from fuel cell OEMs.
- Strengths of this project include the extensive list of contaminants considered, the models of contaminants, and the linkage of mechanisms to classes of contaminants. This project is important work for stack/system design; it is addressing a common problem of fuel cell developers. Development of the website is a valuable tool.
- This is much-needed work, and the approach of model compounds was probably the only way to tackle such a complicated problem. The team has produced lots of data and excellent technical hypotheses on how each contaminant might affect operation. There is excellent cooperation among partners.
- Strengths of this project include the team's (1) high-volume data collection capability; (2) collaboration with GM to provide direction on system contaminants; (3) good use of parametric variations to understand the effects of catalyst loading, condensed water, and other conditions that could cause recovery from contamination; and (4) attempt to focus on “fundamental classes” of contaminants instead of particular compounds.

### Project weaknesses:

- One weakness is the depth of the degradation mechanism analysis and mitigation strategy.

- The use of model compounds to determine the biggest negative impact was not followed up by focusing on that mechanism using real-life components. Also, mitigation strategies were not proposed.
- The lack of developer input on contaminants outside of GM is a weakness. The premise of the project could lead to results that are particular for one developer or group of developers.
- Considering the expertise of the researchers from multiple organizations, it would be interesting to hear about options to manage the degradation effect, especially for species that lead to irreversible loss. The level of contaminant exposed to the MEA is likely to be different, depending on the source and release rate.
- The data have not been checked against a larger active area cell. All results are done at 50 cm<sup>2</sup>. This size is appropriate because a larger cell may mask effects, but some checks should be done. The combined effects of other degradation modes with contamination have not been studied; for example, if ECSA is reduced, it is unclear if the effects will become larger. The effect of catalyst loading is a good addition—the researchers might have considered this as a baseline condition because it would also capture the effects of degradation for current loadings. Correlations of contaminant behavior to cell voltage, or more importantly electrode potential, would provide improved links to mechanisms—only current density is studied.
- The objective to produce a global contaminant model seems unrealistic. It is well known from decades of research on organic and inorganic adsorption on Pt that there are many different pathways to adsorption. Work specific to fuel cells indicates that voltage cycling helps remove many of the contaminants, while some molecules adsorb irreversibly. While it is nice to think that there is some universal process for all adsorbates, it is just not that easy. The work is further complicated by the gas diffusion layer, operating conditions (which vary widely beyond the test conditions probed by NREL), and dose level of the impurity (concentration versus time). It is a very extensive test matrix. The team needs to focus on guiding principles but not a universal model (which does not exist).

#### Recommendations for additions/deletions to project scope:

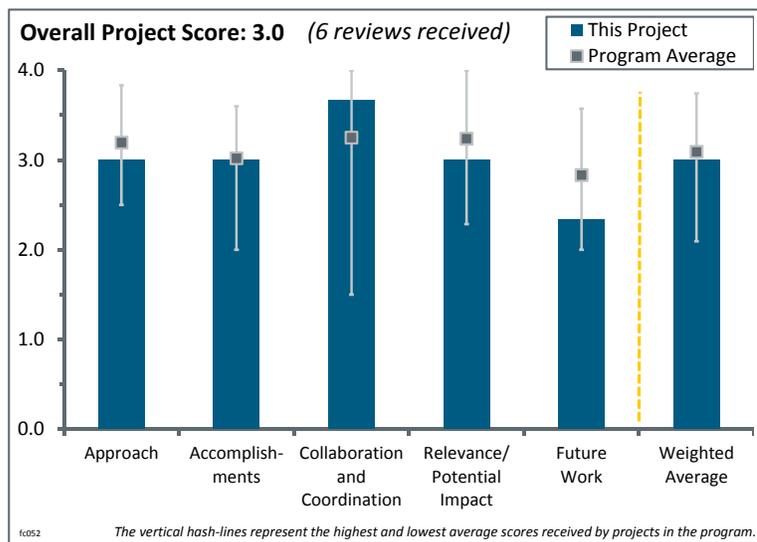
- Only one addition is suggested: reproduction of small-scale results with a larger cell or stack. It would be interesting to see if the results can be reproduced at that level.
- The researchers should classify the contaminants based on their hazard and propose management options based on the researchers' insights. Identifying the effects at various operating conditions should be a lower priority and paid for by the developer.
- There has been extensive testing on mechanisms and characterization of the compounds, as well as selection of model compounds. Because the website will be the legacy of this project, this work should be better represented on the website. It is understood that the website is a work in progress. Interactions with other degradation modes should be pursued.
- The team should focus more on how to recover the performance of fuel cells, rather than try to develop a universal model to explain voltage loss. It would be more constructive to look at "classes" of contaminants and categorize their introduction to the fuel cell as reversible or non-reversible. The team should also identify additives that are strong bad actors.

## Project # FC-052: Technical Assistance to Developers

Tommy Rockward; Los Alamos National Laboratory

### Brief Summary of Project:

Los Alamos National Laboratory (LANL) provides technical assistance to fuel cell component and system developers and includes testing of materials and participation in the further development and validation of single-cell test protocols. This task also covers technical assistance to durability working groups, the U.S. Council for Automotive Research (USCAR), and the USCAR/U.S. DRIVE Partnership Fuel Cell Technical Team (FCTT). This assistance includes making technical experts available to the U.S. Department of Energy (DOE) and the FCTT as questions arise, conducting focused single-cell testing to support the development of targets and test protocols, and participating in working group and review meetings.



### Question 1: Approach to performing the work

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

- The work appears to be serving a useful and accessible function of sharing technical assistance to developers through fuel cell and materials characterization. The work directly supports DOE because DOE is directing the scope and development of assistance.
- This project takes its direction from DOE in terms of its focus depending on the needs of other projects. LANL supports the other projects by studying a broad array of specific issues as directed by DOE.
- This project was mainly focused on water. The work involved hydration of feed gases through a membrane device, gas diffusion layers (GDLs) of different water permeability, and tests of fuel cell performance impedance as well of imaging of water in fuel cells by neutron scattering. As long as Nafion® or similar water-based membranes are used in fuel cells, this work will be very important. The work here is critical to hydrating a fuel cell and balancing water in a fuel cell and was well done.
- LANL has a wide array of analytical equipment and techniques to thoroughly characterize materials in need of improvement. Understanding material changes and underlying mechanisms is a prerequisite to mitigating degradation.
- The objectives, goal, and overall scheme of how to proceed with the project are not clearly identified. Even though this project is directed by DOE, the scheme should be defined by the project leader.
- One assumes that each task that is reported had a reason or objective and a goal or product that was described to the DOE decision committee by the customer before each task was assigned, costed, and conducted. This process was not defined in the poster, but it needs to be to determine whether the project accurately addressed the issue. Although the tasks are related to fuel cell issues, the degree of relevance to other tasks at LANL was not described.

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## Question 2: Accomplishments and progress toward overall project and U.S. Department of Energy (DOE) goals

This project was rated **3.0** for its accomplishments and progress.

- LANL has successfully addressed several technical issues identified by DOE and other principal investigators (PIs). The apparatus and procedures have been developed as needed.
- The poster exhibits a wide range of characterization results, from Fourier transform infrared spectroscopy and relative humidity degradation characterization of membranes to fuel cell performance of GDLs to water imaging across the membrane. Scanning electron microscopy is also presented for GDL imaging, but this seems to be a more generalized imaging technique rather than a fuel-cell-specific diagnostic or characterization capability.
- The exact need by each outside organization could not be fully explained because of the nature of the particular effort. However, the assistance that the personnel at LANL have to offer each requester seems to be sufficient and willingly provided. How well this was incorporated into the outside agency is difficult to measure. Providing the assistance that was described seems to be adequate for the need presented.
- Most work involved characterization to support others. There is not much innovation. The hydration system was run and tested, the GDLs were tested, and fuel cell impedance and fuel cell performance were tested. Water was imaged.
- What is shown as an accomplishment in the presentation is not distinguished with what is usually done by each collaborator.

## Question 3: Collaboration and coordination with other institutions

This project was rated **3.7** for its collaboration and coordination.

- The work was well coordinated over a number of industrial and government laboratories. Results were of high quality. Work was complete and done in a timely fashion.
- The list of “clients” is comprehensive and includes automotive original equipment manufacturers, laboratories, universities, materials and equipment suppliers, and technical institutes. Strong relationships have been established in the course of designing the pertinent apparatus and experimental parameters.
- Participation in DOE working groups supports critical areas that DOE has identified as opportunities for a wide range of developers.
- The project appears to span a wide range of collaborators from government, academia, and industry, as well as across multiple Fuel Cell Technologies Office programs. It is assumed that there is close collaboration with DOE stakeholders. Fuel cell training, demonstration, and class material could serve as a useful input or template for more generalized training materials for the college or university level as part of a greater outreach effort in fuel cell education and to help build a talent pool for further research work in the area.
- Lots of collaborators exist. However, it is difficult to understand the big picture of the collaboration (i.e., how to share the various functions/capabilities and combine them to achieve the goal).
- The degree of interaction with other working groups to learn what activities need assistance and how LANL can provide this seems to be quite good. However, the extent of success in portraying the assistance and availability of personnel and equipment to help overcome specified barriers is not described, and no outline is available because this appears to be a rather ad hoc operation.

## Question 4: Relevance/potential impact on advancing progress toward DOE research, development, and demonstration (RD&D) goals

This project was rated **3.0** for its relevance/potential impact.

- The issues addressed are relevant to DOE’s goals and targets.
- Supporting the efforts of developers with unique equipment and expertise is an important role that national laboratories are very well suited for.

- To the extent that the work can support DOE objectives and DOE working groups, the project is expected to have a consistently positive impact and serve a useful purpose. The relevance is to facilitate technical support and testing of industry, government, and academic partners that are low-cost and reliable.
- This work involved high-quality characterization of fuel cell components pertaining to hydrating and water handling. This is important for DOE in terms of ensuring that performance and durability objectives are met. There has not been much innovation, so progress is not directly impacted by this work, but it has been indirectly impacted because progress depends on the innovation of collaborators being served and the feedback these collaborators get from this work.
- The impact and importance of the assistance are big.
- The tasks seem to be quite well oriented toward assisting fuel cell developmental needs. However, the educational aspect of the reported work seems to fall outside of the intent to assist the advancement of fuel cell technology. Educational efforts should be funded out of a separate fund or category.

### Question 5: Proposed future work

This project was rated **2.3** for its proposed future work.

- Future work will be defined by DOE in support of the other PIs. It is assumed that the work will be relevant and timely.
- The plan is to maintain these capabilities. Not much was planned to address the deficiencies observed, such as the formation of hydration limiting anhydride in the water permeation membranes of the feed gas hydrator.
- Because of the ad hoc nature of the task and the unknown nature of DOE funding for fuel cell work, it is difficult to describe what needs will arise and how to address them. While it is necessary to make LANL's assistance open to all parties, this procedure precludes developing specific ties for continued work with a given research group or company agency, which is appropriate. It is not clear how the plans for funding should be allocated when the work cannot be planned in advance.
- It would be good to see more in the way of proposed future work beyond "to be defined by DOE." For example, perhaps stakeholders could be surveyed for their input on what is most useful in existing technical support and what could be most useful but is currently lacking.

### Project strengths:

- This project provides great support for other laboratories, academia, and companies.
- Strengths of this project include its potential value and that it is directed by DOE.
- Strengths of this project include its high-quality characterization work and timely response to collaborations regarding the results of characterizations.
- Providing personnel and equipment availability to DOE contractors that need this assistance to perform their work but cannot fund these DOE-funded facilities or need only conditional assistance is an excellent idea. The interaction with working groups to advertise this capability is a very positive feature of this work.
- This project's strengths include its wide range of technical services and characterization techniques; responsiveness to DOE needs and requests; and how it is serving a wide range of partners across industry, government, and academia.

### Project weaknesses:

- The objectives and process are unclear.
- This is a support project, so the most important aspect is to provide timely and high-quality characterizations. Still, more interpretation and recommendations to the collaborators about modifications to the materials seem warranted and were not evident.
- Perhaps it is possible to develop some metrics of success beyond DOE Hydrogen and Fuel Cells Program Annual Merit Review (AMR) feedback and evaluation (e.g., how many sample images, utilization of tools, throughput time). Similarly, perhaps the impact of such technical support or characterization can be quantified or semi-quantified (e.g., "this characterization work led to a 10% increase in performance or developed the basis for a new degradation model or mechanism for this customer"). Also, there should be a

mechanism to specifically call out the new or enhanced capabilities on an annual basis. Otherwise, year-to-year progress is harder to assess.

### Recommendations for additions/deletions to project scope:

- If the purpose is to provide service to collaborators, this project is fine as is. However, if the purpose is to improve water handling, then more interpretation by government laboratories and adjustment of materials by collaborators (feedback between the team and collaborators) are warranted to stimulate and accelerate innovation.
- Because this is an ad hoc effort and not specifically identified with a specific need in advance of the issues that arise, it is difficult to determine either the workforce or funding that should be allocated. This may also be a problem with respect to how extensive of an effort can be ascribed to a given problem if the funding is to be spread over several unplanned tasks. While this is a valuable “tool” for assisting the advancement of fuel cell research, a significant amount of time is required to establish how effective it is for assisting other researchers. Perhaps including a broad publication of what is available for assistance with any request for proposals would help in identifying what needs could be met by proposers and researchers through including LANL in the proposal at the beginning.
- There are a few suggested additions: (1) perhaps single-cell protocols can be documented either in the poster or in the supporting publications, and (2) perhaps the short course could be the basis or input to a more general short course that can be made available to the community. One could imagine a “train the trainer” session at a future AMR meeting to spread this course content around the United States. There are no recommendations for deletions, but if there was a metric for utilization of the tools/characterization techniques, then maybe some could be downscaled or re-directed if not used, while others could be prioritized for upscaling/expansion.

## Project # FC-054: Transport in PEMFCs

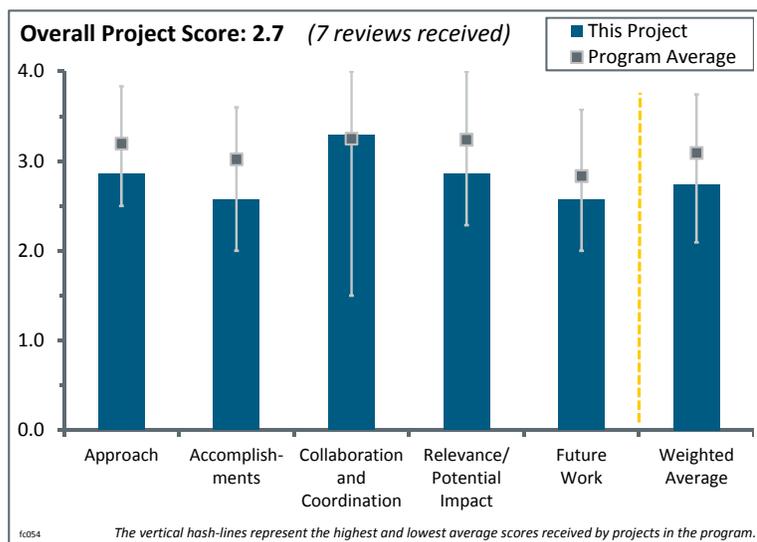
Cortney Mittelsteadt; Giner, Inc./Giner Electrochemical Systems, LLC

### Brief Summary of Project:

The objective of this project is to improve understanding of and the correlation between material properties and model equations. The use of modeling in fuel cell development is widespread, but the fundamentals of modeling are not agreed upon throughout research. This project identifies inconsistencies in design rules for polymer electrolyte membranes (PEMs) and works to standardize the parameters.

### Question 1: Approach to performing the work

This project was rated **2.9** for its approach.



- The approach to measuring water transport numbers in membranes is novel and good, and it apparently leads to a model that has excellent correlation to the experimentally measured water transport values in actual operating fuel cells.
- The approach is good. By widely varying the transport and structural properties of fuel cell components (mainly the membrane), this project seeks to come up with guiding design principles for fuel cell membrane development and maybe other components.
- This project concentrates on model generation and development of relevant transport numbers.
- The project aimed at understanding the correlation of material parameters to PEMFC transport properties through the development of specific ex situ experiments, a transport model, in situ testing, and verification with in situ data. All in all, this is an ambitious project trying to answer questions that may help to improve/design membrane and gas diffusion layer (GDL) materials with specific properties. It uses a sound approach but aims at high-hanging fruit.
- The approach, it appears, is to develop new membrane materials with different transport numbers. A new electro-osmotic drag coefficient (EODC) was developed, and the degree to which the EODC contributes to performance was estimated using modeling. The model was compared with performance and water balance testing in fuel cell testing to link the component to the fuel cell.
- The approach to the project does not directly address critical barriers, but it does provide support in addressing key barriers of performance, particularly at high current density. The project is not particularly well integrated; the key thrusts of polymer synthesis, transport measurements (development of novel techniques), and modeling overlap but do not critically depend on or leverage each other. The development of a model that cannot be widely circulated has limited value as well.
- Elements of this effort, such as the development of membranes with improved water management, can contribute to overcoming barriers that impede fuel cell commercialization. The modeling and other aspects, such as the segmented cell, are generally similar to past efforts and are less likely to contribute to the development of technologies that overcome barriers.

## Question 2: Accomplishments and progress toward overall project and U.S. Department of Energy (DOE) goals

This project was rated **2.6** for its accomplishments and progress.

- The progress in membrane design and characterization and transport modeling appears to be reasonable based on additional reading of the published literature in *ECS Transactions*.
- Very good advances have been made with respect to model verification and experimental results, including water balance predictions and cell performance predictions. Some correlations were established between membrane composition and membrane parameters using previously developed experimental techniques. Other correlations included GDL parameters and performance. No data were reported on Tech-Etch. It is unclear what this company's contribution was.
- The accomplishments and progress toward the overall project goals are reasonable based on the lofty challenge that this project is attempting to meet. More effort to validate the model's predictive power based on two-dimensional data is needed.
- The novel polymer electrolytes and novel techniques developed to measure water uptake, diffusivity, and electro-osmotic drag all have value to the community. Some of the structure–property relationships investigated for multi-block copolymers have provided increased insight into the water-related properties of interesting novel materials. The modeling work is showing reasonable agreement with experimental data, but it is limited in the fact that it has not been presented in significant detail, it cannot be openly circulated at the end of the project, and it seems far less advanced than other models that have been developed. The results to date provide little value to the community, although the comparisons between hydrocarbon and perfluorosulfonic acid (PFSA) materials are interesting, and there is significant concern that at the end of the project little specific information will be created that can be built upon by the community.
- This project features interesting measurements and modeling; however, for much of the work there is a lack of in situ validation. A good example is the local distribution of temperature and liquid water cross sections. These have been measured in situ by different methods, primarily in DOE projects by neutron imaging. These modeling cross sections should be validated by actual experimental data—if not from this project, from data collected by other projects. Model validation needs to be undertaken for both the cross-section modeling and the areal “water film thickness” model as opposed to validation of water concentrations by segmented cell.
- Generally it appears that progress has been made, particularly in the membrane arena, but the situation is confused somewhat by presentation or technical backup slides that are very similar or identical to the previous year but still utilize the terms “new” or “achievements” in the title. While EODC measurements in general are contentious, it is not convincing that this technique is superior, only different. Progress toward the technical targets is not addressed, nor is the relevance of much of the work. For example, start-up is listed as both a barrier and a technical target, but there is no obvious tie-in with the work presented.
- It is unclear what the overall objective of this project is. It is unclear what the benefit is of membranes with more or less diffusivity or EODC in operating fuel cell systems. The researchers do show a polarization curve with higher performance due to less water transport and therefore less flooding of the cathode in high relative humidity (RH) conditions; however, this is in an atypical H<sub>2</sub>/air co-flow orientation of the gas channels. Typical PFSA-based membrane fuel cell systems take advantage of the high water transport and run counter-flow gas channels for air and H<sub>2</sub>; the researchers did not report on this more typical flow channel orientation. Furthermore, in the more typical low RH operating regime, the low water transport of the new Virginia Tech membrane shows a lower polarization curve, making it unclear if high-water-transport membranes or low-water-transport membranes lead to a better fuel cell system.

## Question 3: Collaboration and coordination with other institutions

This project was rated **3.3** for its collaboration and coordination.

- This project benefits from a set of strong contributors that provide the majority of the effort.
- The project features good collaborations with university and other industrial partners.
- This project features a good team that involves organizations with complementary skills. The roles of the team members are well defined.

- The project appears to have a good degree of integration.
- This project features collaborators from industry and academia, as well as clear task separation that leverages the strength of these institutions. It also features the exchange of information and materials required to achieve technical progress. The project and collaborations appear to be managed successfully. The contribution from Tech-Etch remains unclear.
- The collaboration with Virginia Tech and the University of South Carolina (USC) appears to be working well. Some automotive industry input may be useful.
- The team has a reasonably broad group of collaborators, including leaders in the areas of polymer synthesis and membrane characterization. The modeling work being performed by the USC team has little other background in this area beyond this project.

#### **Question 4: Relevance/potential impact on advancing progress toward DOE research, development, and demonstration (RD&D) goals**

This project was rated **2.9** for its relevance/potential impact.

- This project relates directly to DOE's needs for understanding and coming up with design strategies for improving mass transfer in next-generation fuel cell components.
- The project's relevance to the overall program is difficult to assess in terms of the value to the fuel cell industry. The fundamental learnings from component studies will no doubt be useful to researchers in the field, which may indirectly result in progress in fuel cells.
- The project indirectly supports a subset of the DOE objectives. The strongest connection is performance, particularly at high current density.
- The understanding and development of membranes that alleviate water management challenges are of significant importance to the field. As the modeling results are similar to those previously observed or modeled, they are unlikely to benefit fuel cell developers.
- No agreement exists regarding the fundamental parameters used in fuel cell modeling. An agreement would be very helpful for meaningful model development with respect to fuel cell performance and water balance. This work thus contributes to developing the capability to engineer/design materials that have specific transport properties for optimized fuel cell performance and efficiency.
- It is unclear how this project will actually be used by industrial developers. There are questions about whether the model is going to be distributed and how the data will be utilized by developers.
- The barriers claimed to be addressed are performance, water transport in the stack, water management, and start-up/shutdown. It is not clear how this work affects any of these barriers. Perhaps a better study would be water transport studies of the diffusion media rather than the membrane; the researchers do recommend that in their future work, but there is not much time left in the project.

#### **Question 5: Proposed future work**

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

- The future work plans seem to be a reasonable continuation of the current activities.
- There is a reasonable amount of future work for the remaining time period. A comparison of nanostructured thin-film (NSTF) layers to conventional catalyst layers would help researchers understand the feasibility of an NSTF catalyst. Optimizing GDL properties for an NSTF-type catalyst may be the only way to overcome the flooding issues of these catalyst layers.
- Now that the membrane water transport is well understood, the study of the water transport in NSTF electrodes (which are known to be challenged by good water management) and the diffusion media (DM) (where there is currently not much good understanding of the water transport mechanisms) is good future work.
- The purpose of the "Emphasis on Saturated Conditions" is unclear; this is clearly the opposite of what the automotive original equipment manufacturers are doing. Examining flooding of thin catalyst layers (such as NSTF) could be highly useful.
- The future work should probably be limited to membranes, diffusion media, and water management, rather than catalyst effects, so that the scope is less broad and more focused on the strengths.

- The future work focuses on studying saturated conditions (whose primary relevance is only during start-up for automotive applications) and electrode effects. In the area of electrode effects, it is unclear how the researchers plan to approach the areas of high current density.
- Investigating flooding of NSTF layers is proposed in the future work. While important, such an effort is a bit of a departure from the current efforts and is quite challenging considering the time remaining on the project.

#### Project strengths:

- This project features a good, sound approach that addresses many aspects of transport in PEMFCs.
- This project features good experimental methods to measure fundamental material properties, in addition to a good model with good correlation to measured data.
- This project's strengths include its novel polymer electrolyte synthesis and novel water transport studies.
- The membrane development portion of the effort provides the most potential value to the fuel cell community.
- The approach is the main strength of the project. By widely varying the transport and structural properties of fuel cell components (mainly the membrane), this project seeks to come up with guiding design principles for fuel cell membrane development and maybe other components.
- The progress in membrane design and characterization and transport modeling appears to be reasonable, based on additional reading of the published literature in *ECS Transactions*. The collaboration with Virginia Tech and USC appears to be working well. Some automotive industry input may be of further use.

#### Project weaknesses:

- The team needs to better leverage the different project facets (membrane synthesis, water transport, and modeling).
- A poor case is made for the relevance of the various efforts to the “technical targets” and the “barriers to be addressed” listed up front.
- Additional in situ validation techniques could be used. The level of work going on in this project related to hydrocarbon membranes is unclear, as the project is a transport project.
- There is not enough connection made to real fuel cell systems. In addition, it is unclear where the advancement in performance, cost, reliability, and durability comes from for membranes with higher or lower water transport numbers.
- Although the model data seem to predict the overall performance values well, the local performance data shown in the two-dimensional plots of temperature and current look visually discrepant between the model and experimental data. In addition, there are no comparisons to the neutron measurements of water production from [www.pemfcd.org](http://www.pemfcd.org). The model must be able to predict the measured values from neutron radiography as well.

#### Recommendations for additions/deletions to project scope:

- Start-up is listed in the barriers/technical targets and has been mentioned in the past. Correspondingly, some of the future work should be directly linked to start-up.
- With little membrane work in the current portfolio, the membrane studies bring value. The value of models being developed seems small and does not seem to have a clear path forward; it is recommended that the project cease the modeling work.
- The researchers are using segmented cell distribution measurements as validation of their modeling of water and water flux. These data are at best an “inference.” These water concentrations should be verified directly. There are developed techniques to measure the water concentration in situ; for example, the BT-2 beam line at the National Institute of Standards and Technology is funded by DOE/U.S. Department of Transportation as a user facility. The value of the modeling of the hydrocarbon membranes in terms of temperature and liquid water content is unclear, unless a developer is actually exploring using these materials.
- There are no recommendations because the project ends this year.

## Project # FC-063: Novel Materials for High-Efficiency Direct Methanol Fuel Cells

David Mountz; Arkema

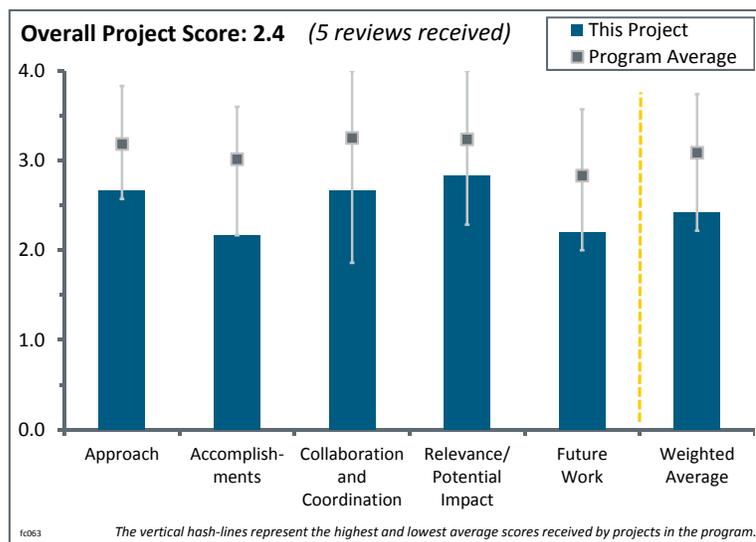
### Brief Summary of Project:

The objectives of this project are to (1) develop a membrane technology having low methanol crossover, high conductivity, and increased durability; (2) develop cathode catalysts that can operate with considerably reduced platinum (Pt) loading and improved methanol tolerance; and (3) combine the cathode catalyst and membrane into a membrane electrode assembly (MEA) achieving performance of at least 150 mW/cm<sup>2</sup> at 0.4 V and costing less than \$0.80/W for the two components.

### Question 1: Approach to performing the work

This project was rated **2.7** for its approach.

- The project team has been thoughtful in eliminating unpromising avenues and staying focused on avenues with promise to meet U.S. Department of Energy (DOE) targets. The focus on combinations of conductivity/MeOH permeability, and on MEA development and diagnostics, are appropriate and wise.
- This project aims to develop a low-cost MEA that has a better-performing direct methanol fuel cell (DMFC) membrane (lower methanol crossover, high conductivity, and increased durability). It also aims to develop a cathode catalyst that can operate with considerably reduced Pt loading and improved methanol tolerance. These are the right issues to address for DMFCs. However, the membrane technology is not significantly new, and the methanol tolerance catalyst was a no-go.
- The main purpose of avoiding methanol crossover seems to be a difficult task, although some progress has been reported. Generation 2 membranes have the same problems reported in the previous year (leaching of sulfur). The use of cross-linking agents did not help. Other approaches (increasing the polyelectrolyte molecular weight) failed, too. Perhaps some modeling would help.
- The team took the right decision of stopping the cathode development approach, which was not effective. Using a commercial catalyst and GDE for conducting membrane performance and durability assessments is the correct approach. However, the performance and durability test protocols being used by the team are very soft and not adequate for predicting material behavior in true DMFC power system operational conditions. The team should consult with DMFC stack/system builders or scientists from a national laboratory to devise correct performance and durability test protocols for conducting performance and durability diagnostics.
- The project focuses on improving DMFC performance and cost through the use of blend membranes and the development of Pd-based catalysts. The Pd-based catalysts have not shown promise, nor is it clear why it was believed that they would show promise in the heavily investigated area of methanol oxidation. The development of blend membranes offers the potential of decoupling mechanical and transport properties; however, efforts from the team lead over the past several years have not suggested that the proposed approach will result in durable and/or improved performance.
- The targets on slide 4 should be set in units that measure the bulk material properties, not in units that depend on membrane thickness. For example, bulk resistivity should be used for material resistivity, not areal resistance. For perfluorosulfonic acid (PFSA) membranes, the industry standard would become 6.3 Ohm-cm instead of 0.12 Ohm-cm<sup>2</sup>, and the proposed Generation 1 membrane with a 1.2 mil thickness and an areal resistance of 0.03 Ohm-cm would have a bulk resistivity of 10 Ohm-cm. Thus, the Generation 1 material does not have a lower bulk resistivity as compared to PFSA; the researchers have simply reduced



the membrane thickness to meet the target. This is furthermore evident when the researchers compare the performance of a 2-mil PFSA and a 1.2-mil-thick Generation 1 membrane that has essentially the same areal resistance and thus the same polarization curve. Thus, there has essentially been no advancement in the state of the art. The approach should therefore be more focused on the bulk material properties of a new material that has better bulk material properties as compared to industry standards. A similar approach should be done with methanol permeability.

### Question 2: Accomplishments and progress toward overall project and U.S. Department of Energy (DOE) goals

This project was rated **2.2** for its accomplishments and progress.

- Progress has been made on a new material that seems to behave similarly to industry-standard PFSA.
- Only the membrane work remains from the original goals, and there are still some obstacles to achieve the desired performance.
- Overall the progress is good, but it appears to be stalled. Generation 2 membranes are not panning out; Generation 1 membranes have been optimized and perform fairly well, but this is relatively old work. The MEA work is sensible and necessary, but it is not very creative in and of itself. The diagnostic work on MEAs will be helpful in understanding failure modes.
- PFSA MEAs presently outperform Arkema MEAs, both in terms of performance and durability. The durability milestone had to be lowered and is awaiting a status update. Interfacial resistance is a common major issue when working with a new membrane. The team has not been able to resolve this issue or have a good understanding of it. The team has made good progress in lowering catalyst loading.
- The objectives of membrane development (Task 1) were not accomplished because of the ionomer instability in the membrane under DMFC conditions. The blending of an ionically conductive polyelectrolyte with a PVDF host matrix did not produce a workable membrane because of the high solubility of the polyelectrolyte. The team should have focused more on developing a stable polyelectrolyte to achieve the objectives of Task 1. The evaluation of the MEA was done under an extremely high air stoich, which is inappropriate for the portable DMFC condition. The team should conduct its testing at an air stoich of 2.0, which is closer to that preferred in portable DMFC systems. The team should test its MEA at a higher temperature (80°C) and a lower air stoich (<2.0) to understand the possibility of using its MEA in a DMFC power system. The 2-mil PFSA, which is very stable, also meets the Milestone #5 target. The developmental PVDF/polyelectrolyte membrane does not offer much better performance than the commercial 2-mil PFSA membrane.
- The progress toward DOE goals for portable power has been minimal. The fuel cell performance shows modest performance gains compared to industry-standard values at fixed operating conditions, but it is unclear that this value represents the state of the art, and other published performance values for DMFCs seem to be higher than the presented values. One of the biggest concerns is the low stability/durability of the different membrane approaches employed (one of which was down-selected owing to extremely poor stability). It is not clear that the properties of the blend membranes employed can meet those of state-of-the-art hydrocarbon membranes, even in initial properties performance, and even if they do, they do not appear to be stable. The properties reported—namely areal resistance and permeability—make comparisons between membranes difficult; conductivity and permeability or methanol crossover and resistance would be more appropriate properties for comparison in order to ensure that the thickness effects do not confuse data interpretation.

### Question 3: Collaboration and coordination with other institutions

This project was rated **2.7** for its collaboration and coordination.

- The lead institution has been proactive in finding the right partners and closing things off with partners that were working in unpromising directions. This is commendable.
- The team consists of good partners, including a university and a catalyst company. However, inclusion or consultation with a national laboratory or DMFC portable power manufacturer could help the team to test and evaluate its membrane/MEA under realistic DMFC operational conditions.

- Most of the work is done at Arkema. There is some collaboration with the Illinois Institute of Technology (IIT), Quantum Sphere, and IRD Fuel Cells, LLC.
- Most of the progress seems to be achieved by Arkema; it is unclear if this is because of the lack of coordination with the partners. The progress is really slow. The team was not able to find an appropriate membrane formulation for the problem of leaching, and the other membrane has a higher permeability than the target (even when the target permeability has been increased from last year).
- A little collaboration exists, but there does not seem to be much synergy or strength in the interactions. IIT no longer contributes to the project, and the Pd catalysis work was tangential to the membrane work. The outsourcing of MEA fabrication and testing does not appear to have much synergistic value and appears to be primarily contract work. Increased interaction with partners that have alternate membrane DMFC testing and MEA fabrication would be beneficial.
- Because this project should be a fundamental material improvement project rather than an MEA project, the project could benefit from university collaborations that help with the fundamentals of the membrane materials and further processing of the membrane materials to improve bulk properties.

#### **Question 4: Relevance/potential impact on advancing progress toward DOE research, development, and demonstration (RD&D) goals**

This project was rated **2.8** for its relevance/potential impact.

- This project aims to increase the performance and durability of DMFCs and reduce cost, which are both relevant to the DOE Hydrogen and Fuel Cells Program (the Program). Its approach to doing this is to develop a better and lower-cost DMFC membrane and cathode catalyst. These are the relevant objectives to pursue with respect to DMFCs and DOE targets.
- The proposed goals are aligned with the Program. However, the slow progress shown so far creates some doubts about the potential impact of this project.
- The project lead is certainly aware of DOE goals and is evaluating project work against them. Progress has been slow, but the team is at least being honest about its findings.
- The project is relevant to the objectives of DOE's *Fuel Cell Technologies Office Multi-Year Research, Development and Demonstration Plan*. The activities are aligned with DOE's goal. This project is focused on low-crossover membrane and MEA for DMFC application, which is very important for the commercialization of DMFC technology. The focus to accomplish the performance and cost objectives is aligned with the fuel cell initiative of DOE. However, the feasibility of the concept is not very clear.
- The project focuses on the cost and performance barriers for portable power. The primary (remaining) focus has been on novel membranes and MEA integration. Issues of catalyst cost—a primary driver for these systems—are no longer being addressed within the project. Meeting system cost goals through only membrane improvements is not likely.
- The research should be focused on a new membrane material that has better conductivity, lower MeOH crossover, and good stability as compared to standard PFSA materials. Pursuing lower-cost membranes compared to PFSA membranes should not be a driver in the membrane development in this project because the amount of precious metals applied in the standard DMFC electrodes is the main cost factor per square meter of the MEAs, not the industry standard of 2-mil PFSA materials. Lower-cost DMFC MEAs should focus on lowering the platinum group metal (PGM) loading of the electrodes.

#### **Question 5: Proposed future work**

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

- The project is wrapping up soon; the proposed future goals are sensible and appropriate.
- The future work described is aligned with the proposed work of the project. The team needs to work with realistic testing protocols and avoid using soft testing methods to achieve performance/durability targets. It should use practical test conditions, which are needed to make DMFC systems commercially viable. Using a high air stoich will lead to high parasitic loss and hence loss in the output power of the system.

- The proposed future work looks reasonable, but the major issue of higher resistance does not seem to be addressed. Post-mortem analysis will help, but the researchers need to diagnose the problem in order to improve the durability.
- The proposed approach for the dissolution issue in the Generation 2 membranes is complex and may not lead to the expected results. Thus, the overall success of this project is limited.
- The future work focuses on more crosslinking studies, MEA optimization, and some post-mortem testing; it has little relevance toward eliminating barriers or advancing the Program.
- The project has essentially ended (June 30, 2013).

#### Project strengths:

- A strength of this project is having an industry lead with the capability to develop new materials.
- The project team has vast experience with PVDF, which is a potentially good candidate material in ion-conducting membranes.
- The team is well organized and capable of developing DMFC membranes and MEAs. The team is equipped with the necessary resources required for the success of this project.
- Prospects for making very low-cost membranes that also exhibit high performance were good. The approach to testing their ideas is good.
- Membrane development is the strength of this project. However, the researchers have encountered many difficulties.
- The project's strength is in membrane development, but the new membrane is not significantly better than the PFSA membrane.

#### Project weaknesses:

- There were poor advances in materials in both the membrane and catalysis areas.
- The Generation 2 membranes and proposed low-PGM catalysts did not work out.
- Durability tests of the MEA are complicated owing to the uncertainties associated with commercial electrodes. The team did not correctly select the appropriate partners or failed in the overall coordination.
- The team could have benefited from consulting with a national laboratory or DMFC company to determine an adequate testing procedure for the DMFC. The team also needs to move quickly to consolidate on the final membrane and MEA structures to facilitate initiation of durability testing.
- The project objectives and approach are good, but the execution and final product were not delivered. The catalyst and MEA development/expertise were lacking.
- Too much time was spent on making MEAs on materials with essentially similar properties to PFSA materials.

#### Recommendations for additions/deletions to project scope:

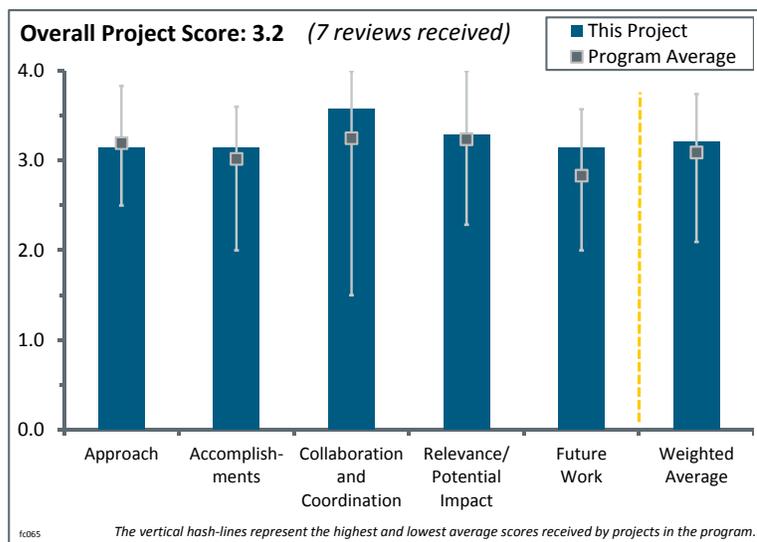
- Because the project is close to completion, there should not be any deletions at this stage.
- The project is ending soon; plans for closeout are appropriate.
- Given the team's strength in membrane development and the time left in the project, the team should focus solely on Tasks 1 and 4. The team should drop Task 3, especially the goal of 150 mW/cm<sup>2</sup> at 0.4 V. This goal seems to be a long shot, and presently there is no indication that the goal is achievable. By dropping Task 3, the team will have more time to complete the other two tasks—Task 1 and Task 4.
- DOE has funded for several years the study of blended membranes for improved fuel cell performance. If anything, it appears that the stability of these materials has gotten worse. Further investigation of PVDF blend membranes should be stopped because of the poor properties and advances, despite the reasonable levels of investment to date.

## Project # FC-065: The Effect of Airborne Contaminants on Fuel Cell Performance and Durability

Jean St-Pierre; Hawai'i Natural Energy Institute

### Brief Summary of Project:

The objective of this project is to identify and mitigate the airborne contaminants that are adversely impacting automotive fuel cell system performance and durability. The University of Hawai'i (UH) identifies contaminants and determines tolerance limits for filter specifications. The project supports recovery of the fuel cell system after exposure to contaminants by identifying fuel cell stack material, design, operation, and maintenance changes to remove contaminant species and recover performance. The 2012–2013 objectives are to establish degradation mechanisms and quantify performance loss for key contaminants to assist mitigation.



### Question 1: Approach to performing the work

This project was rated **3.1** for its approach.

- The project is well designed and starts with a list of contaminants, then prioritizes them, and studies their effects at various operating conditions.
- The project's focus on air contaminants is an important task, and the identification of potential contaminants will help fuel cell developers in their selection and the formulation of electrode catalysts.
- The approach is good. The principal investigators (PIs) are using the available data from the field to establish the most common contaminants in the air and the impact of these contaminants on performance and durability.
- The approach is good, straightforward, and based on down selecting from various contaminants. This project addressed most of the concerns from reviewers by studying the effect of down-selected airborne contaminants on voltage loss as a function of operating conditions. This project also addressed the effect of calcium sulfate from a de-icing agent on degradation.
- The approach is good because it used multiple, industrial sources for the selection of contaminants to evaluate. The approach attempts to identify how to recover the fuel cell system from contamination and quantify the performance impact.
- The approach is very reasonable for the evaluation of each contaminant; however, contaminants need to be studied according to their merit. The study has focused extensively on acetylene. This is a relatively exotic source of contamination. Cars will overwhelmingly never see this contaminant. The initial findings show a complete reversibility of contamination and exposure does not cause long-term impacts on the stack (as soon as the contamination is removed, the stack performance comes back). It may be worthwhile to prioritize all the contaminants of interest and to proceed quickly, studying them one by one.
- The combination of experimental determination of impurity effects and modeling is effective. The breakdown of impedance data to extract kinetic, ohmic, and mass transfer resistances is beneficial. This is mostly coordinated with past and present impurity studies to avoid the duplication of efforts. However, it is not clear how cation poisoning work differs from what has been done in the past. The use of low loaded catalysts ( $0.1 \text{ mg Pt/cm}^2$ ) is a major improvement. The addition of cleaning agents and coolants to the contaminants list is appropriate. The PI needs to work at impurity levels expected in the real world;

acetylene tests performed at 4,030 ppm are not relevant. Even in a welding shop, concentrations should not be this high. Likewise, propane concentrations of 1,000 ppm are quite high and not expected to be relevant.

### Question 2: Accomplishments and progress toward overall project and U.S. Department of Energy (DOE) goals

This project was rated **3.1** for its accomplishments and progress.

- The team has demonstrated how to approach the identification and evaluation of air contaminants. The examples of “recovery” are interesting; however, many recovery protocols are well known in the industry.
- Significant progress has been made with respect to the impact of the contaminant on various sources of voltage loss. Further, the current distribution using a segmented cell sheds some light into the propagation of contaminants in a fuel cell system.
- This project has made good progress studying the effects of four contaminants. The performance loss results are supported by interpretations of an underlying mechanism. Tests with lower Pt loading are more relevant considering the direction of the fuel cell developers. The development of a filtering system is mentioned. The mitigation strategy is important.
- Steady and excellent progress has been made so far by identifying and down-selecting various contaminants that cause degradation in the performance of fuel cells. The detailed understanding of the mechanism should help to understand the effect of these various contaminants on different types of catalysts. Novel materials are being evaluated as cathode catalyst materials for fuel cells. These mechanisms would help to mitigate the effect of these contaminants on the newer electrocatalyst materials.
- The project continues to make good progress evaluating potential contaminants. It would be good to see data showing mitigation/restoration for 90% of cell performance for the seven contaminants that this has been completed for, and information on the mitigation/restoration strategies used for the contaminants. The step-change in effect of the C<sub>2</sub>H<sub>2</sub> contaminant on voltage at a concentration of about 200 ppm needs some explanation and investigation to see if similar results occur at lower concentrations with lower catalyst loading.
- The team has thoroughly examined acetylene. It may be prudent to run parallel evaluation on multiple contaminants as that will provide technology developers with timely feedback regarding potential red flags. This testing should serve as an early warning system to alert manufacturers that certain contaminants need to be addressed in real-car designs. Acetylene appears to be a non-issue and it may have taken efforts away from more important contaminants.
- The team has built up a database of common contaminants with an explanation of the effect on performance and the ability to remove the impurity. It is not evident that the recovery of an acetylene contaminated cathode removed all of the acetylene or if the acetylene was oxidized during removal and left a carbon layer that reduced the active surface area. The researchers did not address this point and did not consider partial oxidation. There was no explanation of why the H<sub>2</sub> peroxide rate increased. It is not clear if specification sheets are being developed in this program, but they should be. The authors stated they would “quantify spatial variability of performance loss,” but there is nothing indicating this in the accomplishments and progress. It was unclear if the cartoon in slide 15 was the proposed mechanism and if there was some explanation of the drawings.

### Question 3: Collaboration and coordination with other institutions

This project was rated **3.6** for its collaboration and coordination.

- UH has assembled a good team for collaboration.
- UH has sound collaboration with appropriate partners.
- The collaborations appear to be very well established and working effectively.
- This is a good team of researchers with many organizations contributing to the project. If the partners contributed to the presented experimental results, the credit is not evident from the slides.
- The coordination with other impurity projects is good. It appears to be getting input from most of the fuel cell developers. It is not clear how cation poisoning work differs from what has been done in the past.

- While the project has a reasonable list of collaborators, more stack manufacturers are needed to update the project on the catalysts used in systems that are either in field trials or being readied for commercial release.
- This group should work much more closely with car, bus, and forklift original equipment manufacturers (OEMs). Ballard is a great company to collaborate with; however, real-world contaminant concerns come in where the rubber meets the road in vehicles. OEMs should really be the ones expressing and prioritizing contaminants and methods of exposure.

#### **Question 4: Relevance/potential impact on advancing progress toward DOE research, development, and demonstration (RD&D) goals**

This project was rated **3.3** for its relevance/potential impact.

- The effects of contaminants must be determined for widespread commercialization.
- This study supports the performance durability of the fuel cells by looking at the airborne contaminants.
- This type of project is extremely important as it can act as an early warning system for OEMs regarding real-world exposure risks. Based on studies like this, OEMs can decide to ignore, monitor, or design system features to deal with key contaminants.
- This project has developed a useful protocol for evaluating the effects and mitigation of air contaminants on fuel cell operation. It will serve as a valuable model for the fuel cell industry with their internal evaluations in the future.
- Understanding the voltage loss from sources is good. The impact of the project could be higher if they provide ways of translating this data into a meaningful trade-off between the stack and system design like the specification for the air filter.
- The establishment of a contaminant database will benefit all fuel cell parties and provide a reference for future development activity. This codes and standards database is one of the many that will be needed for future fuel cell commercialization.
- Understanding the effect of airborne contaminants and contaminants from other possible sources on fuel cell performance is very critical and the objective of this project works to understand that. Degradation mechanism due to various contaminants would help mitigate the voltage loss at the system or material level.

#### **Question 5: Proposed future work**

This project was rated **3.1** for its proposed future work.

- The proposed future work is sound.
- The work plan is consistent with the project objectives. The effect of the remaining four species will be studied and mitigation strategies will be developed.
- The plans to perform tests with concentrations closer to atmospheric concentrations and with 0.1 mg Pt/cm<sup>2</sup> should be done sooner. The plans to look at contaminant mixtures are relevant and should be expedited.
- The project's future work proposal is well focused and aggressive. One possible improvement would be to "down-select" the possible catalyst systems and focus on those few that are most likely to be introduced in near-term commercial applications.
- The proposed future work is in line with the objective of the project; however, detailed understanding of the degradation mechanism would add lot of value to the project. Also, the effect of contaminants with longer exposure times and different concentrations for low-loading catalysts would provide great information for future fuel cell systems. The effect on non-platinum group metal (PGM) catalysts (if any) and ultralow PGM catalysts would be helpful to anticipate any future challenges for these materials.
- It would be beneficial to streamline such processes and address multiple contaminants in short periods of time. It would also be beneficial to begin to look at interactions of contaminants. Cocktails of contaminants are a traditional means of testing a system; for example, bulk diesel exhaust will be encountered by vehicles on a daily basis. It is unclear if that is acceptable. It would be good if the project could explain this more.

- The spatial variability of performance will be explained (March 2013); that should have been ready for the AMR. It was not clear if there was an explanation of the spatial variability mechanism. The research is addressing low catalyst loading at the end of the project, but it is unclear why this was not an early priority based on known DOE automotive targets.

#### **Project strengths:**

- UH has excellent screening techniques.
- This project has strong collaborations and a well-thought-out approach for down-selecting contaminants.
- The capability of the researchers and the quality of the facilities strongly support the continued development of the contamination database.
- The project's participants have made significant contributions regarding the evaluation and analysis of the effects of air contaminants, including mitigation strategies.
- Tests have been conducted with lower Pt loading. Tests have been conducted to evaluate the effects of both contaminant concentration and exposure time. Performance loss mechanisms are being developed.

#### **Project weaknesses:**

- There are too many contaminants to deal with.
- The contaminants' concentration tolerances need to be specified. A detailed understanding of the mechanism is lacking.
- The project's work scope may need adjustments to focus more on the established catalyst systems and less on the broad and ever-changing list of experimental catalysts that may never make it to market.
- Considering that bromomethane is identified as a "red" contaminant, it should receive a higher evaluation priority. The mitigation strategies for the tested species are yet to be developed. It is not clear how determining the spatial variability will help mitigate the problem.
- The team may need to focus on publishing data in a format easily utilized by industry. It is not clear what the spatial variability mechanism defines. It is unclear if this is this another way of saying the contaminant adsorbs on the surface of the catalyst and blocks sites for electrochemical reaction. It is unclear if this takes into account reactions at the surface.

#### **Recommendations for additions/deletions to project scope:**

- The project's work scope may need to be re-focused and build on its accomplishments to date by placing more emphasis on near-term commercial systems.
- UH needs to decide what is a reasonable concentration of a given contaminant that might show up in the air stream. This team should classify the hazard of the contaminants based on the mechanism and the reasonable contaminant concentration. It is suggested that this project maintain the focus on the lower Pt loading.

## Project # FC-077: Large-Scale Testing, Demonstration, and Commercialization of Fuel Cell Coolant (SBIR Phase III)

Satish Mohapatra; Dynalene

### Brief Summary of Project:

The objectives of this project include understanding coolant durability requirements by working with different fuel cell types developed by various fuel cell manufacturers and understanding what the cost of coolant should be relative to current automotive coolants. Coolants should maintain low electrical conductivity and other thermo-physical properties for over 5,000 operating hours and should be compatible with a variety of typical fuel cell components.

### Question 1: Approach to performing the work

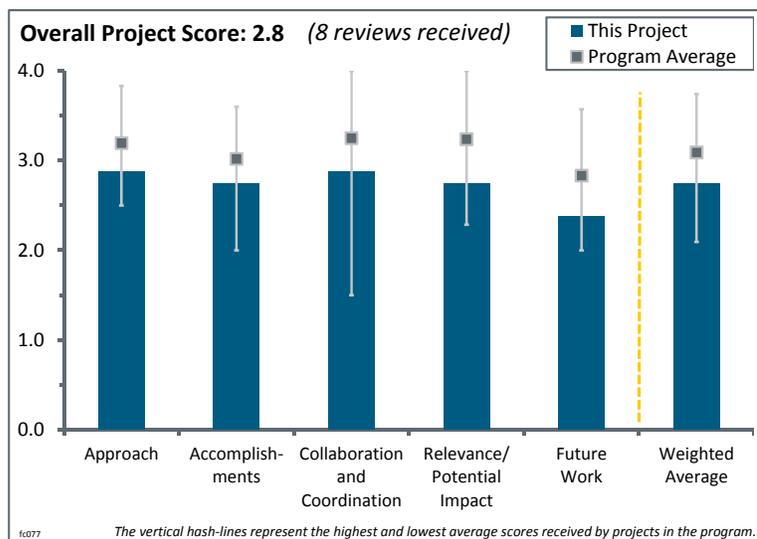
This project was rated **2.9** for its approach.

- The approach is effective and innovative.
- The approach is novel and, based on the data presented, effective at reducing ion contamination in fuel cell systems through a variety of means.
- The project's approach to developing an improved coolant for fuel cells is very good. The nano-sized particles for reducing ion concentrations are particularly interesting.
- This is a thorough and comprehensive approach, although experiments may lack consideration of the effects of direct contact of the coolant with the fuel cell system. It is unclear what the contaminating effect of the coolant is when it is in contact with the fuel or oxidant feed streams.
- This activity is not complicated. The project developed a heat transfer fluid and then will test that fluid and see if the results suggest it has economic viability.
- The approach is limited by the fact that long-term testing is really needed to determine its value; however, reliable, short-term tests are not available to extrapolate value.
- The approach lacks clear metrics for achieving project objectives and addresses only a small scope of the potential solutions. There is no evidence of "large-scale testing" as indicated in the project title.
- The use of the fluid overcomes the barriers of other fluids. Low conductivity and corrosion inhibitions appear possible. The particles remain suspended with surfactants. It is unclear if surfactants will degrade. It is not clear why the nano-particles themselves do not contribute to conductivity. The Dynalene fluid has several advantages over current fluids including no de-ionizing filter, lower pressure drop (smaller pumps), higher performance, lower cost, and no clogging.

### Question 2: Accomplishments and progress toward overall project and U.S. Department of Energy (DOE) goals

This project was rated **2.8** for its accomplishments and progress.

- This project has shown good progress towards meeting the DOE requirements for fuel cell coolants.
- A substantial amount of work has been achieved, but questions remain around colloid stability over time.
- This project has been running through its various phases since 2004. There is a good probability that this project will result in a commercial fuel cell coolant product that is superior to what is presently available.



- This project developed a clear understanding of what type of materials these coolants can be used with. Unfortunately, the materials do not seem to include structural or other plastic materials, which may be the materials of choice for automotive applications due to weight and cost considerations.
- The project addresses a clear need for applicable coolants able to meet the requirements of a PEM) fuel cell. The improvements in system performance, cost, and durability are likely secondary in nature. There are existing solutions in use by many original equipment manufacturers (OEMs), such as DI filter beds. This project will result in the incremental improvement of fuel cell systems, but it is not as groundbreaking as more fundamental work on catalysts, gas diffusion layers (GDLs), and membrane technology.
- The contractor has scaled up 100 L, developed quality assurance/quality control methods, and reduced final fluid cost. Also, the 100-hour test with Protenex is positive and had no increase in conductivity. The fuel cell coolant optimization and scale-up has been completed and Dynalene is capable of producing Dynalene fuel cell coolant in large quantities. It is not certain that conductivity and corrosion tests are conclusive to date; the testing times seem short.
- This project has no clear, relevant quantitative results. The principal investigator referenced about 5,000 hours, but the presentation only included results of 100+ hours. A lot of pictures were shown without a clear explanation of their relevance (e.g., corrosion samples). The presentation creates some doubts about the relevant results and progress. Using nano-particles to avoid corrosion seems to be more of a hypothesis than a real possibility, particularly when it comes to long-term durability and stability of suspension of the coolant liquid.
- The selected fluid, a solution of glycols (this fluid is not described, but one can guess it is propylene glycol and distilled water), is very similar to the most commonly used heat transfer material in the millions of domestic hot water heaters that decorate roofs globally. The engineering requires that fuel cell high-temperature fluids need to also have very low electronic conductivity, unlike the usual heat transfer applications. This requirement results from the fact that fuel cell stacks must be cooled; however, the voltage of the stack increases from plate to plate and the heat transfer fluid addresses each conducting plate. A conducting fluid would short the plates, which is not a good result. This proposal includes ionic scavengers, chemicals that absorb cations, and others that absorb anions. These scavengers are micro particles and are clearly insoluble particles that are entrained in the water-glycol mixture. It appears that progress has been made. The presentation suggests an emphasis on the scavenging, and perhaps that is the only real value.

### Question 3: Collaboration and coordination with other institutions

This project was rated **2.9** for its collaboration and coordination.

- The collaborations have improved and are good.
- It would be nice to see this coolant tested in more fuel cell systems than just Protonex.
- The collaborators are capable and certainly contribute to the project's progress.
- The contractor collaborates with Protonex, the Naval Research Laboratories, the University of Tennessee – Knoxville, and Lehigh University.
- The group assembled for the given task is satisfactory. There were again only vague statements and having more than 15 fuel cell companies does not really say anything.
- The collaboration could be stronger. It would be good to see high-voltage testing in relevant automotive systems. This could be ongoing, but is proprietary.
- This project used the university collaborator for determining the effects of using the coolant on the fuel cell. The partner from the fuel cell industry is providing a system for long-term tests and other companies will field test the developed coolant. It is unclear if information will be relayed back to project.
- The collaboration appears to be more like a vendor-buyer relationship. The small-scale fuel cell testing is not convincing. Obviously the hot fluid needs to be compatible with a specific set of polymers, metals, coatings, gaskets, pumps, etc. What works in one fuel cell design may not be useful in another.

**Question 4: Relevance/potential impact on advancing progress toward DOE research, development, and demonstration (RD&D) goals**

This project was rated **2.8** for its relevance/potential impact.

- As long as there are no quantitative results, the impact is not clear.
- Coolant performance is important in system performance and maintenance.
- The project is certainly relevant to the success of both automotive and stationary fuel cell technology.
- An improved coolant for fuel cell systems is supportive of the Hydrogen and Fuel Cells Program's goals.
- This project is of high interest to the fuel cell community. This interest is also indicated by the amount of companies that test the coolants.
- The relevance and impact are moderated by the fact that coolants exist. This project improves on the performance metrics of the available coolants and so it is an important achievement.
- The project will support the goals of cost reduction and durability. The impact on performance is not clearly demonstrated. It would be useful to see fuel cell voltage degradation rates over time with Dynalene and a DI water control.
- It seems like there are reliable and useful fuel cell stack coolants around. Many fuel cell vehicles have been manufactured and each has a useful thermal management system. Obviously, a lower cost coolant has the advantage; however, if a component has a small cost, it does not save significant money by making that small part cheaper.

**Question 5: Proposed future work**

This project was rated **2.4** for its proposed future work.

- The completion plan is acceptable.
- The project ends at the end of fiscal year 2013.
- To complete only some of the work is not really a good plan; the project needs to achieve its goals.
- The project is about to end; a focus on long-term testing results is critical and will determine overall value.
- More work on the effects of polymer-based materials that are of interest to the automotive industry would create a significant value increase in the project with respect to automotive applications.
- The future seems to be "ship product," which is obviously the goal. There must be some appreciation about the competition, and some need to think about how this work could result in a strategic commercial advantage.
- The future work will validate corrosion inhibitors in a 5,000-hour test, increase anionic particle surface charge to match cationic at 500 µeq/g, and include compatibility and thermal degradation studies at temperatures exceeding 100°C. This project will perform long-term testing of final coolant formulation in three separate fuel cell systems.
- The future work focusing on 100°C testing is important; however, performance should be tested at higher voltages. Given that the fluid uses ionic nano-particles as its primary mechanism for controlling conductivity, it would be good to see how this fluid stands up to voltages around 100 V DC, which may be more common in automotive fuel cell power plants. It would also be good to see full-scale field testing, which is a more accurate determiner of actual fluid performance in the market than the limited lab-scale testing currently underway.

**Project strengths:**

- This project is very relevant to fuel cell operations
- The innovative use of nanoparticles for improved coolant is a strength.
- This project is sharply focused on the development of an improved coolant for fuel cell systems.
- This project has a novel approach that can provide modest improvements in fuel cell system cost and possibly durability.
- The company running this project is leveraging its experience with coolants for developing a fuel-cell-specific coolant. This work appears to benefit strongly from the experience of the company.

- This is a commercialization project, which is not a bad thing. Getting a reliable solution for durable coolants certainly has merit.

#### Project weaknesses:

- The long-term tests have not yet been completed.
- It is unclear how much collaboration with automotive OEMs has been performed in this project. Using these coolants with light and cheap non-metal materials may be key for automotive applications, but to date they are questionable at best.
- There is a lack of full-scale field testing of the fluid in relevant systems. Also, the presentation claims that the fluid can be non-toxic, but the health effects of many nano-particles are unknown and the claims of non-toxicity should be validated prior to being promulgated further.
- Some real technical questions remain with respect to colloid stability over time. The tests should be run under load as well. The effect of contaminants, such as di- and tri-valent ions, is unknown other than assuming that any corrosion of the metal plates would have delivered contaminating ions. This assumption may be true, but the purposeful addition of ions would have determined boundary limits since almost all colloids are ionic-strength sensitive.
- The necessary metrics for a good heat transfer fluid must include no plugging of the flow path within the radiator and no fouling of the heat exchanger (HEX) surfaces, especially by putting a thermal barrier on the HEX surface. The downside here is all about the wisdom of pumping the micro particles through the fuel cell stack. Small particles can agglomerate and it seems like this approach adds risk to achieving the reliability demanded by the targeted market. Certainly, fouling in a specific stack involves an interaction between that fluid and the stack components. This type of consideration appears to be missing.

#### Recommendations for additions/deletions to project scope:

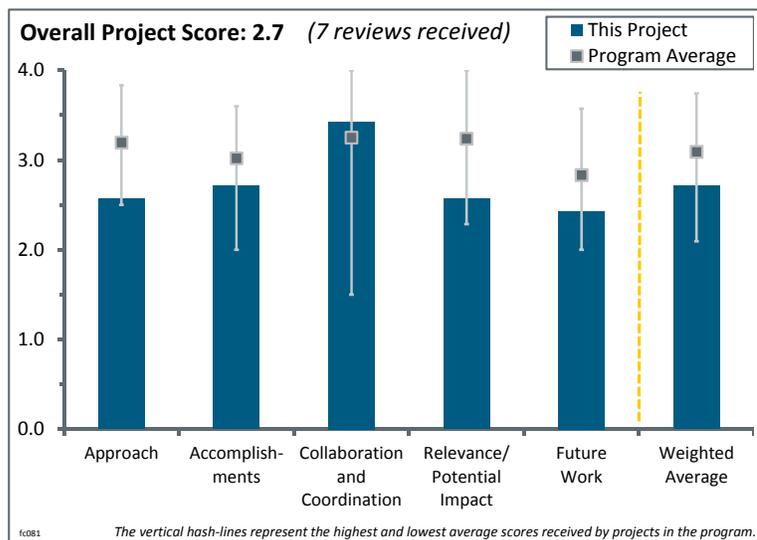
- Three reviewers commented that they had no recommendations as the project is ending.
- This project should continue to work to its conclusion. Temperature has a strong influence over the results.
- Future research should consider full-scale field testing at high voltages in a relevant system.
- The researchers should work to understand the effect of the coolants on structural plastics and other materials that may be used in automotive fuel cell systems.
- This project uses biofuels and glycols synthesized from a biological starting material. Although it is admirable to use these products, they add some uncertainty to the results. Biological products are derived from available feed stocks, and they tend to be variable. This approach is rather unlike using high-purity methane as a starting point for glycols derived from a chemical plant. It is certainly true that the two products are similar. Even so, there are two formulations in sight. There is the chemical glycol with additives and the bio glycol with additives. It makes sense to first test with a glycol formulation that has assured quality and then repeat the test with the new bio-sourced organics. Most likely the tests will give similar results. However, for now there can be some question. There should be some thought given to using a stationary “filter” sort of scavenger hardware, an ion exchange sort of device that remains outside of the stack. Certainly, if that were in-line with the principal flow, there would be a pressure drop. However, the entire heat transfer volume is being pumped around; therefore, all of it will be contacted by a well-placed, impurity-catching gadget. This gadget could be positioned in a side arm, a fraction of the total flow, or it could be placed in the reservoir tank. Such alternatives need to be considered. It is also important to test the concept on a stack designed for automotive applications. This hardware has extreme power density on a volume basis and necessarily has HEX components with small-gap heat exchanger flow paths. If things are going to plug up, these small slots will be the site for that precipitation. So, there will be a need to do coolant testing of prototypical hardware. Tests could be done on a “used” stack—one that is no longer making design voltage but has a complete thermal management system. This project should install an inline heater to heat the coolant and then pump that around for a few weeks. They should then address flows through each of the plates and show that no blockage occurred.

## Project # FC-081: Fuel Cell Technology Status – Voltage Degradation

Jennifer Kurtz; National Renewable Energy Laboratory

### Brief Summary of Project:

This independent assessment of state-of-the-art fuel cell technology benchmarks the fuel cell durability status using uniform analysis and reporting methods to evaluate proprietary data from leading fuel cell developers. Data from developers is collected annually, analyzed, and compiled into two products: detailed data products, which contain confidential material and are shared with each contributor individually, and composite data products, which list aggregated data without revealing any proprietary information and are shared with the public.



### Question 1: Approach to performing the work

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

- This project seems well organized, well managed, and successful.
- The project offers the fuel cell industry an excellent methodology to evaluate fuel cell stack durability, even at the prototype stages of development.
- The approach to obtaining and analyzing the data is very good; there are considerable efforts pursued to access data and report out on the analysis using a variety of metrics. The areas of concern are identified by the researchers, and an additional effort could look into ways to address these concerns.
- The National Renewable Energy Laboratory's (NREL's) approach in this project is very good and clear. This project is reaching out to as many fuel cell developers across the world as possible to gather real-world data. One objective, studying the difference between lab and field data, is of prime importance to know the readiness of fuel cell technology and challenges. NREL is using already established tools for this data compilation and analysis, which is useful for getting the most out of the funding provided.
- NREL's approach to evaluate the data they are given from developers is reasonable. There are so many unknowns about the data sets and they cover such broad ranges of protocols that the value of the compiled data is small. It would be good to see them focus on gleaning information about other targeted metrics, such as power density loss or quarter power efficiency loss, in addition to the time to 10% voltage loss at a fixed current. Also, the steady-state data for automotive systems is irrelevant.
- The project has been shown to be responsive to the objectives of benchmarking the available technology. However, some of the fundamental characteristics of the fuel cell systems involved are missing from the analysis. Some examples of these characteristics include precious metal loading, membrane thickness, measures to maintain membrane durability (additives, reinforcements, etc.), operating conditions, carbon type, system mitigation strategies, and other characteristics. In terms of providing the U.S. Department of Energy (DOE) with status information, the project appears to work best for providing durability information. However, even this data still leaves its audience with an incomplete feeling. It is not clear what systems have reports on durability and what technologies those numbers represent. The project does some good in showing that there is a sincere difference between laboratory and field data, but questions still remain as far as which technologies might provide the greatest disparities between the laboratory and the field and why.
- The overall approach of this project is flawed. As currently constituted, it is difficult to understand how this work contributes to the barrier of addressing the durability of fuel cell stacks and systems for several

reasons. First, it combines different types of fuel cells (polymer electrolyte membrane [PEMFC] and solid oxide fuel cells [SOFC]) into one homogenous set of data. It is unclear how one can identify the current state of the art when all of the different fuel cells are combined into the same pot. Second, the operating conditions in the lab are much different from those in the field. The lab conditions can be closely controlled while the field operations are not. For example, the effects air contaminants encountered in the field have on the performance of the fuel cells is unclear. The effects will be different for different operational environments. A forklift operating at the factory door where a tractor trailer truck may be idling and emitting sulfur diesel exhaust that is being ingested by the fuel cell will be different from the same brand of forklift operating inside the bowels of the warehouse. It is unclear if the project's results are getting better. There was nothing in the slides that offer any conclusions that the results are getting better over time. This work should identify what areas need to be addressed. The desire to keep the identity of the different fuel cell suppliers secret may be self-defeating when trying to understand the current state of the art. This information needs to be segmented by fuel cell type. The bottom line is that it is unclear what meaningful information is being identified in this project. It seems to be more of a modeling exercise rather than a search for specifics. Most (if not all) of the slides address modeling and not the outcomes. This effort is not useful.

### Question 2: Accomplishments and progress toward overall project and U.S. Department of Energy (DOE) goals

This project was rated **2.7** for its accomplishments and progress.

- The data is starting to provide a view of fuel cell durability for a number of applications.
- If one accepts this reviewer's premise that the basic approach is flawed, it would be impossible to make meaningful accomplishments and progress.
- The project's data handling and statistical analysis of expected durability provides an excellent model for adoption by the fuel cell industry.
- In some ways, this is a "reporter" sort of effort. The daily reports come in, records are made, and the results are distributed on the Internet. It does not cost very much to do and makes for interesting reading.
- Excellent progress has been made so far. NREL or the principal investigators (PIs) have reached out to fuel cell providers outside the United States, which is very important. Sixteen data sets were gathered last year; this is great progress. This project is very transparent with the results and presentations by publishing them on the website, while also protecting the intellectual property of various data providers very well.
- The main objective of this project is to benchmark state-of-the-art fuel cell durability. There is no way to know whether the technology being analyzed is, in fact, state of the art. The project also does not directly track progress towards DOE's durability goals, as protocols are not disclosed. For example, if data for cells/stacks run was analyzed using the DOE automotive durability cycle, it would be much more informative.
- Unfortunately, the presentation was constrained to reporting what data sets exist, as opposed to the meaning that could be extracted from the data sets. For the data to be more meaningful to developers, NREL will have to be more aggressive about having data contributors be more open about material sets, Pt loading, carbon types, membranes, operating conditions, system mitigation, flow-field designs, etc. The volume of data generated was impressive along with the 99 different data products that the analysis conceived. Despite the amount of data, the data still suffers from a lack of details about systems.

### Question 3: Collaboration and coordination with other institutions

This project was rated **3.4** for its collaboration and coordination.

- The project has worked hard to obtain data from numerous entities.
- NREL has received data from 15 developers; without their collaboration there would be no project.
- The entire effort is based on collaboration, which involves input from the global community. The project team obviously operates a trusted procedure in which results are given, but those who generated those results are not identified. Such collaboration requires a perfect record in keeping identities protected, and that is what NREL is doing.

- The project does not exist without collaboration. Just to have the data that the project has, collaborative relationships had to be established. Some question exists as to whether the collaborations were able to sufficiently leverage the relationships. Since many material sets, cell designs, and operating condition parameters were left unknown, there is some uncertainty about whether the investigators were able to understand as much about the stacks and systems as they should have.
- While many potential collaborators (fuel cell manufacturers) were invited, few have participated, which is somewhat understandable given the competitive and confidential nature of an emerging industry.
- There have been many companies contacted to try to get more data. While the 15 entities that have shared the data represent 98 data sets, this data set is still quite limited. It is unclear if there are cost-effective ways to get more companies involved, either through reassurances or by offering incentives.
- The fact that 68 developers were contacted and the project was able to gather data from 15 developers is commendable. As this data sharing is voluntary, it is very necessary to reach out to as many developers as possible and the PI and NREL have done an excellent job collaborating.

#### **Question 4: Relevance/potential impact on advancing progress toward DOE research, development, and demonstration (RD&D) goals**

This project was rated **2.6** for its relevance/potential impact.

- The fuel cell activities supported by DOE clearly have commercialization as the goal. This project maps a part of that success. It seems essential and certainly relevant.
- There is some relevance. The main value of the project is to report public status numbers and to illustrate to DOE how the lab data is often different from vehicle data. For developers specifically, the project is not relevant. Progress towards meeting the program goals would proceed with or without the project.
- This project provides the needed durability benchmark status and progress concerning the emerging commercial applications of the fuel cell industry. The “third-party” expertise and analysis provides the necessary credibility to substantiate manufacturer’s claims during the pre-commercial stages of introduction.
- It is very critical to know the readiness of the fuel cell technology and this project is helping a lot by collecting and comparing real-world or field data with lab data, which at times can be misleading to know the current real-world readiness of the technology. This information fits well and helps with DOE’s Hydrogen and Fuel Cell Program’s long-term goal.
- Fuel cell performance is going to be addressed by the individual fuel cell developers. The market competition is going to drive them to improve performance. DOE needs to analyze the data to see if there is some systemic issue common to all the developers that can be address at an overall programmatic level. The work done in this project does not do that.
- This project may provide some value for the developers who provide the individual data sets, assuming they do not have the capacity to do this analysis themselves, and help to assess the voltage degradation of their technologies. The compiled data is of limited value due to the unknowns and variations in the protocols, materials, and designs. Plus, this project only addresses voltage decay at high power. It may have more impact if it also addressed other failure modes, such as efficiency and power density loss.
- The data is highly relevant as it provides a view on the status of durability over a range of applications. This data is important for DOE to understand how the industry is progressing, and it is valuable for companies to benchmark themselves against others. However, some of the relevance may be lessened due to the inclusion of such a broad range of types of data (e.g., from accelerated to steady state and from short stack to system).

#### **Question 5: Proposed future work**

This project was rated **2.4** for its proposed future work.

- The future work proposed is to keep counting and reporting.
- The proposed future work is well thought-out and fills the gaps in current analysis. The system-level voltage degradation data for automotive seems to be minimal or missing. If NREL could get this information from original equipment manufacturers, it would really help with understanding the real-world

challenges. The proposed price information addition and other aging parameters for fuel cell durability would be great.

- The future plans, such as compiling results by test protocols and by current density (especially low-current density), are good ideas. Investigating start/stop and soak time is also a good idea. The plan to add price information may be valuable, but it is unclear how NREL will get and verify such information from its data providers.
- This project needs to be fundamentally redesigned to get meaningful results that will support systemic changes that can be supported by the fuel cells program. If this cannot be done, then the project should be discontinued.
- The project's proposed work effort seems to be too broad. Focus should remain on stacks and not expand to single cells. The benchmark data for PEMs, SOFCs, and direct methanol fuel cells (DMFCs) would be useful to the industry for "comparisons," but it may be difficult to get the interest of enough suppliers of SOFC and DMFC stacks to provide data.
- The future work as outlined is reasonable. However, the highest needs should be to 1) increase the number of data sets and 2) increase the comparability of the data. For example, including single-cell data will help the former, but at the expense of the latter. More effort should be put into adding additional companies so they can contribute data and add additional requested parameters to better compare data.
- The future work must attempt to convince developers to provide information about the characteristics of their systems. Without this information, there is little quality information that will come from the project to advance the Program toward its goals. In fact, without further information about system or stack characteristics, the project may serve to misinform the public or government officials in either a negative or positive light about the progress of fuel cell technology.

#### Project strengths:

- NREL has outstanding analysis capabilities and access to a wide variety of durability data.
- The project's ability to analyze data and validate durability is excellent. This capability may develop into a "service" for those manufacturers unable to perform these evaluations in-house.
- This project has a strong team and a clear approach. The use of already developed NREL tools for the data compilation and analysis is a strength.
- This project has confidential data input and industry-relevant output, a non-biased view of achieved durability by application, and extensive data analysis.
- The NREL team is doing a good job and the strength is there. It is also apparent that this is a unique effort, and many people are reading the results. However, the NREL team is the core strength.
- This project has a vast array of collaboration. The information gathered has been treated with considerable analytical prowess. The project has been a public source for fuel cell durability information.

#### Project weaknesses:

- This project's lack of shared details of data sets makes the compiled analysis of little value.
- This is not a weakness but a limitation as only data is shared by the developers and not the material information or other details on understanding the mechanisms of degradation.
- The project needs some way of obtaining a material set and an operating condition and cell design context for all of its data products. The project is dependent, by definition, on information generated by others.
- The work is very important, but this reviewer is concerned that the confounding factors seriously impact the quality of the data set. It is understood that the data is what they get and they cannot influence that. It should be considered whether there is a way to adjust data for better comparisons.
- This is a flawed approach. This project is homogenizing the fuel cell performance of many types of fuel cells including large stacks, short stacks, SOFC, and PEMs with no attempt to analyze the data to determine what research and development needs to be done on a systemic basis.
- This is not necessarily a weakness, but more of a barrier to success: the extensive data requirements and confidential nature of the industry protects the material and system-design information and durability performance. Manufacturers will assume the responsibility to provide performance warranties and the expanding fuel cell applications will make comparisons (as currently done) more difficult. As mentioned during the review, "too many bins" (unique applications) will eventually dilute the comparison data.

- The information gathered, as in almost all reporting, is only as credible as the source. There are many reasons for distorting history. Bad data could be changed to “look good.” There could be outstanding data, but it is undesirable to alert the competition before the project is ready and those numbers might be obscured. The data set is, in truth, very small, so credibility is an issue. The error bars tell the story, perhaps.

#### **Recommendations for additions/deletions to project scope:**

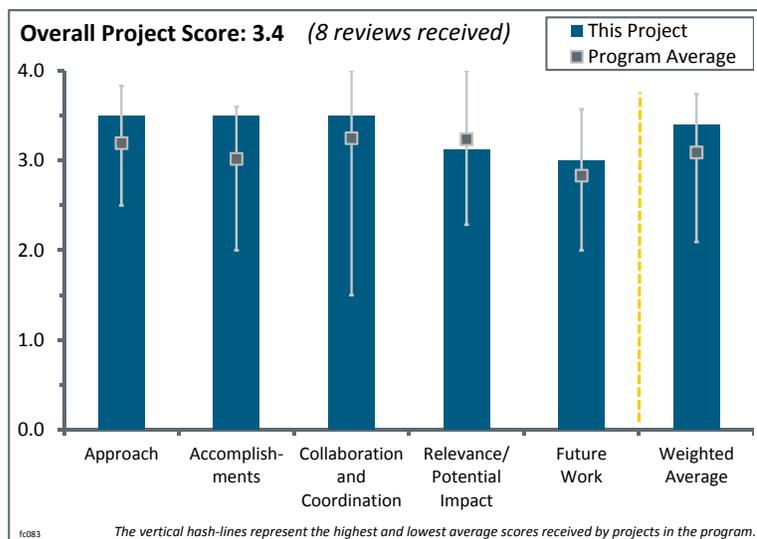
- This project needs to get background information on the stacks and systems it has analyzed.
- The investigators should totally overhaul this project to get meaningful results that address the barriers. If that cannot be accomplished, then the project is of little value.
- The project team should explore how a “service” might be provided to the industry, similar to what is done by others (e.g., Oak Ridge National Laboratory with clients for “characterizations of fuel cell materials”). This project should develop examples and publish protocols for the industry, including the relationship of voltage degradation as a function of operating parameters, etc., which is one of the items in the list of future work.
- This project should not include any steady-state data sets in the compiled automotive data; it should track the time to 10% quarter power efficiency loss and to 10% peak power density loss. This project should separate data sets with and without voltage recovery procedures and do a separate analysis for tests runs with the Fuel Cell Technical Team’s recommended durability protocol. For automotive data sets, this project should run an analysis at maximum current points that meet the Q/ΔT requirement.
- It would make sense to have some large-scale durability tests conducted under DOE sponsorship and then have NREL include numbers derived from actual, well-defined hardware. That is, incorporate some data that is verified and serves as the “reference,” perhaps several in each application class. There is no question that good data is verified data. It would also be interesting to collect some details about operational conditions, such as duty cycles, average current density, and operating temperature. This suggestion may not be possible, but it might make sense to try.
- Some data could be adjusted to account for various effects (e.g., model effects of current density on voltage degradation) and then use that to adjust the data. This project should then show data as both collected and adjusted data. The inclusion of the accelerated testing is of significant concern. Many accelerated tests are designed to fail within a few hundred hours or less. It is not clear how much acceleration is included. Following are some possible approaches : (a) when collecting accelerated data, the project should also request an acceleration factor and adjust the data accordingly, possibly with a large error bar; (b) the project should gather information on stressors and cycle times used in the accelerated data in order to adjust the data using known factors, although this would likely be more difficult in terms of data gathering. The inclusion of steady-state data is also a concern on the opposite end of the spectrum, but it at least shows the product capability given benign operating conditions.

## Project # FC-083: Enlarging Potential National Penetration for Stationary Fuel Cells through System Design Optimization

Chris Ainscough; National Renewable Energy Laboratory

### Brief Summary of Project:

The objective of this project is to build an open-source tool that helps combined heat and power (CHP) fuel cell developers, end users, and other stakeholders determine the appropriate sizing to reduce cost; integrate commercial building control and heating, ventilation, and air-conditioning (HVAC) systems to maximize durability; compare performance relative to incumbent technologies; determine optimum system configuration; and evaluate potential market penetration. These activities will help drive economies of scale and cost reduction in full-scale systems.



### Question 1: Approach to performing the work

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

- The approach to the model formulation in this project is excellent.
- To build a flexible, modular software framework that allows the addition of a wide variety of modules is a good approach. The cost and durability challenges are addressed.
- The approach taken in this project appears sound. It leverages existing models and information, works with organizations to access valuable databases and to improve those databases, works with original equipment manufacturers (OEMs), validates the model with existing data, and has a go/no-go step.
- This project incrementally improves upon the work done under previous years, which strengthens the confidence in this project. It directly targets the cost barrier by utilizing open source to allow multiple different users and suppliers to have some idea of the bottom line prior to initiating and allocating funding.
- The project has a solid, realistic, and unbiased approach. It exploits and analyzes a huge data volume and, thus, gets very good results. Analyzing 16 model buildings (even considering their vintages) and 16 climate zones is impressive and provides valuable local data. A web-based tool was realized and is helping local decision makers see if fuel cells will be of benefit. Guidance by a user group strengthens the project.
- The approach is solid and comprehensive. It is detailed enough to work as a planning tool, but lacks thorough benchmarking with competing technologies outside of the CHP sector (e.g., comparison to or in combination with heat pumps and better insulation).
- This project is well-focused on three critical barriers: cost, durability, and performance relative to the incumbent. In the presentation, the researchers make it clear how both of these barriers relate to DOE goals and how the research specifically addresses these barriers. While the approach addresses these barriers, the late and still somewhat limited outreach and coordination with other efforts raises a question about whether and how this work could be more effective.
- The project has included a very comprehensive survey of energy usage in buildings. This inclusion makes the study very realistic and relevant. The idea of the user group is pertinent. However, assuming a constant cost for fuel cell systems over a wide range of rating (100 kW–3 MW) may not be valid. The model is not flexible enough to incorporate technical aspects of individual developers: some can load follow better than others, some cannot load follow, etc.

**Question 2: Accomplishments and progress toward overall project and U.S. Department of Energy (DOE) goals**

This project was rated **3.5** for its accomplishments and progress.

- Progress so far has been very good.
- Excellent progress has been made on model development. There should be more comparisons of the model to real-world operational stationary fuel cell systems.
- The progress within the scope described is very good for its comprehensiveness, detailed character, and applicability.
- The progress of the project and the additional measures taken to make the results even better are worthwhile. The interaction with other projects, particularly regarding cost, is very good.
- There has been good progress on the model and a significant database on data across the country and for many building types, as well as the addition of new control cases.
- This project currently has models for 400 kW phosphoric acid fuel cells (PAFC), 300 kW molten carbonate fuel cells, and the natural gas genset (as a control). It is developing models for polymer electric membranes (PEM) at 1, 5, 25, and 100 kW and for solid oxide fuel cells (SOFC). The movement toward cloud and open source computing is a good direction.
- This provides an excellent reference to past reviewers' comments that have strengthened the program and directly impacted the progress made this funding period. Getting Commercial Buildings Energy Consumption Survey (CBECS) inclusion for industry feedback was a critical success and should help validate model assumptions made thus far. Updating the model to include 15-minute increments that allow for thermal storage requirements is a great step. The means used to predict the storage and power needs of the system for the next day in order to reduce the thermal cycling of the fuel cell are interesting. It is unclear if there are predictive patterns or a connection to the National Weather Service.
- The researchers have made significant progress toward the project's objectives and have addressed most of their stated barriers. In particular, the effort to integrate with commercial building controls and HVAC systems to maximize durability could benefit from added efforts to reach outside of the National Renewable Energy Laboratory (NREL) and make use of resources at other national laboratories, such as Lawrence Berkeley National Laboratory (LBNL) and Oak Ridge National Laboratory, and the emerging resources from the DOE Buildings Innovation Hub. Making use of these broader resources will provide the researchers with more opportunities for evaluating the reliability and overall performance of their scenario analysis.

**Question 3: Collaboration and coordination with other institutions**

This project was rated **3.5** for its collaboration and coordination.

- The industry involvement has been broadened. The open source collaboration is an excellent tool.
- This project has very good collaboration with its project partners. User groups need to be expanded and members need to provide feedback on the model's usefulness.
- The "consortium" is big enough to cover all topics and small enough to be efficient. The introduction of a user group adds value and the collaboration with other projects is well performed.
- This project leverages other DOE-funded work and the establishment of a user group is valuable. This project has a good collaboration with the University of California, Irvine (UCI). However, it is not clear how committed the user group is to the project or the amount and quality of the feedback that they will provide.
- Although there has been an effort to expand collaboration relative to last year's review, this area still needs some improvement. The presentation identified collaborations, but it did not provide clear evidence of whether and how these collaborations have benefited the approach and outcomes.
- Some important stationary fuel cell manufacturers are absent from the collaborations (e.g., Bloom Energy). It does not seem that there are very many commercial building organizations associated with the user group.
- This project has good collaborations with NREL's Electricity, Resources, and Building Systems Integration Center; UCI, which is subcontracted for controls and integration work; LBNL, which has a tie-in with a

separate DOE project (FC098) for manufacturing cost analyses; Strategic Analysis, Inc.; and Battelle. Stationary fuel cell OEMs are providing product data sheets and supporting information.

- This project is leveraging separately funded projects from DOE that have the information needed in this program to provide a much more efficient program and reduce duplicative work and wasted funding; this project makes good use in this area. Forming a user group is a critical step toward validating that the model is able to be customized for proprietary inputs and still provide useful data. A user group is an excellent use of collaboration since both this project and the user can benefit greatly once validation and refinement occur.

#### Question 4: Relevance/potential impact on advancing progress toward DOE research, development, and demonstration (RD&D) goals

This project was rated **3.1** for its relevance/potential impact.

- The analysis is important. It can have a high impact on implementation since it provides guidance for planning and might also be used to enhance the confidence of investors in stationary fuel cell systems.
- The project addresses some of the program's goals and objectives. However, the project does not address the critical issues of meeting the cost and reliability targets, as these issues are not within the project's scope.
- The project has a strong impact due to the many different cases investigated and thus provides valuable data for decision makers with regard to new buildings or even retrofitting old ones.
- The goals of this project are aligned well with the DOE Hydrogen and Fuel Cells Program (the Program), but the researchers seem to be working in isolation and have not planned ways to test and evaluate model performance through interactions with other researchers, other similar models, and a broader number of data sets.
- This project covers two major potential impact areas: (1) users, who by inputting grid information and building type, can see what type of fuel cell set-up is best for their application and get controls, HVAC, and cost analysis, and (2) developers, who can see how many users could be impacted prior to making investment decisions and committing funds. This is a versatile tool that can impact both sides of the technology used and can help avoid wasting funds.
- This project supports CHP application implementation by providing an analysis tool for fuel cell CHP developers. This analysis is currently a strong barrier for fuel cell developers, requiring access to data they might not be able to source and significant analysis time. This tool should enable a strong understanding of value propositions for fuel cells as a function of geographic location and use type.
- Stationary fuel cell manufacturers already consider the factors that the model summarizes into their business plans. They have relatively little need for a global model that evaluates their potential market penetration. The primary users of this model are companies that are trying to decide if fuel cell stationary power systems make sense for their organization. It is not clear what steps are being taken to "sell" this modeling activity to the user group. There is a need for such an evaluation model for business users who are seeking to determine if stationary fuel cell power makes sense for their commercial buildings.
- This project is highly relevant to deployment success. The tool is relevant and will be used to minimize lifecycle costs, lifetime greenhouse gas (GHG) emissions, or installed capital costs of fuel cell installations; characterize the largest segments of the U.S. building inventory for use in the tool, leveraging the CBECS; characterize building control systems and include in the tool, advanced control strategies for integrating fuel cell systems, and building control systems; validate the model outputs against real-world data from stationary fuel cell installations; and use the tool to determine the set of the most favorable system sizes and types to achieve national GHG emissions and energy-demand reductions.

#### Question 5: Proposed future work

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

- This project has a clear scope of future work.
- This project has continuity between existing progress and future goals in most aspects.
- The proposed future work items are sound. Benchmarking to systems other than CHP are recommended.

- The proposed future work is straightforward with meaningful objectives. A decision for continuation should be taken.
- There is an upcoming go/no-go decision point on this project. The project seeks to develop participation in the user group.
- The future work was not discussed as it is contingent upon a go/no-go decision. The future work should include addressing other goals described in slide 3.
- While the investigators have included a validation step for the model, it is not clear how extensive this validation will be. They have not outlined risks associated with this validation. The inclusion of high-temperature PEM would be useful.
- In reference to Verizon, it is unclear if this project can utilize data from installed systems to validate the model as part of future work. As Europe and Japan have been in the CHP game for a long time, this program should set up models of European buildings, utilities, and rates to help validate the model's concepts on actual ongoing CHP systems.

#### **Project strengths:**

- The modeling approach is comprehensive.
- This project has excellent collaboration and has created a user group.
- This project addresses issues that are important for the Program and includes visualization methods for viewing model outputs.
- The major strength is the detailed and comprehensive character of the project. It has the potential to be used as a realistic planning tool.
- The development of an open source tool that is applicable to multiple fuel cell developers is a strength of this project. This project also considers realistic and comprehensive data for electricity usage in distributed generation.
- This project should result in a valuable tool to model the applicability of fuel cell CHP systems for various building types around the country. A validated model will provide an essential tool for fuel cell developers. The use of a user group to validate the model is good. The incorporation and leveraging of significant data sources that may not be available to fuel cell developers provides a strong data set for the model and a significant advantage for use by fuel cell developers.

#### **Project weaknesses:**

- This project needs to strengthen the user group's participation.
- With CHP programs ongoing around the world, this project could validate these models and present the data.
- A small fraction of fuel cell developers have joined the user group. The project does not consider the customers' input. It is not clear what the requirements of the customer are besides cost.
- It is not clear how much validation will occur. Go/no-go criteria were not defined and success depends on use by fuel cell developers. Since the users are not an integral part of the project, there may only be limited evaluation.
- The researchers seem to be working in isolation and have not planned ways to test and evaluate model performance through interactions with other researchers, other similar models, and a broader number of data sets.
- The restriction to CHP is the major issue. It is understood that benchmarking to other competing technologies cannot be done as comprehensively as the CHP analysis. Nonetheless, for certain cases, it should be included to avoid working with a sub-optimum model. Such an analysis should yield a feeling for when alternative technologies have to be considered and analyzed in detail. This analysis is required for the model's use as a comprehensive planning tool and, moreover, to win over potential investors.

#### **Recommendations for additions/deletions to project scope:**

- This project should add users with committed roles, as opposed to a voluntary user group.
- This project should build in more capacity for model performance evaluation.
- This project should consider the relatively higher costs for smaller (e.g., <100 kW) fuel cell systems.

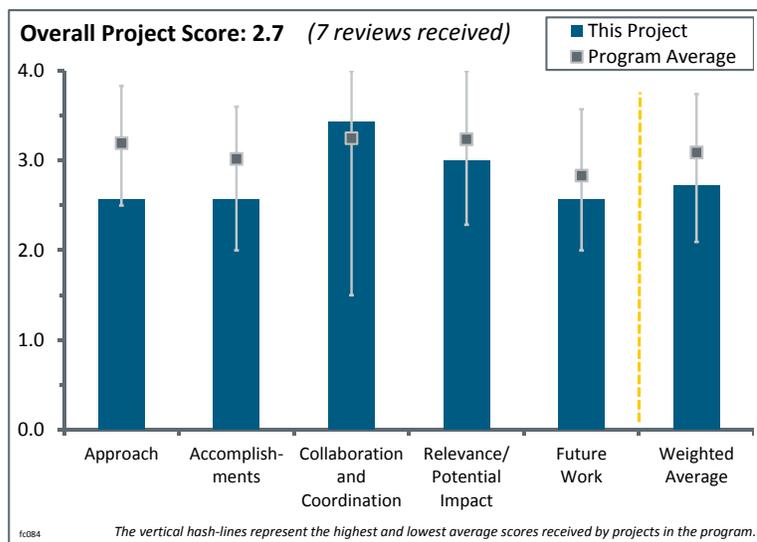
- DOE is funding a cost analysis for large-volume manufactures of automotive PEM stacks. It seems worthwhile to check if there could be synergy with this effort. Looking at different fuel cell technologies (e.g., PAFC, high-temperature PEM, and SOFC) may be difficult, but would be interesting.
- This project should continue the work. It needs to continue working very closely with marketers in fuel cell companies. User groups are very important and the project needs to provide some value for them. Fuel cell operators and building managers may not have the capability in-house.

## Project # FC-084: WO<sub>3</sub> and HPA-Based Systems for Durable Platinum Catalysts in PEMFC Cathodes

John Turner; National Renewable Energy Laboratory

### Brief Summary of Project:

The objective of this project is to improve electrocatalyst and membrane electrode assembly (MEA) durability and activity through the use of Pt/WO<sub>3</sub> and heteropoly acid (HPA) modification of carbon support to approach automotive proton exchange membrane fuel cell activity and durability targets. Enhanced platinum (Pt) anchoring to the support is expected to suppress losses in Pt electrochemical surface area under load cycling operations and to increase electrocatalytic activity. Lowering corrosion of support materials will increase durability under automotive startup/shutdown operation and suppress Pt agglomeration and electrode degradation. Ultimately, improvements to the electrocatalyst durability and performance will simplify the fuel cell system and lower system costs.



### Question 1: Approach to performing the work

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

- This project demonstrates the performance in working devices.
- As WO<sub>x</sub> has been unsuccessful and SnO<sub>2</sub> becomes the current focus, this project seems to rely on trial-and-error.
- The principal investigator and his team are sharply focused on critical U.S. Department of Energy (DOE) goals and barriers and are pursuing sensible, but creative, approaches to their work.
- The stated objective is to use Pt/WO<sub>3</sub> and HPA to achieve performance and durability targets. There is no hypothesis as to why this would work and no attempt has been made to combine them. WO<sub>3</sub> and HPA were just ideas that might work. In fact, WO<sub>3</sub> has been tried before and found to have issues.
- This project is working to develop more durable catalysts with a two-pronged approach: using WO<sub>3</sub> as the support and synthesizing catalysts using HPA. Neither of these approaches seems to be aimed at increasing the mass activity of the Pt, which is required to meet DOE's targets. The use of advanced characterization techniques, such as EXAFS is good to provide basic information.
- The approach is quite standard and based on the experimental screening of promising materials. WO<sub>3</sub> was dismissed earlier this year (2013) as an option, given the poor performance. The program approach should have been crafted to reach this conclusion in a much faster time frame than three years. This way, the program partners would have had more time to explore and work the other options (e.g., HPA).
- The goal of using a non-carbon support to get around the degradation of traditional carbon supports under start-up/shut-down operations and at high voltages is to be lauded. There is much potential for scientific return in this approach, especially if the team continues the search for oxides and compounds with better conductivity. There are numerous paths to explore, but non-stoichiometric WO<sub>x</sub> and SnO<sub>2-x</sub> are marginal pathways. The use of atomic layer deposition (ALD) processing to obtain conformal Pt coatings at low loadings is also commendable. Given that ALD processing is still in its infancy, compared to wet-chemistry or sputter-coating techniques, there is much to be learned from this project. ALD processing shows the promise of cost-effective scaling to large volumes.

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**Question 2: Accomplishments and progress toward overall project and U.S. Department of Energy (DOE) goals**

This project was rated **2.6** for its accomplishments and progress.

- The materials show improved durability, but low mass activity.
- The team made good progress towards its objectives. The return of knowledge was worth the effort, even if DOE's performance metrics were not achieved.
- The work on  $\text{WO}_3$  could have been accelerated to achieve the go/no-go decision earlier in the program. The progress on HPA seems encouraging.
- Refocusing on Pt/SnO<sub>2</sub> and Pt/C-HPA is a good move that yielded promising results for durable catalysts with improved activity.
- SiW<sub>11</sub> does not seem like a hetero poly acid (figure 3 slide 8), as some O<sub>2</sub> is missing. All the efforts in  $\text{WO}_3$  did not produce any benefit, as shown in the literature. The HPA work did show some promise, at least in durability. The Pt/SnO<sub>2</sub> is just a distraction; the project should focus better. SnO<sub>2</sub> is only conducting in a reducing environment and will not survive startup and shutdown transients.
- This project synthesized, characterized, and measured the performance of a number of materials based on the  $\text{WO}_x$  support. Mass activity measurements indicate that these are not competitive with traditional Pt/C catalysts, let alone more advanced alloyed (or dealloyed) catalysts. The Pt/C-HPA results indicated that some improvement of durability to the accelerated stress test cycling protocols is achieved; however, no initial increase to the mass activity is made, thus the modifications do not help the catalysts make the activity targets.
- The work on HPA-modified carbon appears promising and is being pursued in a sensible way that will yield actionable results and reveal the positive attributes of this approach to improve durability. The team has worked very hard on the other system involving  $\text{WO}_3$  and Pt and has been careful and thoughtful in their approach. Even though that system ultimately did not make the milestone needed for the go/no-go decision due to insufficient support conductivity, the team is commended for their approach to the work.

**Question 3: Collaboration and coordination with other institutions**

This project was rated **3.4** for its collaboration and coordination.

- The project appears to be very well coordinated with the partners.
- The collaboration on this project was well organized.
- This project has good, productive collaborations with industry, national laboratories, and universities. However, the role of the University of Colorado-Boulder (CU Boulder) is not clear when  $\text{WO}_x$  is no longer included.
- The collaboration between CU Boulder and the Colorado School of Mines (CSM) is clearly evident with the materials being produced and transferred to the National Renewable Energy Laboratory.
- It is good to see catalyst suppliers involved, represented by the Tanaka Kikinzoku Kyogo Group (TKK). Andy Herring (at CSM) knows what he is doing with HPAs. It is early yet for scale-up and commercialization.
- There is clear collaboration among the partners. However, it is not clear if collaboration with TKK (and the use in this program of a commercially available catalyst) is relevant to accomplishing the objectives of the program.
- The collaborations appear excellent on both materials and characterization fronts. The team will soon be moving forward on MEA fabrication and testing, and they are encouraged to take advantage of the many resources available in DOE for making and characterizing MEAs, including both performance and microscopy.

**Question 4: Relevance/potential impact on advancing progress toward DOE research, development, and demonstration (RD&D) goals**

This project was rated **3.0** for its relevance/potential impact.

- This is a relatively low-cost approach to improving the effectiveness of Pt catalysts.
- The durability of catalyst supports is currently a critical path item. Sadly, progress here was limited due to distractions from what actually worked.
- This project is working to stabilize catalyst activity from degradation mechanisms. This work should be expanded to increase the mass activity of catalysts so that they meet the DOE mass activity targets.
- The corrosion of catalyst supports and loss of Pt ECSA are very important problems; the project's work is highly relevant to solving problems in these areas.
- It is ideal to have a corrosion-resistant support for catalysts; however, its cost needs to be justified because there is a way to mitigate carbon support corrosion at the system level.
- The goals for this project are well aligned with the Hydrogen and Fuel Cells Program's RD&D objectives; however, the team has not fully addressed how the cost benefits will be obtained solely from using more durable support.
- The pursuit of novel catalytic structures to address durability, cost, and performances is definitely in line with DOE's goals. However, these new structures are far from being at the maturity level needed to turn them into commercially available products. Alternative work, focused on the optimization of the catalyst layer for existing carbon-supported Pt, has been proven to be effective to approach DOE's targets. In particular, the optimization of the water management in the catalyst layer is a big opportunity to accelerate the achievement of the goals.

**Question 5: Proposed future work**

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

- The work plan is excellent and will help achieve project goals.
- The proposed future work is feasible with a focus on Pt/SnO<sub>2</sub> and Pt/C-HPA.
- The focus should be on HPA and the project should forget everything else. It should take HPA to subscale testing.
- The proposed preparation and characterization of MEAs is sensible. The team probably needs some new ideas on other areas to pursue. Some work aimed at revealing mechanisms by which HPAs improve performance will be helpful.
- The future work does not appear to continue with the Pt/WO<sub>x</sub> materials and to date there is no data to support that this work is promising. Moving the Pt/C-HPA to a graphitized carbon will probably provide more positive results. However, the value of the HPA is questionable, as the HPA has not improved activity to date and it is already clear that the graphitized carbon is more stable than carbon black.
- The program will sensibly focus on testing the most promising configurations (HPA and Pt/SnO<sub>2</sub>). The value of testing the Pt/SnO<sub>2</sub> is not fully understood. Given that it is a commercial catalyst, the majority of work should be aimed at assessing performance of HPA, which has been the main output of the program up to now.
- The plans build on past progress, with logical down-selects chosen. However, the project ends in April 2014 and the use of carbon-stabilized HPA phases or sub-stoichiometric tin oxide needs to be supported by additional materials development beyond stating that the team will explore wet chemistry Pt deposition of alternative support carbides, etc.

**Project strengths:**

- The right experts are involved with HPA.
- There is lots of collaboration with strong academic and industrial partners.
- This project has a strong team, particularly on electrochemical characterization.
- The use of lower cost materials with improved corrosion resistance is a strength of this project.
- This project has done good fundamental work on a promising system combining HPAs with Pt on C.

**Project weaknesses:**

- Low mass activity.
- There is no desire to narrow down to a conclusion.
- There is limited value in short- and medium-term plans for fuel cell commercialization.
- With work on  $\text{WO}_3$  a no-go, the project is relatively narrow. Some new initiatives are probably needed.
- This project really only concentrates on improving the durability of catalysts, not improving the mass activity, and the mass activity of the catalysts are low compared to standard benchmarks. The durability improvements are mostly only marginal.
- This project lacks the theoretical analysis to help the development of corrosion resistive support. For example, the impact of electronic conductivity on catalyst activity should have been predicted by a mathematical model that considers electron conduction.

**Recommendations for additions/deletions to project scope:**

- As  $\text{WO}_x$  has been excluded from future work, this project should include a theoretical analysis to explain why  $\text{WO}_x$  is not as good as  $\text{SnO}_2$  as a catalyst support.
- The future work should address the question of whether the HPA modification of carbon helps to prevent carbon corrosion and/or Pt sintering. Also, the project should consider the proposed idea of combining  $\text{RuO}_2$  with  $\text{WO}_3$ .
- There should be a focus on the HPA work and a drive to demonstrate its value for improved durability in subscale fuel cells. This project should engage TKK to scale up this catalyst to allow some original equipment manufacturer (OEM) testing. This project should find an OEM willing to evaluate it in the short stacks.
- It looks like the work with Pt/ $\text{WO}_x$  should be discontinued; it is hard to see any benefit. The project has not really examined the detrimental aspects of the electronic conductivity yet, which is about eight orders of magnitude lower than carbon. This project needs to look at the stability of the Pt/ $\text{SnO}_2$  in terms of this and past work. These Pt/Sn materials were explored about a decade ago by the Phil Ross group with the conclusion that the activity was not stable. ALD does not seem to be amenable to cost or to make materials with high catalytic activity; this does not seem worth pursuing. More data on the activity of colloidal Pt/C-HPA and how it relates to the benchmark of Pt/C in rotating disk electrodes and DOE activity targets would be beneficial to understand the value of these materials and if modifications can be made to increase the mass activity.

## Project # FC-085: Synthesis and Characterization of Mixed-Conducting Corrosion Resistant Oxide Supports

Vijay Ramani; Illinois Institute of Technology

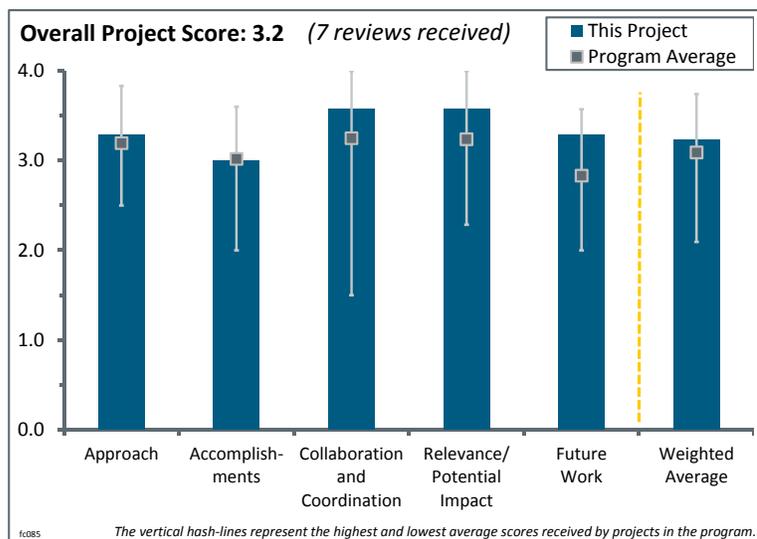
### Brief Summary of Project:

Research objectives in this project are to (1) develop and optimize non-carbon mixed-conducting materials with high corrosion resistance, high surface area, and high proton and electron conductivity; and (2) concomitantly facilitate the lowering of ionomer loading in the electrode for enhanced performance and durability by virtue of surface proton conductivity of the electrocatalyst support and reduced ruthenium (Ru) content in support materials. This project also will develop a cost model for the optimized support materials.

### Question 1: Approach to performing the work

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

- Exploring mixed conducting oxides as an alternative to conventional carbon supports is a sound idea. In terms of stability, the materials examined are clearly superior to carbon. The RuO<sub>2</sub>-TiO<sub>2</sub> system looks promising, but the non-platinum group metal supports, such as indium-tin-oxide (ITO), are even more interesting and worthy of greater attention.
- This project has some very interesting approaches and has rightfully narrowed work to the most promising the RuO<sub>2</sub> supports. However, divergence from U.S. Department of Energy's (DOE's) and U.S. DRIVE Partnership's automotive cycling protocols is not good at all. It is fine if the Illinois Institute of Technology (IIT) team thinks it has found a better way, but it is essential to do the standard test for comparison.
- This project should use DOE protocols for catalyst cycling (0.6 V–1 V at 50 mV/second). The reason these exist is to make sure you can compare material sets being developed by various projects. There is nothing wrong with doing the more severe carbon corrosion test; in fact, the U.S. DRIVE Fuel Cell Tech Team has already adopted this accelerated stress test. The Nissan Technical Center North America (NTCNA) wants to run their own protocols, but it will be useful to DOE to have the same materials evaluated under DOE's protocol. The summary slide included this information, "< 30 mV electrocatalyst support loss after 100 hrs at 1.2 mV"; it should have said, "< 30 mV electrocatalyst support loss after 400 hrs at 1.2 V."
- The support materials chosen are directed towards a more durable support. SiO<sub>2</sub> is more durable than carbon black, as are most oxides. The key component is RuO<sub>2</sub>, which is deposited on the SiO<sub>2</sub> to provide electronic conductivity and the ability to deposit small particles of Pt on the modified support. It is unclear if Ru will dissolve and move into the membrane or anode of a membrane electrode assembly (MEA) in a fuel cell. It is also unclear if RuO<sub>2</sub> also provides a protonic conduction and if the ionomer can be eliminated. These questions should have been answered by the third year. Ex-situ measurements on electronic and ionic conductivity of RuO<sub>2</sub> have not been reported.
- The approach addresses the key obstacles in improving and demonstrating support durability and includes testing under relevant conditions. The much higher density of the mixed metal-oxide (MMO) supports compared to carbon suggests that the Pt loadings should be adjusted to lower Pt loadings to achieve comparable volumetric loadings for Pt/C. Assuming a 50-50 RuO<sub>2</sub>-TiO<sub>2</sub> ratio, the Pt loadings should be reduced by a factor of two to three for RuO<sub>2</sub>-TiO<sub>2</sub> compared to Pt/C (i.e., should be 13%–20% Pt on RuO<sub>2</sub>-TiO<sub>2</sub> to compare to 40% Pt on carbon). In<sub>2</sub>O<sub>3</sub> has an even higher density, so Pt loadings should be reduced even further for the ITO support. The different electrical and proton conductivities in the MMO supports



may lead to different optimized Pt loadings, but it would seem that starting at the same volumetric loading (rather than mass ratio) would be a good starting point. It is not clear if the Pt loadings used were at 40% because the loadings on carbon are also 40%, or if they were optimized based on electronic and protonic conductivity considerations. Water management in the catalyst layer can have a large impact on performance. The project has not yet looked at the effects of changing the catalyst layer structure (removing ionomer, changing hydrophobic C to hydrophilic oxides) on water management. Tests should be done under conditions where flooding may occur to see if water management issues arise from changing the support material to a less hydrophobic material.

- The overall approach is to develop alternatives to carbon supports in order to mitigate the corrosion problem. This approach is particularly important from the perspective of start-stop operation, lower humidity operation, and conditions that could cause cell reversal, such as fuel starvation, etc. The approach, therefore, is based on developing metal oxide support materials to replace carbon. These metal oxides, besides providing for a more corrosion-resistant support, also provide for greater wettability and proton transport (under dry operating conditions). The attempt to use metal oxide supports to replace carbon is not new and, therefore, not terribly innovative. The choice of materials proposed and followed through in this effort is interesting. Particularly interesting are those that are well known to form underpotential deposition and even bulk deposition within the operating window of fuel cell operation. These include Ru and tin oxides. Both have the potential for dissolution at higher electrical potentials, and their ability to re-deposit on Pt may have debilitating consequences on oxygen reduction reaction (ORR) activity. In addition, any migration to the anode would be even more devastating as they form bulk depositions below 0.3 V versus RHE. It is interesting to note that these MMOs (some with SiO<sub>2</sub>) are stable when cycled at high potentials.
- This project demonstrates a good knowledge of what properties a non-carbon support requires to yield improved durability electrocatalysts for fuel cell applications while at the same time being compatible with catalyst and MEA preparation. The integration with an original equipment manufacturer (OEM) partner is apparent and at an appropriate level. With their partner, the project has adopted an accelerated testing procedure to probe rates of corrosion. The project has adopted a laudable “fail fast and move on” approach that enables testing a much wider array of materials that may have promise. Perhaps an improvement in their approach would be to do less “front end” characterization of surface areas and crystallite sizes via X-ray diffraction and more materials testing, saving the more detailed characterization for materials that offer demonstrated advantages, or doing post mortems of materials that have unanticipated poor corrosion properties. Sometimes focusing on outliers at both ends of the spectrum can reap rewards to faster rates of progress. While keeping an eye on materials cost is a good thing, one may not want to narrow ones view too early at the expense of developing the learning and knowledge of what structures and compositions lead to the desired properties. In terms of the community and their fixation on surface area, one might want to consider not the surface area/mass, but rather the surface area/volume. It is the surface area contained within the reactor volume that is relevant in most cases. In the case of the MEA, it is the MEA that is the “reactor,” and so it is the surface area available in the volume of the support in the catalyst layer that is important, not the number of grams of support in the catalyst layer. Thus, one might want to consider normalizing surface areas per unit mass to surface areas per unit volume by multiplying by the density of the material. Otherwise, one is comparing mostly apples to mostly oranges.

## Question 2: Accomplishments and progress toward overall project and U.S. Department of Energy (DOE) goals

This project was rated **3.0** for its accomplishments and progress.

- This project has made good progress on the RuO<sub>2</sub> supports. They do not normalize for mass activity, they only do ECSA; this omission is a major mistake.
- The divergence in goals for e- and H+ conductivity is confusing. Using a typical telegraph model for a catalyst layer, the electrical conductivity can be much lower until it becomes limiting.
- The milestones and go/no-go criterion outlined in slide 8 were all satisfied in the 2012 review. The dispersion of Pt on ITO looks great, but it is unclear why the electrode was inactive. It will be nice to see if the group can get to the bottom of this in the remaining grant period.
- This project is making good, steady progress toward controlling corrosion/loss of ECA. Hopefully, the work on the Ru cost model did not hold up progress in the more important areas of screening more

materials. Although highlighting the influence of durability on cost is always good to remember, cost modeling is not the principal investigator's (PI's) strength; materials development is. The progress included some very valuable knowledge gained from accelerated testing studies to benchmark a variety of materials. This occurred with good feedback from the OEM partner.

- The technical accomplishment of Pt/RuO<sub>2</sub>-TiO<sub>2</sub> with only a 34% ECA loss compared to a 49% loss when cycled in the voltage range of 0.6–1.0 V, is not spectacular. The same results can be obtained with Pt/graphitized carbon black. The initial surface area of the Pt/RuO<sub>2</sub>-TiO<sub>2</sub> is half that of Pt/HSAC; therefore, since the Pt particles are large, their dissolution is lower. This is not an indication of an improved catalyst. On slide 13, the limiting currents for the RDE measurements vary from sample to sample, which has been explained as due to the dispersion of Pt on the support. This explanation is fundamentally incorrect since both poly-Pt with a very low area and Pt/C with 10–100 times higher area have the same limiting current for a given O<sub>2</sub> partial pressure. It is good to see a cost model being presented.
- This project has good MEA results. It is unclear how the proton conductivity of the support (stand-alone) was measured. More details on this need to be provided. It is not clear if the project has run fuel cell drive cycle measurements with the catalysts. At low potentials, it seems the RuO<sub>2</sub> could be reduced and alloyed with Pt to decrease the ORR. It seems the project has to take these supports to lower voltages in order to evaluate that effect. It is not clear if any other comparisons have been made with other supports such as Vulcan carbon (e.g., MEA studies). Those supports might be a fairer comparison for durability since the Pt ECSA of these catalysts is far lower than the HSACs and might be more comparable to Vulcan, which will obviously have better durability than the HSACs (slides 7 and 8). If possible, a highly graphitized support should also be included for comparison. There is a good cost model included with simplified assumptions.
- The accomplishments in this effort are good. The durability measured under the DOE durability working group's recommended metrics show a high state of durability. These measurements are under both 100% and 40% relative humidity operating conditions. Even though the surprisingly high durability results are reported with oxides, which typically dissolve into soluble valance states below pH 1, no clear underlying studies are reported on how this feat is accomplished. Some impedance data, together with conductivity measurements as a function of potential, would be interesting and important for future consideration of these materials as mixed-oxide supports. Traditional reports in a direct methanol fuel cell with PtRu and Pt on RuO<sub>2</sub> show very different results, wherein Ru dissolves and ultimately kills the cathode and anode electrodes. The absence of this behavior in a slightly different format where RuO<sub>2</sub>(OHx) is used as a support is most interesting and needs an explanation.
- The stop-start cycling (1.0–1.5 V) results for Pt/RuO<sub>2</sub>-TiO<sub>2</sub> are very encouraging. The lack of negative impact of RuO<sub>2</sub>-TiO<sub>2</sub> support in catalyst dissolution cycling protocol (0.6–1.0 V) is encouraging, but needs to be repeated with samples of similar Pt particle sizes. Previous results compare cycling at 0.6–1.0 V for Pt/C and Pt/MMO were not of comparable Pt particle sizes. Recent efforts to prepare smaller Pt particles on RuO<sub>2</sub>-TiO<sub>2</sub> should lead to a more appropriate comparison. The much higher density of RuO<sub>2</sub>-TiO<sub>2</sub> compared to carbon indicates Pt loadings should be adjusted to lower Pt loadings on the support in order to achieve comparable volumetric loadings for Pt/C. Assuming a 50-50 RuO<sub>2</sub>-TiO<sub>2</sub> ratio, the Pt loadings should be reduced by a factor of two to three (i.e., they should be 13%–20% Pt on RuO<sub>2</sub>-TiO<sub>2</sub> to compare to 40% Pt on C). If the loadings are decreased to give comparable volumetric loading as for Pt/C, it should be easier to achieve the smaller particle sizes desired. The initial cost study shown was based on the initial performance of Pt/RuO<sub>2</sub>-TiO<sub>2</sub> with much higher Pt loading for the RuO<sub>2</sub>-TiO<sub>2</sub> support than for Pt/C. Based on volumetric loading arguments, this loading should be able to be reduced substantially. This loading suggests that RuO<sub>2</sub>-TiO<sub>2</sub> supports will have cost advantages due to increased durability once the Pt loading for this system is optimized. A true cost comparison should be on optimized Pt/RuO<sub>2</sub>-TiO<sub>2</sub> loadings. The initial work with ITO is encouraging, but a synthesis providing higher surface areas while maintaining conductivity is needed. It is not clear what impact the order of magnitude lower electrical conductivity, compared to RuO<sub>2</sub>-TiO<sub>2</sub>, will have on performance. If the performance is significantly impacted, the cost differential between ITO and RuO<sub>2</sub>-TiO<sub>2</sub> will be overshadowed by the increased Pt cost due to lower performance.

### Question 3: Collaboration and coordination with other institutions

This project was rated **3.6** for its collaboration and coordination.

- The collaboration between IIT and NTCNA is working well.
- The collaboration with NTCNA is very good.
- This project has excellent interaction with NTCNA. This interaction is a major strength of this project and keeps the project relevant to automotive applications.
- The collaboration with NTCNA appears to be fruitful although the data between NTCNA and the IIT do not appear to match well.
- This is a small group, which is good. However, they should continue to follow the Fuel Cell Tech Team's recommendations for comparisons.
- The IIT project lead indicates that NTCNA has been an excellent partner. Hopefully, they can get the performance and durability studies of the Pt/ITO system completed in the remaining grant period. It is unclear what is going on with the sulfated tin oxide system.
- The project review resulted in many examples of excellent integration and communication between the PI and the OEM partner in developing materials, properties targets, and accelerated test procedures to make more rapid progress. Sending students to interact with colleagues at the OEM is extremely valuable for the student. Hopefully, this interaction can continue.

### Question 4: Relevance/potential impact on advancing progress toward DOE research, development, and demonstration (RD&D) goals

This project was rated **3.6** for its relevance/potential impact.

- Durable, non-carbon supports have the potential to significantly increase durability.
- They are doing exactly as asked; however, automotive OEMs are saying that they have good strategies to avoid carbon corrosion all together so the need for these supports is questionable.
- The work has clearly demonstrated that RuO<sub>2</sub>-TiO<sub>2</sub> support exhibits superior durability compared to traditional carbon supports.
- Alternative supports for Pt are a critical area, but this is not so easy to solve because the materials that are corrosion resistant are usually electronically insulating and also have a low surface area resulting in low Pt dispersion. Select projects on alternative supports need to be continued.
- The PI provided some cost estimates, which look promising. However, the use of Ru and Sn still seems risky. The impact of this effort is based on the ability for this process to be scaled up and implemented by a commercial entity.
- The development of corrosion-resistant supports will help the DOE program achieve its research and development goals. This project, if successful, can help commercialization of fuel cells by providing an alternate to carbon, which is the only support used today. The authors have provided a good cost study that helps alleviate concerns regarding Ru costs.
- Improving support durability and overall catalyst stability is highly relevant to DOE's goal of advancing progress toward less-costly commercial fuel cell systems. The development of alternative support materials for fuel cell applications that avoid the shortcomings of carbon supports, while providing advantages beyond what carbon offers, is very relevant to DOE's objectives of providing durable, cost-competitive fuel cell systems. This project is well focused on the relevant barriers and is well-integrated with an OEM to maintain the project's focus on acceptable materials for contemplated future use in commercial systems.

### Question 5: Proposed future work

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

- The proposed future work is adequately addressed.
- The emphasis on lowering Pt particle size is good, but the project did not speak to what is limiting them now. IIT should consider alloys following the PtCo and PtCoNi materials on carbon now. Specific activity should be measured.

- The proposed experimental work appears to be sharply focused on what is required for continued progress to meet relevant DOE objectives. This reviewer would recommend that any cost modeling work after the materials down selection should be held to the appropriate level. The strength of the project is in the capabilities directed at the materials development and learning what some of the composition and function relationships are for alternative supports. The substantial cost modeling efforts would distract the project team from their strengths of materials development and the development of accelerated testing protocols for alternative support materials. IIT should study lower loadings, especially when looking at reducing ionomers. IIT should try not to use loadings over the DOE 2015 targets.
- The project should see how the ITO and sulfated tin oxide support work in terms of catalytic performance and durability. It is not clear what lies behind the inability to measure the activity of the nice Pt dispersion on ITO shown in slide 20.
- The future plans address optimizing Pt particle deposition and decreasing Pt particle size. The future plans discuss a down-selection of supports. Water management in the catalyst layer can have a large impact on performance. The project does not appear to have plans to look at the effects of changing the catalyst layer structure (removing ionomer, changing hydrophobic carbon to hydrophilic oxides) on water management. Tests should be done under conditions where flooding may occur to see if water management issues arise from changing the support material to a less hydrophobic material and removing the ionomer.
- In addition to the future work proposed, electronic and ionic conduction measurements as well as surface area measurements should be conducted ex-situ. These measurements should guide the possibility of success in electrochemical measurements. Such measurement may help the selection of materials for further work. For example, it is unclear how one can expect to deposit 2–3 nm Pt particles ( $100 \text{ m}^2/\text{g}$ ) on an ITO support after having a BET surface area of  $40 \text{ m}^2/\text{g}$ . It is unclear if Ru is found in the membrane and anode side, and if the ionomer content can be reduced due to the use of  $\text{RuO}_2$ .

#### Project strengths:

- This project addresses critical needs for the DOE Hydrogen and Fuel Cells Program. This is a reasonable approach to solving the problem and has good collaboration with industry.
- Nissan provides accelerated testing expertise and knowledge of system requirements. The potential cycling test results were very encouraging.
- This project makes a compelling fiscal argument, the RuOx is viable. RuOx is definitely a real technical possibility.
- This project has good interaction between NTCNA and the IIT. The durability offered by  $\text{RuO}_2\text{-TiO}_2$  is impressive. It will be good to hear more about the performance/behavior of other Pt ITO.
- This project has great collaboration with NTCNA and good, promising initial results. There needs to be high activity on these promising supports.
- This project has a strong PI-OEM interaction and communication that has led to a focus on materials requirements and the appropriate accelerated testing protocols to screen against. There is a good focus on benchmarking test protocols and materials against the best currently available materials.

#### Project weaknesses:

- This project needs to improve ex-situ diagnostics and measurement of material properties to guide electrochemical work.
- The project should not lose its focus on materials development to cost modeling in the future. The strength is in materials development.
- The project is still looking at too many supports. It is good to look at various things at the beginning of a project, but the team needs to focus as the project gets mature (it is 65% complete at this point).
- There is a need to measure specific mass and surface activity and compare two automotive targets. This project needs to do long-term testing. It is unclear if these catalysts ripen. The project needs to hunt harder for Ru dissolution over the long term.

**Recommendations for additions/deletions to project scope:**

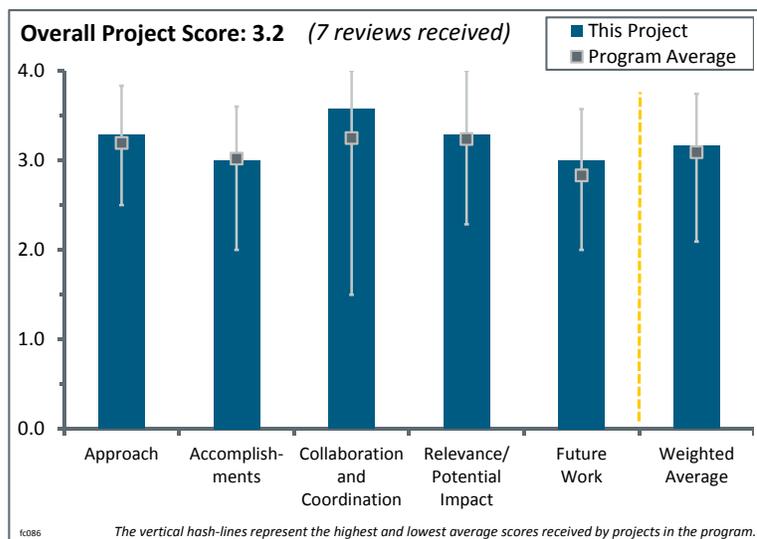
- The scope is appropriate at this time.
- This project should sample the materials to external groups for characterization as well.
- The investigators should see how the Pt/ITO and Pt/sulfated SnO<sub>2</sub> supports perform and/or what prevents the effective activity measurements.
- This project should ensure the balance between materials development and cost modeling makes sense. They should consider engaging others in the “alternatives” community to share samples and do some round-robin testing against the best-in-class, carbon-supported catalysts. Perhaps the PI or DOE can consider taking on this initiative.
- It is difficult to evaluate how much of the effort is being spent on developing the ITO support and the other three supports in addition to the RuO<sub>2</sub>-TiO<sub>2</sub> support that has already been developed, and how much is being spent on developing a workable catalyst on the RuO<sub>2</sub>-TiO<sub>2</sub> support that has already shown great promise. The best approach is not sequential, such as the one the PI is following. The research team has the one support and are optimizing the catalyst on that support and now are exploring another support and plan to optimize that too (maybe doing this five times in total). It is better to down select one or maybe two supports and do all the optimization (MEA, durability) work on that one or, at most, two supports.

## Project # FC-086: Development of Novel Non-Platinum Group Metal Electrocatalysts for PEMFC Applications

Sanjeev Mukerjee; Northeastern University

### Brief Summary of Project:

This project will develop new classes of non-platinum group metal (PGM) electrocatalysts to meet or exceed U.S. Department of Energy (DOE) 2017 targets for activity and durability. This will enable decoupling of polymer electrolyte membrane fuel cell (PEMFC) technology from platinum (Pt) resource availability and lower membrane electrode assembly (MEA) costs. The science of electrocatalysis will be extended from its current noble metal catalysts to a wide array of reaction centers that have a greater tolerance to poisons, which typically affect Pt and Pt alloys.



### Question 1: Approach to performing the work

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

- This approach is an exceptionally good ramification of early work on pyrolyzed macrocycles.
- The approach includes computation, catalyst and electrode design, powder preparation, out-of-cell and in-cell testing, and stack testing.
- The approach of this project is valuable and systematic. It covers all relevant aspects that should be considered for the class of catalyst that may revolutionize fuel cell technology.
- This presentation was one of the best. The approach used to develop the non-Pt-based catalysts shows a high degree of understanding of physics, chemistry, and materials science. This project shows that there is strong promise in this area.
- This project is following a multi-pronged approach to developing non-PGM oxygen reduction reaction (ORR) catalysts to significantly reduce the cost of PEMFCs. Three organizations are pursuing three approaches to synthesizing Fe-C-N<sub>2</sub> catalysts. The project also shows a balanced approach in determining the active site and ORR mechanism using computational chemistry, XPS, X-ray absorption, and RDE studies. The project originally had other types of catalysts, but these have been down-selected due to low ORR activity.
- The overall approach to performing the research is reasonable, with a good materials development strategy. The collaboration approach also seems reasonable and appropriate for the project. What is not clear in the approach is the parameters to be reported on the electrocatalyst activity and active sites for ORR. The principal weakness of a poor ORR electrocatalyst is that the loading would have to be very high resulting in high thickness of the electrodes. Although the units of A/cm<sup>3</sup> is a good choice to take into account in terms of electrode thickness, the actual electrode thickness, loading, and resistance (using EIS, not HFR) should be clearly measured and reported for simplicity and transparency.
- This area is important to explore, but the project's approach is incremental relative to an earlier attempt at co-pyrolysis of CHN precursors with metal ions/complexes. The team's approach to this important area will not lead them to raising the bar in the search for non-PGM electrocatalysts. This pyrolysis approach, while yielding materials that have demonstrated some PGM-like activity and some durability, necessarily leads to uncontrolled catalyst properties, such as structure and composition. That is OK, but it makes it very difficult to make rapid progress in understanding the underlying principles of this class of catalysts, and the researcher's approach should recognize the degree of difficulty and apportion resources appropriately. The

principal investigator's (PI's) approach should be a little more careful not to oversell the ability to control active sites, electronic structure, and metal-support interaction as there is no supporting evidence that any of this is possible at such an early stage in research. For example, there is not any definitive evidence that the activity is metal-centered. The approach to understanding ORR electrocatalysis by spectroscopy and computation is laudable, but it encounters the usual problem in catalysis in that the minority species that go missing by "the usual" approaches may be responsible for all of the catalytic activity. What is seen is not generally what is doing the catalysis; it may be a mere "spectator" along for the ride. The theory and spectroscopy efforts have leapt to assuming there is some M-N<sub>x</sub> center(s) responsible for the catalysis. This assumption is not supported by any direct evidence; correlation is not causation. The approach at this early time should focus on very elementary catalysis characterization approaches rather than on the approaches that are more appropriate to more well-understood catalyst systems. There is value in learning what makes these things tick, even if the activity and durability is not yet on par with PGM.

## Question 2: Accomplishments and progress toward overall project and U.S. Department of Energy (DOE) goals

This project was rated **3.0** for its accomplishments and progress.

- The milestones and go/no-go points are being met. The results approach DOE performance targets in some conditions. There needs to be more operation and testing with air. Durability seems to be an issue with some formulations and operating conditions.
- Substantial progress has been made over the last fiscal year and the PI was able to address challenging critical barriers. Moreover, the project brings an overview of an entire new class of catalysts and it spans from lab to scale-up efforts that engage research labs and industry.
- The materials shown exploit the Fe<sup>2+</sup>/3<sup>+</sup> redox couple. The researchers should focus on modifications of the chemical moieties where the local atomic-scale environment (e.g., near-neighbors, coordination, and short-range ordering might result in shifts in the E<sub>1/2</sub> value to higher potentials [reduced over-potential]).
- A lot of excellent work has been carried out, but the main deficiencies of these catalysts have not been reduced. The major issue is their stability, and another issue is their activity. Considering that the cost of production cannot be low and there is still insufficient performance, it appears that approaching PGM catalysts will not be an easy task.
- The progress is incremental with respect to earlier efforts in this area. Progress in performing computations and modeling "active sites" and advanced spectroscopic studies is of dubious value as there is simply not yet even an elementary understanding of how or what these catalysts are functioning as. For example, it is not clear if these are metal-centered or not. Hence, the progress in "mechanistic understanding" is of yet more dubious value.
- In slide 7, the current density has not been reported, so only the relative values of current at 0.8 V are known. In slide 8, the resistance of the catalyst layer and its thickness should both be reported; no activity values are reported or extracted from the curves. In slide 9, millivolts at 200 A/cm<sup>3</sup> is reported and the back pressures are arbitrarily different. No attempt has been made to identify the active sites, estimate the number of active sites, or obtain the turnover frequency. A study of the effect of loading might enable one to estimate the values that are critical in understanding how these non-PGM materials work. In slide 11, the DOE Durability Working Group (DWG) protocol for non-PGM has a cycle from 0.2 to 1.1 V. This range is not realistic for an automotive fuel cell. The ranges used by Nissan and by the DWG for Pt-based catalysts are much more reasonable. There is no reason why a non-PGM material should have a special protocol that deviates from a protocol used for Pt-based catalysts and simulates automotive conditions.
- The project has shown excellent progress towards enhancing the ORR activity of the Fe-C-N<sub>2</sub> catalysts and characterizing the active site. Whereas last year they were quoting ORR volumetric activities at 0.8 V based on extrapolation from higher potentials, this year they are reporting directly measured ORR activities at 0.8 V which are approaching DOE targets. While the MEA performance is still well below that of Pt/C, the progress demonstrated by this project and in other labs working on the same type of catalyst show that these materials are becoming viable both in terms of activity and durability. This project is behind schedule in meeting its milestone for the in situ measurements for degradation and electrocatalytic pathways for ORR.

**Question 3: Collaboration and coordination with other institutions**

This project was rated **3.6** for its collaboration and coordination.

- The team seems to be operating coherently.
- This project has excellent collaboration.
- The collaboration team for this project is excellent.
- Collaboration between mostly top experts for this topic appears to be very good.
- The team includes an automotive OEM, universities, national laboratories, and materials suppliers.
- Very good team effort is demonstrated throughout all phases of the project that enabled a systematic approach in tackling challenging issues in non-PGM catalysis.
- This project has an excellent breadth of experience and balance between academia, national laboratories, and industry. The Nissan participation is vital to keeping the project relevant to automotives. A new partner has been added to the project this year. Though this partner's work was not presented this year, it is apparent from the supplemental material that they are scaling-up the most promising catalyst materials. A cost estimate from Parajito powders on industrial-scale catalyst synthesis would benefit the project.

**Question 4: Relevance/potential impact on advancing progress toward DOE research, development, and demonstration (RD&D) goals**

This project was rated **3.3** for its relevance/potential impact.

- The work addresses the issues of Pt cost and availability by replacing Pt as the catalyst.
- The realization of Pt-free materials for the cathode in PEMFC will be a game changer.
- The project, if successful, will significantly advance fuel cells as a power source; however, considerable research will be needed to realize the possibilities of this approach.
- The project aligns very well with the Hydrogen and Fuel Cells Program and serves as a valuable source and foundation for future considerations of non-PGM catalysts.
- If this project is successful in improving the ORR activity of the non-PGM catalyst even further, the results of this project would be of enormous benefit to the Program as it would eliminate one of the major barriers to commercialization—cost.
- Non-PGM materials need to be studied for the next decade before they can achieve targets comparable to platinum group catalysts. Projects of this nature need to be funded even though the progress might seem slow. Better fundamental electrochemical measurements, along with improved analysis, are partially lacking. The targets should be rigorous and identical to that for platinum-group materials, so that there is relevance for automotive targets. The impact of success in such a project will be disruptive, but it will speed-up automotive PEMFC commercialization.
- The goal of discovering, characterizing, and utilizing non-PGM catalysts is highly relevant to DOE objectives in making progress toward active, durable, cost-competitive electrocatalysts to support future fuel cell vehicles. Where the relevance falls off in spite of the promise for the future, is that the approach taken by this team will not likely produce successful results as quickly as it might. The project's emphasis on modeling and advanced spectroscopies is too early in the development cycle and saps resources from an effort to do some of the very elementary catalyst and materials characterization steps. In this very early stage of catalyst discovery, focus needs to remain on developing some of the elementary systematics of how, why, and what this catalyst might be. This is necessary so that in the future, meaningful experimental input can be given to the theorists and carefully chosen, well-designed experiments can integrate spectroscopy into the experiment—spectroscopy—theory cycle. This should be done; otherwise, the project will be of limited relevancy.

### Question 5: Proposed future work

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

- The proposed future work is logical and in line with the overall project approach and goals.
- This is a good path forward. Again, this project should focus on reducing the over potential and then try and get kinetics.
- Although the future work sounds reasonable, the key task is to meet the DOE activity target at 0.80 V and 0.90 V in  $\text{A}/\text{cm}^3$  with a better understanding of the actual active sites of the catalyst for ORR.
- Spectroscopic mechanistic studies should be compared with the RRDE data, which can clearly determine the sequential mechanism, and with diagnostic criteria involving formal electrode kinetics.
- The project has well-focused future tasks; however, several milestones in this project are only 50%–70% accomplished. Considering that the project is entering the last phase, there is a concern about whether these milestones will be met.
- There is some value in placing these early non-PGM materials into an MEA; but of course, the risk is that these catalysts will be far from optimal, will not perform as well as PGM at this early point, and that this approach will be discarded before the true potential of these catalysts can be shown or one can conclusively identify that there is no path forward. This is a wordy way of saying to stay the course on the materials discovery aspects of this project.
- While the overall thrust of the project—improving catalyst activity and mass transport—is on the right track, it would have been beneficial if there were more details given as to the approach that would be used to achieve these goals. The modeling of catalyst layer transport would presumably provide guidance for the design of catalyst layers with improved mass transport, but this was not presented and was relegated to the backup slides.

#### Project strengths:

- This project's scientific approach is a strength.
- This project has a strong research team of top experts on the topic.
- The multiple classes of materials and collaborations to choose from are a strength of this project.
- This project is working on an important topic in catalysis that has implications beyond fuel cell catalysis. The project is potentially very relevant to DOE objectives in thriving (to zero) PGMs.
- This project has novel systems and non-PGM catalysts, a systematic approach from fundamental atomic scale to real applications, and a strong team effort.
- This project has many approaches to synthesizing Fe-C-N<sub>2</sub> non-PGM catalysts. The X-ray characterization of multiple catalysts and correlation of characterization results with activities to determine active site and mechanisms is very good.

#### Project weaknesses:

- Pt-free anode materials are a weakness.
- This project has partially achieved their milestones. The volumetric activity to actual fuel cell performance is not well defined and the durability issues are substantial.
- Need a report on electrochemical activity results under conditions that are comparable and with sufficient detail that allows one to determine whether one is approaching the activity of baseline Pt/C. Fundamental electrochemical measurements with improved analysis is partially lacking. The targets should be rigorous and identical to that of platinum-group materials so that there is relevance for automotive targets. Although the future work sounds reasonable, the key task is to meet the DOE  $\text{A}/\text{cm}^3$  activity target at 0.80 V and 0.90 V with a better understanding of the actual active sites of the catalyst for ORR.
- The approach is not well-aligned with realistic catalyst discovery approaches. There is not enough information at this point to feed to theorists, and there are not enough elementary catalyst characterization studies. There is also not enough information to determine if the metal plays a role in the electrocatalysis, or if it is important (or crucial to know) for the formation of a non-metal active site. This project is not staffed with conventional catalyst characterization types that can approach answers to these rather elementary questions.

- The presentation lacked details on how the proposed improvements were to be made and also details on the various catalyst synthesis methods, making it difficult to evaluate the merits or feasibility of the proposed future work. The roles of Los Alamos National Laboratory and the University of Tennessee-Knoxville (UTK) were not clear in the work that was presented. A discussion of mechanisms was interesting and important, but it could have been greatly abbreviated to allow for highlighting the results from other aspects of the project, for example, the UTK transport modeling work.

**Recommendations for additions/deletions to project scope:**

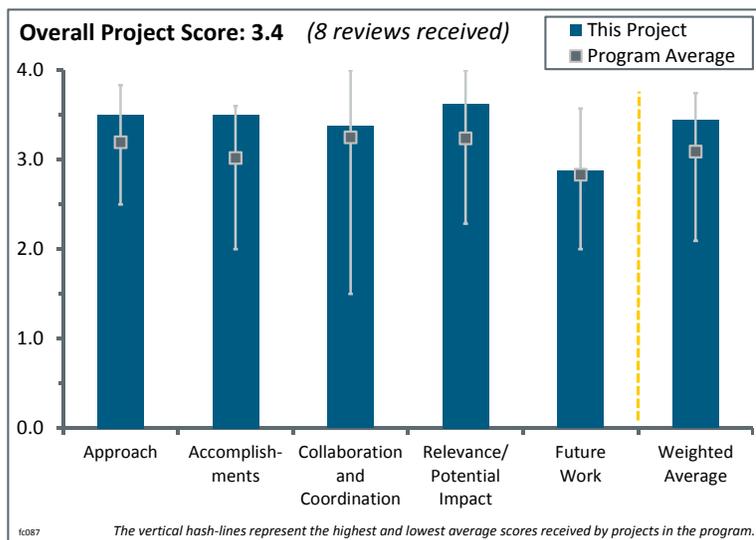
- Modeling the structure of the active site is not appropriate at this time. A useful modeling effort needs additional elementary information about what the active site properties are. This is not to say to keep the theorists out of the loop, just that performing modeling on a very incompletely defined system is not productive. This project should stay the course on materials discovery; the community needs more potential non-PGM materials, and thus an effort to go look for them.

## Project # FC-087: High-Activity Dealloyed Catalysts

Anusorn Kongkanand; General Motors

### Brief Summary of Project:

The objectives of this project are to overcome cost barriers and increase the durability and performance of fuel cells using dealloyed catalysts. Research should (1) demonstrate reliable oxygen reduction reaction kinetic mass activities that achieve the U.S. Department of Energy (DOE) target in hydrogen/oxygen ( $H_2/O_2$ ) fuel cells using manufacturable synthesis and dealloying procedures, (2) achieve high-current-density performance in  $H_2$ /air fuel cells that meets DOE heat rejection targets and platinum (Pt)-loading goals, (3) demonstrate the durability of the kinetic mass activity against DOE-specified voltage cycling tests in fuel cells, (4) determine where alloying-element atoms should reside with respect to the catalyst-particle surface for durable activity, (5) demonstrate the durability of high-current-density performance, and (6) scale up to full-active-area fuel cells.



### Question 1: Approach to performing the work

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

- The approach is systematic and focused. Investigating different leaching methodologies is important in optimizing and “stabilizing” the catalyst.
- This is a very well organized program that is following a sound approach based on intensive collaboration with partners and an iterative experimental process. The program team has done a very good job defining the milestones to progressively increase confidence in the findings and is oriented toward identifying a practical solution for commercialization.
- The approach is good. There could be some additional challenges for further scale-up, such as: quality control of the dealloying process, resulting in a higher cost; approximately 40 mV voltage loss due to dissolved Ni can have a significant impact on performance and cost, considering fuel cell electric vehicles (FCEV) total life; and modeling capability to validate demonstrated performance/durability is preferable.
- The focus on large-scale catalysts provided by a catalyst supplier allows this project to have very strong short-term benefits. Shifting the focus to Co and Ni only prevents some of the poisoning concerns from Cu that had been in the project. Reasonable cases are made for the performance of these materials being acceptable after accelerated test protocols. Longer term testing in short stacks under vehicle-relevant conditions would be interesting to confirm that the accelerated stress tests (ASTs) are relevant for the durability concerns of these alloy catalysts.
- The project is working on developing cathode catalysts to meet DOE mass activity targets. The main approach is exploring dealloyed materials based on Pt. The initial precursors include  $PtCo_3$ ,  $PtNi_3$ ,  $PtCu_3$ , and other combinations that include Ir, Au, and Pd. Some of these appear to be good approaches; others appear to be less valuable and more questionable, including the use of Cu and Ir, especially in view of past comments from General Motors (GM) about using Ir.
- The project is focused on demonstrating catalysts that meet the DOE activity and durability targets and that can be manufactured in large batches. The approach to try to improve the formation of core-shell particles by controlling rates of base-metal dissolution and Pt surface migration is sharply focused on the major barrier of the durability of these materials.

- The group is focused on exploring the role of dealloying in the performance and durability of Pt-Ni and Pt-Co electrocatalysts that will be central to any meaningful progress in the engineering of polymer electrolyte membrane (PEM) fuel cells. The efforts of GM, Johnson Matthey Fuel Cells, Inc. (JMFC), and the Massachusetts Institute of Technology (MIT) are well represented in this report.
- The approach in this project has significant weaknesses and does not bring new insight into catalyst properties. Moreover, it does not consider any novel class or type of catalyst. It is mainly focused on catalyst performance that cannot be correlated to the physical/structural properties of the catalysts due to the lack of consistency in particle size and elemental distribution.

### **Question 2: Accomplishments and progress toward overall project and U.S. Department of Energy (DOE) goals**

This project was rated **3.5** for its accomplishments and progress.

- All the 2012 milestones have been met.
- The progress is excellent. The validation for scale-up has progressed gradually. The gas transport measurement is very helpful and effective in addition to the activity in terms of catalyst microstructure.
- This project has made excellent progress toward the project objectives. The further loss of Co and Ni with fuel cell operation is not surprising. It is expected to affect membrane and catalyst layer ionomer, thus voltage loss analysis could shed some light on the loss mechanism. In order to understand the impact of the carbon support on the observed performance loss, it may be valuable to test the equivalent Pt/C catalyst.
- A big improvement was shown in this year's work in terms of improving the initial Pt particle size distribution. The researchers have met initial activity and durability criteria. They are demonstrating that the concept of dealloyed catalysts has promise for improving the state-of-the-art cathode ORR catalysts. The work has been accomplished at a good scale for these catalysts.
- The progress over the past year in this project included materials that met DOE targets in the initial activity and added the ability to meet durability targets when tested under AST conditions. The materials set expanded to include Co as well as Ni. These materials have shown a good capability to meet DOE's targets and currently represent the state-of-the-art for fuel cell catalysts in membrane electrode assembly (MEA) and a significant step forward to commercially competitive systems.
- This project has made substantial increases in mass activity over the past year, from 0.5 A/mg to 0.75 A/mg platinum group metal (PGM). They have made substantial increases in the durability of dealloyed PtNi<sub>3</sub>. JMFC has made good progress in improving the particle size distribution and has decreased the maximum particle size from greater than 25 nm in the old synthesis to approximately 10 nm. The project has also demonstrated catalysts with mass activity greater than 0.5 A/mg Pt after 30,000 potential cycles. PGM loading (g/kW) has not decreased despite substantial increases in mass activity, suggesting mass transport issues need to be addressed. Ni leaching from catalysts into membrane and catalyst layers still needs to be reduced.
- This project has made significant headway exploring the performance and durability of the Pt-Ni nanoparticle system. This includes studying the influence of variations in the synthesis and dealloying procedures, although the details of the former were not provided. Slide 13 demonstrates completion of milestones 1 and 2. Interestingly, variations in the dealloying process led to a significant range of Pt/Ni net composition ratios (from 0.8 to 1.8), yet the performance and durability milestones were still satisfied after 30,000 cycles. The results indicate that the new alloys are very forgiving in terms of sensitivity to the dealloying treatments, and speak to a certain robustness of well-engineered PtNi catalysts. From a different perspective, the compositional heterogeneity of the dealloyed particles speaks to the net Pt/M ratio as not being the essential parameter that specifies catalyst performance. Going forward, the scientific and technological impact of this work would be greatly enhanced if the size and compositional scatter of the precursor particles could be improved. It is not clear why the project adopted the synthetic path reported by the Argonne National Laboratory group in 2012. The presentation is nominally focused on PtNi<sub>3</sub> precursors, yet slides 11 and 12 indicate that the milestone satisfying material is closer to PtNi stoichiometry.
- Most of the conclusions from the project are already known and do not add new insight into the functional properties of these catalysts. The progress made since last year's report is not obvious.

### Question 3: Collaboration and coordination with other institutions

This project was rated **3.4** for its collaboration and coordination.

- The project represents a well-coordinated team effort that is led by GM.
- The project is well executed; the collaboration between all partners is excellent.
- JMFC appears to be coordinating well with the GM activities.
- The team is well structured with an automotive original equipment manufacturer (OEM) as the prime and a material developer and universities as subcontractors. The roles and responsibilities of the partners are clear and the reviewer thinks the technical results are the outcome of a strong collaboration.
- The project has several partners and defined roles. The inclusion of a leading OEM and a catalyst synthesis company are particularly strong and the efforts of team members appear to be well defined. How the efforts of Northeastern University (NEU) and George Washington University (GW) were leveraged in the rest of the project is unclear.
- The collaborations appear to be transferring knowledge from universities to catalyst supplier and from OEM to catalyst supplier to provide information on what makes active catalysts and feedback on performance and durability, resulting in an improved catalysts produced in large batches.
- The link between the work at GM, JMFC, and MIT is clear. Hopefully more insight will be forthcoming from MIT, NEU, and GW once the “rush of fascinating used MEA-samples” that satisfied milestones one and two have been examined.
- The collaboration is going well, but it seems independent of each pair. More organic and effective collaborations can be carried out among the collaborators.

### Question 4: Relevance/potential impact on advancing progress toward DOE research, development, and demonstration (RD&D) goals

This project was rated **3.6** for its relevance/potential impact.

- The work has satisfied the 2017 DOE mass activity and loss targets and is approaching the PGM total loading goals.
- This project, led by the OEM, covers three major challenges that are very important for automotive commercialization.
- The project addresses cost and durability barriers and is directly targeted at meeting cost and durability goals in the DOE *Fuel Cell Technologies Office Multi-Year Research, Development, and Demonstration Plan*.
- The project is well aligned with the DOE objectives that aim to reduce cost and improve the durability of PEM fuel cells. It focuses on dealloying PtCo<sub>3</sub> and PtNi<sub>3</sub> catalysts to improve durability, while maintaining high catalytic activity of the alloy catalyst.
- Catalyst mass activity and catalyst durability are key target metrics that require parallel improvement for long-term commercialization. This project is addressing the Pt particle durability and the mass activity, and thus, cost. However, the project neglects the other portion of catalyst durability, which is the catalyst support.
- The project is well aligned with DOE goals and objectives. It addresses the key fuel cell concern of catalyst cost and durability while maintaining performance. In the past year, the team has been able to meet the DOE targets for electrocatalyst and MEA performance using industrially relevant materials and approaches.
- The adoption of low-Pt loading materials (retaining performances and durability) is crucial to achieving the cost targets allowing broad commercialization of FCEVs. The reviewer wonders whether this work should be combined with the optimization of catalyst-layer properties (e.g., water management) that is perceived as a big driver to be able to fully leverage the low-Pt materials.
- Considering the lack of novelty in this project, it is hard to envision the substantial impact to the Hydrogen and Fuel Cells Program. Despite the unfortunate choice of systems and poor quality of samples, the team is capable of conducting a systematic approach that spans from fundamental insight to real application. For that reason, the set of knowledge accumulated from this project may serve in the future as a valuable set of results that justify utilization of Pt alloy in PEM fuel cells.

**Question 5: Proposed future work**

This project was rated **2.9** for its proposed future work.

- The shift to short stack is good. The model validation of demonstrated performance change/durability is preferable.
- The proposed future work addresses the most important issues. With little time remaining in the program, a down-selection of catalyst systems in order to focus on one system seems appropriate.
- This project is ending in this fiscal year, and the outcome does not seem to serve as a foundation for the future work on dealloyed catalyst.
- The future plans seem adequate, but are possibly a little aggressive for the remaining six months of the project.
- The work performed to date on the project has yielded significant benefits. The future work is focused on minor tweaks to the system as optimized to date, with a focus on fine-tuning dealloying, employing thinner membranes, and modifying syntheses/treatments. It is unclear that these materials can offer much in terms of further improvements. Clear rationales explaining why further improvements in performance or durability are possible, or why the approaches being suggested are likely to succeed, are missing.
- A number of the future work items seem to be from reviewer comments from the 2012 DOE Hydrogen and Fuel Cells Program Annual Merit Review, instead of the comments being addressed in the past year. The future work should include measurements of the catalyst durability, including the support durability. If this project is relying on the synthesis of the catalysts on nonviable supports, this effort could be wasted. It is unclear what they are actually going to do in terms of “Advanced Characterization.”
- The future work seems to be in line with the strategy to progressively increase confidence in the technology. It is not clear to the reviewer how the porous catalyst will interact with water and whether the project team has investigated this aspect. In particular, if ice formation could happen in the porous structure or its proximity as a consequence of low-temperature events, the reviewer would invite the researchers to conduct degradation studies to better understand this phenomenon. On a similar note, it would be interesting to understand if the catalytic structure has an impact on the water transport (e.g., if a higher retention of water may yield to a lower dynamic response when passing from low to high current density).
- The NEU/GW side of the team needs to move forward with the “rush of used MEA samples” provided by GM. In addition to characterization of the aged specimen’s closer correlation, like that shown in slide 11, the as-formed catalysts are called for. Throughout the presentation, the as-formed materials are referred to as PtNi<sub>3</sub> (e.g., slide 12), yet the composition of the as-formed catalysis appears to be a function of the particle size (e.g., slide 11). In this regard, attributing variations in the composition of the dealloyed particle-to-particle size might be misleading without a proper assessment of the variations evident in the precursor. The parting limit for face centered cubic alloys (Erlebacher and Newman) is thought to be near 58.4% of the reactive metal. How this impacts the aging trajectory of the nanoparticle population is an interesting question, with the authors presenting some very useful data in this regard.

**Project strengths:**

- This project is led by the OEM.
- The project has a strong and well-coordinated team.
- This project has good collaborations across the project.
- Commercially relevant materials with the ability to meet DOE’s targets have been demonstrated in fuel cells and have maintained performance following ASTs.
- This project has a strong team effort. The potential to conduct systematic evaluation of the structure function correlation is positive.
- Excellent progress has occurred in the last year that includes satisfying milestone one and two. The characterization work shown in slides 11 and 12 is most welcome. This program represents the key bridge that connects exploratory laboratory activity with real-world applications, and, as such, is a key pillar in the DOE Hydrogen and Fuel Cells Program portfolio.

**Project weaknesses:**

- The ability to further advance these materials beyond what was demonstrated in the project is unclear.
- Poor-quality samples and a lack of novelty in the approach and choice of systems are weaknesses.
- The quality control/cost for further scale-up and the model's capability to validate demonstrated performance change/durability related to material structures are weak.
- It will be nice when the full power of the NEU/GW subcontractors characterization capabilities are brought to bear on the latest generation of catalyst that satisfied milestone one and two. Improvements in the compositional and size dispersion of the precursor catalyst particles would greatly improve the quality and strength of the conclusion and insight that will come from this study.
- The lack of samples due to GM's relocation from New York to Michigan is a weakness. They state that "0.6–1.0V cycling is too aggressive for vehicle operation. Could induce carbon corrosion. More relevant tests than 30,000 cycles at 0.6–1.0 V are probably required." However, they have yet to examine whether the catalysts being developed are being put onto stable substrates. The substrate plays a key role in the particle precipitation, yet they are ignoring this key parameter, and appear to want to go to a "less stringent" testing protocol.

**Recommendations for additions/deletions to project scope:**

- This project should continue going full steam ahead.
- At this point, much of the need for these systems likely lies in the scale-up, introduction, and long-term testing under relevant operating conditions of these materials.
- This project should compare durability of the dealloyed PtCo/C and PtNi/C catalyst durability with the equivalent Pt/C catalyst.
- Without knowing the stability of the carbon support, the progress in this project is still unclear. It is not clear if high surface area carbon (HSAC) or a more stable graphitized carbon is being used. It is easier to get higher dispersions with the HSAC, but these catalysts are less stable during the higher potential ASTs. It is recommended that the catalyst support and the stability of this support, as well as AST testing of these materials, be conducted and presented. GM should end all activities for Ir as their own company guidance to other developers is that Ir will never work. If this is a reasonable path, it seems odd that there are comments in the past from GM to other projects to never use Ir. The ternary systems work should concentrate on other components that are low cost in contrast to the Au, Ir, and Pd explored to date. The effect of de-alloying different atmospheric conditions should be explored (in air versus N<sub>2</sub>). The researches should also examine the effect of Ni leaching on the performance and durability of the other components in the system. It would be interesting to understand how this work compares to the similar catalyst develop by Stonehart et al., for phosphoric acid fuel cells in the 1980s.

## Project # FC-088: Development of Ultra-Low Platinum Alloy Cathode Catalyst for PEMFCs

Branko Popov; University of South Carolina

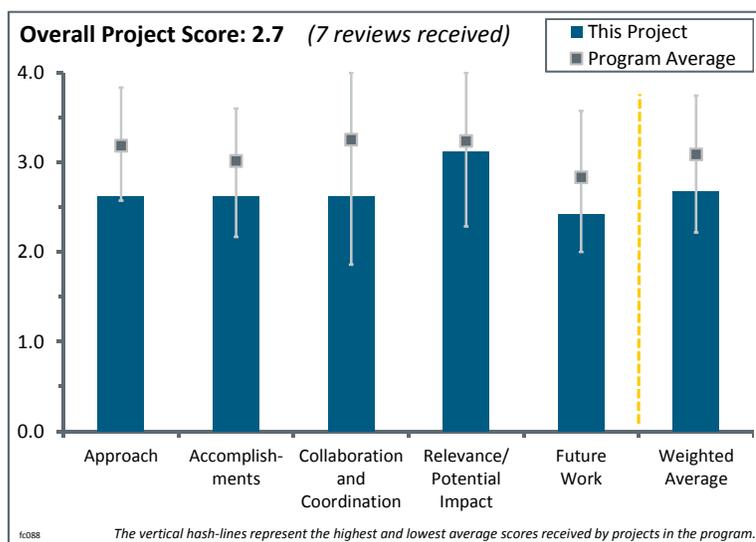
### Brief Summary of Project:

The objective of this project is to develop high-performance, low-cost, durable cathode catalyst and support. The research focused on optimization studies of carbon composite catalyst (CCC) supports, development of a process for the in-house synthesis of carbon nanocages (CNCs), development of an advanced hybrid cathode catalyst (HCC) based on a CCC support with low-platinum (Pt) alloy loading catalyst, development of CNC supported Pt-alloy catalysts, and development of high-volume procedures for the synthesis of a promising catalyst.

### Question 1: Approach to performing the work

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

- The approach has been consistent in terms of trying to meet the targets set out by the U.S. Department of Energy (DOE).
- The basic approach to develop a catalyst-support system with a corrosion-resistant, heat-treated support is valid and seems to result in high activity electrocatalyst systems that are close to the DOE targets.
- The approach based on synthesizing graphitized carbon and then finding adequate Pt deposits apparently worked well. However, there is no information on why it worked and if the Pt-C interaction is determining the activity and stability. Only the degree of graphitization is considered.
- This project seeks to simultaneously develop more durable support materials, some of which have O<sub>2</sub> reduction activity, and more active Pt-based catalysts. The experimental approaches taken towards these ambitious goals are reasonable and have produced some positive results. It is not clear that the membrane electrode assembly (MEA) testing is yet state-of-the-art and capable of demonstrating the true potential of these catalysts. The idea of combining some ORR activity of the support (to carry current primarily at low potential/high loads) with low loadings of Pt (to provide current at high potential/low loads), the HCC really needs to be checked by modeling that can adequately handle the mass transport losses in the thick films needed to get useful currents out of the active support. Not enough results from the modeling shown in the reviewer-only slides are given to demonstrate that this issue has been adequately considered. It is essential that the hybrid catalysts be tested under H<sub>2</sub>/air conditions, and it appears that this work is just starting now.
- In general, the approach has significant weaknesses. First of all, the designing “rules” for the ORR are ill defined and it is still difficult to understand what is unique with PtNi and PtCo preparation methods. It is more like making materials and testing them.
- The principal investigator (PI) claimed in his talk that Pt is better than any alloy. This seems to contradict several other speakers and undermine the very title of this project (alloy). The researchers must provide more proof when making such claims. It is not clear why alloys are being studied in this project. It seems to meet all targets based on DOE protocols. This project needs to evaluate the new U.S. DRIVE Fuel Cell Tech Team accelerated stress tests (ASTs) on carbon corrosion (1–1.5 V cycling instead of 1.2 V hold). This is a new change and should be followed for the rest of the project. The PI did not answer questions satisfactorily. He started talking about H<sub>2</sub> crossover when asked about H<sub>2</sub> evolution in the cyclic voltammograms (CVs). The electrochemical surface area should be determined from CVs that do not go



down to the H<sub>2</sub> evolution region. The approach could be better stated with a slide that shows exactly what gains they hope to achieve by using active supports. It is not clear if the support is actually contributing to better activity or if the activity of Pt overwhelms anything from the support. The support corrosion durability is also being improved by increasing graphitization temperature. All this should be stated simply in one slide with clear criteria for go/no-go decisions.

- The overall project approach and objective are unclear from the presentation. While it appears that the approach is to utilize an ORR active support for platinum group metal (PGM) catalysts to reduce the cost of the catalysts, the loading of Pt on the CCC support is as high as what is utilized in current state-of-the-art materials, and an initial performance benefit was not demonstrated. The Pt-based metal catalysts are achieving high ORR activities, but these are similar to or lower than what has been demonstrated for the same classes of Pt alloy catalysts on traditional carbon supports. It is not clear if the approach of this project is to enhance the ORR activity of non-PGM catalysts by adding Pt, or if it is to enhance the ORR activity of Pt by supporting it on an ORR active support.
- The approach appears incremental, at best. Pyrolysing carbon blacks at a variety of temperatures with or without additives have been a part of heterogeneous catalysis and electrocatalysis for a long time. This project does not move the dial very far, if at all. Giving a new name to an old carbon does not make it new, nor does placing Pt on it make it either “advanced” or “hybrid.” The project approach would be improved by bringing some focus to explaining what, if any, the differences are between commercial carbons and the CCC or CNC, why those differences may be important in durability/activity, and how the comparative characterization/electrocatalysis/durability data supports their hypothesis. The electrocatalytic studies are appropriate; the accelerated durability testing parameters could be better defined or illustrated.

## Question 2: Accomplishments and progress toward overall project and U.S. Department of Energy (DOE) goals

This project was rated **2.6** for its accomplishments and progress.

- The team has made good progress year after year, especially in terms of evaluating the catalyst technologies developed and making some key advances in understanding how to control Pt particle size on the support material. The team has a very short list of candidates that have the capability to meet the DOE targets.
- The PIs made a small amount of progress towards the objectives, especially if the results are compared with the catalytic activity of ORR obtained from the other groups.
- The catalysts’ performance and durability are close to DOE’s targets for 2017, but they are not yet there. There is no information on the alloy composition after the tests of durability. The Co content in Pt<sub>1</sub>-Co<sub>1</sub> alloys should be known given the devastating effect of Co<sub>2</sub><sup>+</sup> or Ni<sub>2</sub><sup>+</sup> on a membrane’s conductivity. The project needs techniques that provide more basic structural and molecular-level information.
- High catalyst activities close to DOE’s target at the beginning of life have been demonstrated in this project in the MEAs of fuel cells. Although the support is supposed to be very durable after very high-temperature heat treatment, the support still corrodes and results in activity losses of approximately 50% compared to the baseline Pt/C in durability studies, as seen in slide 15. The goal of a more durable support has not been achieved.
- The activities and durability of the Pt/CCC should be compared to state-of-the-art Pt/C rather than comparing the activity of HCC to Pt/C, which includes the effects of both the unique carbon support and the alloying effect. An impressive number of iterations have been synthesized and tested in this project. The most promising at this point are the Yonsei University (YU) catalysts, but these should be compared to their counterparts using traditional high-surface-area carbon (e.g., Ketjen) and graphitized carbon for a valid comparison and to validate the premise of the project.
- The project accomplished a lot of work if work is measured by the sheer number of data panels on the slides. There is far too much data, far too little interpretation in the presentation to result in any clear accomplishments and progress. To deflect criticism that these materials are not novel, effort should be put into demonstrating that the carbons that result from the modification of carbon black is somehow different than, say, the pyrolysis of carbon black. The evolution of products is not clear; they could arise from the methanation of the amorphous fraction of the carbon black. The fate of the surface modification additives is also unclear (e.g., where does the O<sub>2</sub>, N<sub>2</sub>, etc., from the additives go?). The project should use a TGA/MS

to at least give some idea as to mass recovery and off gases of the pyrolysis step(s) such that reviewers can ascertain the “novelty” of the support. Essentially, there are no elemental characterizations of the carbon or of the catalyst to allow one to determine the uniqueness, if any, of the compositions.

- Progress since the 2012 review appears to be limited. The 2013 slides show only one catalyst, the YU Pt<sub>2</sub>Ni/CNC (in both unleached and leached forms), meeting both the initial activity of 0.44 A/mg of Pt and the loss of less than 40% of the mass activity after 30,000 cycles 0.6–1.0 V. The same catalyst was shown meeting these targets in the 2012 slides. The 2012 slides showed a University of South Carolina (USC) Pt<sub>2</sub>Ni/C at 0.45 A/mg of Pt, but in 2013 this is listed as 0.43 A/mg of Pt (not a significant change), and presumably the result of additional experiments pulling down the number slightly. New and productive work was done on new generations of the modified carbon supports (CCC), including more durability testing. The performance of MEAs at moderate- to high-current density in H<sub>2</sub>/air testing is still below the targeted values, even before aging and even with iR correction, which is not commonly applied to H<sub>2</sub>/air tests.
- The ECSA losses reported are artificially low since the ECSA scans are taken down to very low potentials (<0.85V) where there is significant H<sub>2</sub> evolution. The PI should repeat these measurements down to a reasonable voltage and then report the percentage of losses. These will be significantly higher than those reported in this talk. Once they do this, they will find that their ECSA percentage losses are a lot more consistent with their mass activity losses, which are far greater than ECSA losses now. In slides 10 and 11, the cycling is done to an upper potential of 0.925V, but in slides 12 and 13 the upper potential is 1.0V. The DOE protocol is 1.0V. It is unclear why there is this discrepancy. More post-characterization data and the particles sizes and electrode layer thicknesses before and after the various durability tests should be presented. These should be shown in addition to the polarization curves. A slide summarizing the behavior of all three catalysts (fresh and after the two AST protocols) would be very useful. It is not very easy to evaluate the progress since the details are missing. While there is lot of polarization data, there is no link to what was done to achieve this improvement. The reasons behind the improved performance of the various catalysts are not clear, nor is the difference between the 2012 and 2013 catalysts (first generation and second generation HCC). The durability of the CCC is not clear. After durability tests, it is not clear if the transition metal is still there. It was also not clear if there are any post characterizations of the carbons used in this study, if they still retain activity, or if they contribute to the activity of the overall catalysts (not just the overall catalyst activity controlled by Pt).

### Question 3: Collaboration and coordination with other institutions

This project was rated **2.6** for its collaboration and coordination.

- The collaboration is strong and this is a strong component of this project.
- This project has significant collaboration with the Korean universities and companies.
- There are many collaborators, some for a short time. The coordination of their efforts should be improved.
- The collaborators from YU appear to have made a very significant contribution in terms of helping the team to reach their milestone for the project.
- This project is rather narrow in its collaborations versus other catalyst development projects, especially in the area of characterization and computational studies. Some of this was apparent in the reviewer-only slides, but the impact of the characterizations and the impact of modeling on catalyst layer design should be indicated.
- It is not apparent what the level of collaboration, communication, or coordination was with the other partners as few references were made to them. This perception may, in part, be due to the overwhelming data content of the presentation.
- The official partners on this project are YU and Hyundai. YU and USC are developing their own catalysts and Hyundai had no funding last year. This is not a good collaborative effort. The PI did not mention the percentage of effort or funding that went to the collaborators. The PI needs to interact better with other players in the field (original equipment manufacturers, laboratories, and other universities) to help scale up and validate these catalysts. The additional interactions on the TEM studies are good.
- The presentation did not make clear whether the activities of the prime- and sub-contractors are coordinated, or if they are essentially independent activities. The presentation did not make clear where the MEA testing was done. In the absence of such clarification, one must assume that it was done at USC. The

level of involvement of the automotive subcontractor was not at all clear, and the line about the interruption and restart of funding leaves the reviewer with unanswered questions. The data on the YU catalyst with good activity seem to be the same as those presented in 2012. The collaboration might be better facilitated if the PI made a conscious effort to listen to, and thoughtfully consider, what others have to say and to achieve greater brevity in his own answers to questions.

#### Question 4: Relevance/potential impact on advancing progress toward DOE research, development, and demonstration (RD&D) goals

This project was rated **3.1** for its relevance/potential impact.

- The project aligns with cost reduction and activity targets for catalysts.
- The project is focused on PEM fuel cells development.
- The project is developing catalysts that can meet the DOE targets and, as such, is very relevant.
- The project is relevant to obtaining high activities and durability of catalyst systems to lower costs and speed up the commercialization of automotive PEM fuel cells.
- Most project aspects align with the Hydrogen and Fuel Cells Program and DOE RD&D objectives.
- Given the highly incremental nature of this approach, it is unlikely that this project will significantly advance the state of the art in fuel cell electrocatalysis.
- The topical area of developing ultra-low Pt catalysts having appropriate durability is highly relevant to DOE's objectives in developing long-lived, cost-competitive components for fuel cell vehicles. This project is aligned with those goals, but the approach will not significantly advance RD&D toward the goals.
- The potential impact of a synergistic effect between an ORR active support and a PGM catalyst in reducing PGM loading and cost is large. In theory, this project is relevant to DOE's goals if the PGM catalyst loading can be vastly decreased using this concept. However, what was presented this year utilized high Pt loadings on the support and appeared to just reduce Pt loading through alloying, which is the focus of many other DOE projects.
- This project addresses the activity and durability of catalysts, supports, and complete MEAs and, as such, is well positioned to improve the state of the art of PEM fuel cells for a wide range of applications. The modest progress on several fronts and the weaknesses in MEA performance to date, coupled with the inadequate modeling analysis of the prospect of the hybrid catalysts, raise doubts as to whether the project can achieve enough of its very ambitious goals to positively impact the field.

#### Question 5: Proposed future work

This project was rated **2.4** for its proposed future work.

- The proposed work appears to result in small incremental improvements. Similar treatments of the catalyst's components have been already tried.
- It will be important to have the industry-led evaluation of the technology/other proof points from independent groups.
- The proposed future work should focus on reducing the Pt loading on support by increasing the ORR activity of both the alloys and the non-PGM support.
- It is not clear how the go/no-go decision is going to be made. It is unclear if the best of the three tested catalysts can automatically go forward and if this catalyst needs to meet some minimum requirements. There needs to be some comparison made to state-of-the-art catalysts that can be purchased commercially. Currently, all catalysts are being made at USC.
- Future work seems evolutionary with small modifications to materials. The corrosion resistance of the CCC and CNC should be carefully measured in ex-situ measurements and compared to Ketjen Black and Vulcan and graphitized Vulcan to get a quantification of improvement of these new materials. Currents in A/mg and A/cm<sup>2</sup> carbon should be plotted to investigate if these carbons truly have better corrosion resistance that is worth the expensive heat treatments. The supplementary slides showed an effect of Pt loading that is highly questionable and reverses the trends of what is expected. This may have to do with the method of catalyst deposition or spraying onto the membrane.

- The future work section appeared to be mostly regenerated from ongoing work. The goals for future materials improvements were stated, but the pathway to reach those goals was poorly explained, if at all. Carbon modification plans included purification, etc., but the underlying justification for doing this, which was perhaps obvious, went unstated as did the methods for obtaining and confirming that the purification process resulted in changes in compositional/structural properties of the supports. The future approach would be improved by detailing what the hypothesis behind the surface modifications and purification is and then addressing the data to be obtained to prove or disprove the hypothesis.
- The proposed work under the no-cost extension is reasonable, though proper modeling of the hybrid systems, using the kinetic data from the support-only ORR data, and adequate inclusions of traditional treatments of mass transport within the catalyst layer should receive greater emphasis. Making good high-activity electrodes that meet DOE activity and kinetic durability targets on corrosion-resistant supports, as done in this project, is very difficult and modest shortfalls versus numeric targets should not necessarily be taken as a major failure. The viability of the work proposed under Phase II (if the go/no-go is passed) is dependent on improved MEA and short-stack testing capability, either at USC or through partners.

#### **Project strengths:**

- This project used great teamwork to get to the milestone.
- This project closely meets the DOE targets for activity.
- This project has plenty of performance data on various novel catalysts.
- This project is focused effort on two to three factors determining catalyst performance.
- Any strengths were difficult to ferret out of the extremely voluminous amount of material presented.
- The PI has a strong background in carbon chemistry and in electrochemistry. The PI is highly experienced with synthesizing materials with unique stability and activity.
- Some progress was made in taking on simultaneous improvement of support stability and catalyst activity/durability. The project's modified carbon supports do appear to be significantly more stable against corrosion (as would be seen in unmitigated start/stop) than are conventional carbon supports. Progress has been made in achieving reasonably high activities with low levels of corrodible, non-noble metal atoms in the electrodes. The development of partially chemical pathways for producing graphitized carbon supports is a strength, compared to the inert thermal annealing at much higher temperatures than is commonly used.

#### **Project weaknesses:**

- Heat-treated CCC and CNC support do not show high corrosion resistance.
- There was no comparison to commercial materials, no clear understanding of the role of the catalyst carbon support and its contribution to HCC activity, and no clear understanding of the durability of the CCC.
- This project would benefit from techniques that can provide relevant basic structural and spectroscopic information. Protocols used to judge the technology may not be aggressive enough and may thereby give a false sense of security in terms of applicability to industry.
- The systems are in general ill defined. The measured activity/stability is subject to debate. The PI is still questioning the existence of Pt-Ni/Co alloys. If it is not an alloy, then it is not clear what it is. More fundamental knowledge is needed to improve the stability and activity of the systems.
- This project has far too much data and too little interpretation and supporting evidence to support the researchers' hypothesis that these materials are "novel." This project appears to be incremental.
- The kinetic activity targets before and after cycling were met, at best, marginally. The MEA performance at moderate and high-current density is below expectations, and catalyst utilization numbers at higher loadings are unusually low. There was a lack of adequate modeling analysis of the extent of advantages at high-current density that can be realistically expected from use of a carbon support with limited ORR activity.

#### **Recommendations for additions/deletions to project scope:**

- One-to-one Pt-to-Ni or Pt-to-Co alloys are not likely to provide useful electrocatalysts.
- This project is unlikely to lend support to moving DOE's RD&D objectives forward and should be considered for redirection or early completion.

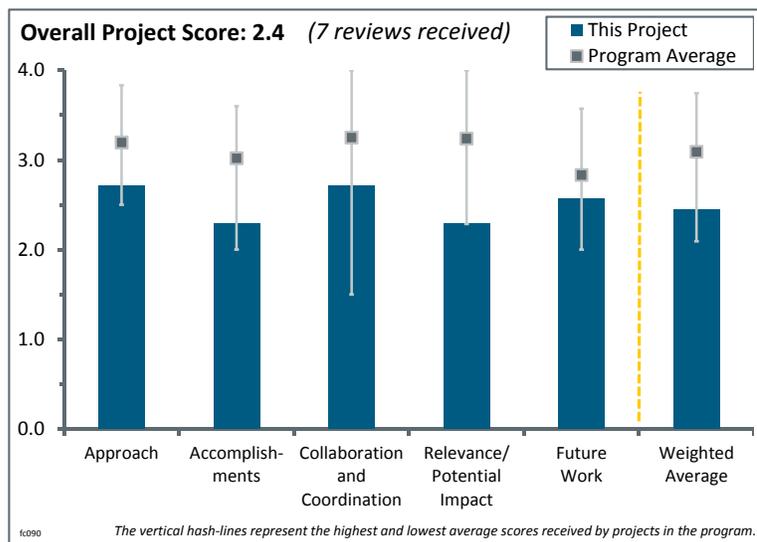
- Only those catalysts that show improvement over state-of-the-art commercial catalysts should go forward to Phase II. Hopefully, these are evaluated somewhere other than at USC, maybe at Hyundai, who is one of their partners.
- The proper modeling analysis—using available kinetic data and standard analyses of mass transport within an electrode layer—of the magnitude of advantages that could be realistically expected at high current density in H<sub>2</sub>/air for a hybrid catalyst incorporating a low loading of Pt on a carbon-based support. It is not clear if one can get a meaningful augmentation of total performance at high current density from the ORR-active support in a layer sufficiently thin that it does not throttle off the performance through mass-transport limitations.

## Project # FC-090: Corrugated Membrane Fuel Cell Structures

Stephen Grot; Ion Power

### Brief Summary of Project:

The objective of this project is to pack more membrane active area into a given geometric plate area, thereby allowing both power density targets and platinum (Pt) utilization targets to be achieved. The project aims to demonstrate a fuel cell single cell with a two-fold increase in the membrane active area over the geometric area of the cell by corrugating the membrane electrode assembly (MEA) structure. An ultra-low, Pt-loaded, corrugated MEA structure will be incorporated in a single cell that achieves the U.S. Department of Energy (DOE) 2015 Pt loading target while simultaneously achieving power density targets.



### Question 1: Approach to performing the work

This project was rated **2.7** for its approach.

- This project has a good approach to increasing MEA area.
- The approach of making corrugated, three-layered MEA (five-layered MEA, including the gas diffusion layers [GDL]) is a good approach to condense larger active surface areas within the confined, two-dimensional (2-D) space. By moving from a 2-D, flat MEA geometry to a corrugated MEA geometry a factor-of-four improvement in power density can be realized. The approach clearly addresses the high power density barrier and is well integrated with the DOE goal.
- The approach is interesting, but there are questions regarding how the stack is going to be assembled.
- The creativity and ambition of the project are commendable; however, there are many challenging technical issues with the approach.
- Corrugated MEA may increase the surface area and potentially enhance the performance, though there are a number of challenges to making that happen.
- While this is an interesting approach to increase the volumetric power density of a PEMFC stack through a corrugated cell and flow-field design, it is very technically challenging and requires a completely new flow-field material set and cell support structure.
- The corrugated MEA approach is unlikely to overcome the cost and performance barriers as this project intends. The complex MEA construction and the use of a metal wire screen will likely lead to higher costs. The corrugated structure may have performance issues related to heat and mass transfer, electrical resistance, and durability. The latest performance results in slide 17 are still substantially lower than conventional MEA design.

### Question 2: Accomplishments and progress toward overall project and U.S. Department of Energy (DOE) goals

This project was rated **2.3** for its accomplishments and progress.

- The project has gotten into modeling and structural/thermal/electric analysis, which provides a clear view of the potential challenges and risks. The project has also moved on to a practical way to demonstrate if it

can eventually be made. The modeling can be improved by introducing a swelling change and by a related conductivity change.

- Progress was made on GDLs. The project needs to address membrane swelling in corrugated structures. Based on the figures shown, current densities may be larger in MEAs and GDLs without changes in cathode/anode plates. It is unclear how this will impact MEA durability and whether General Motors (GM) will be able to support the development of improved seals.
- Most of the results in the last year were modeling by one of the subcontractors. It is not clear how much progress was made by the project lead and the other subcontractor. The overall progress is modest.
- Many tasks are behind schedule due to the demanding nature of the design and materials property requirements. There has been good progress in the modeling of structural and thermal stresses and voltage drops.
- Some progress has been made in establishing the feasibility of the approach. It is unfortunate that the cell design is already limited to a maximum current density ( $1.2 \text{ A/cm}^2$ ) to avoid overheating, as this undermines the original premise of increasing power density.
- It is unclear what the gain is in terms of cost and processing, especially with the higher areas. GM's move from New York to Michigan impacted the project significantly, and there needs to be a plan going forward or the project is delayed. The researchers need to understand how membrane swelling is going to impact durability and performance. There are problems getting the membrane to hold its shape. This project has a good analysis of operating conditions, but this could be a big limitation.
- Very little progress has been made in corrugated MEA development, which is the most important part of the project. The membrane forming tool was made, but the membrane could not be formed into a corrugated pattern. Polymer membrane, such as Nafion®, is known to change its dimension and morphology upon humidity change, and it is not expected that the membrane can be formed into a permanent, rigid, corrugated structure. The team should take the initial approach of making a corrugated GDL, which will support the MEA to remain in a corrugated shape in the cell. It is not clear why the team is taking a Cu membrane approach to meet the cell-compression, mediated, cell-impedance target. The target should be met with a functional, corrugated fuel cell MEA, not a Cu membrane. The team should focus more on making a functional corrugated-structured MEA that can be evaluated in the cell.

### Question 3: Collaboration and coordination with other institutions

This project was rated **2.7** for its collaboration and coordination.

- The collaboration has led to data comparison and improvement—even though only limited data are available.
- The team consists of good partners, GrafTech and GM, who can address the GDL and testing/validation of the corrugated MEA concept. GM and GrafTech can help develop a workable stack using corrugated MEAs.
- It is evident that this project has many relevant collaborations. The team is well-balanced and has an automotive original equipment manufacturer (OEM) to insure that the project is relevant to automotive applications.
- This project has good collaborations with the OEM that should be able to provide input into feasibility. This project should also look into working with other suppliers of GDLs, including those who work with open field and foam structures. With the removal of GrafTech, it is unclear what is going on with their portion and involvement.
- The researchers need to improve the overall design architecture with GM.
- The suppliers appear to be responsive to the effort; the subcontractors are less so.

### Question 4: Relevance/potential impact on advancing progress toward DOE research, development, and demonstration (RD&D) goals

This project was rated **2.3** for its relevance/potential impact.

- The project is relevant to the objectives of the DOE *Fuel Cell Technologies Office Multi-Year Research, Development, and Demonstration Plan*.

- The activities are aligned to DOE's goals. This project brings in an unconventional approach of using corrugated MEA to access higher active areas and, hence, harvesting higher power density from a defined stack volume.
- The researchers have to wait until a fuel cell stack using the corrugated MEAs shows promising results.
- Any changes that can realize a two-times increase are good to explore. However, the project has not fully described an end-to-end solution for making a cell. Perhaps this was in earlier presentations.
- New approaches to overcoming the limitations of current conventional hardware are relevant to the field, but the potential impact of this project is low due to the many challenges inherent in the approach.
- This project falls in the high-risk, high-reward category. It could have a large impact on volumetric power density and reduce the cost of the stack attributed to bipolar plates; however, it is not certain if the manufacturing costs, which would appear to be higher for this non-planar structure, will outweigh the cost savings from reduction in a bipolar plate area.
- It is not necessarily fair to compare on the geometric basis instead of membrane basis, and an effort should be made to compare it to a non-corrugated system with the same membrane area. This can be used to determine the specific targets that one could gain with the corrugated structure. Pt utilization was not presented in this talk.

### Question 5: Proposed future work

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

- The reviewer is looking forward to seeing more data come out of the project.
- The actual operation of a convoluted MEA is, of course, critical and justifiably the primary focus of the future work.
- The de-bug work and approach to fixing the sealing issues are not described. The plans that are on the table to solve these problems are not clear.
- The proposed future work was very broad and what was shown in the presentation is the deliverable of the project.
- The project is ending and not much was presented. It is not clear if the researchers will meet the go/no-go and what will happen in the last few months after that.
- The future work described is partly aligned with the proposed work of the project. The team not only needs to focus on sealing issues, but also on the corrugated MEA fabrication. So far, the team has not come up with a fabrication method of a good performing corrugated MEA. There is no clear outcome on the types of GDL, membrane, catalyst materials, and fabrication process that will be used to make such corrugated MEA. The team also needs to plan the performance and durability studies of corrugated MEA under various temperatures and relative humidity (RH) cycling.

### Project strengths:

- The MEA area increase is a strength.
- The novelty and strength of collaboration is a strength.
- This project's strength is providing a high-surface-area MEA.
- This is an interesting way to change volumetric power density.
- The team is well organized and capable of evaluating such a different idea.
- The strength of this project is creativity, starting with the original idea and then formulating solutions, such as the ability to quickly develop an alternative wire mesh-based GDL when the original was inadequate.

### Project weaknesses:

- The complexity of design and a need for new materials sets is a weakness.
- The project needs to address the catalyst accessibility versus high MEA geometric surface area.
- While significant technical challenges should not necessarily be perceived as a weakness, the magnitude and variety of formidable technical challenges are overwhelming in this project.

- This project does not appear to be a game changer, only a way to increase MEA area. The impact on cost needs to be shown, especially on an MEA area basis, and the problem of being able to only run at lower current densities seems to limit the applicability and gains in volumetric power density. There are membrane and formation issues.
- The concept may have some theoretical merits, but the proposed technical approach may also lead to performance issues related to heat and mass transfer, electrical resistance, and durability. The project timeline has passed the 60% mark, yet the results and progress so far are not encouraging. One of the barriers this project is trying to address is cost; yet there is no cost target. It is very likely that the proposed cell structure will incur a higher cost, and a cost target should be established.
- The team does not have a clear plan for fabricating corrugated MEAs. The team should down-select GDL membrane and catalyst coating methods that are appropriate for making corrugated MEAs. The team assumes that, in a corrugated MEA system, it would not incur any additional stress around the corrugation during temperature and RH cycling. The team also needs to consider the heat dissipation mechanism along the wall of the corrugated surface of the GDL/MEA, which is not in contact with the bipolar plate; hence, the effect of coolant will be very little along the walls of the corrugated surface and can give rise to heat-spots resulting in the formation of pin-holes in the membrane. The heat management and, hence, the cooling of the MEA in a stack, is always a challenge and the team should consider heat management challenges for corrugated MEA seriously.

#### Recommendations for additions/deletions to project scope:

- It is suggested that the project make full cell stacks to figure out all the issues and then lay out the plan to address those issues.
- The whole project approach lacks a solid fundamental and engineering foundation; its lack of progress is not a surprise. It is questionable what we can really achieve by continuing the project.
- While modifying the hardware for obtaining proper compression of the membrane for sealing purposes, the team should get the appropriate MEA materials for making rigid and corrugated MEA that can be compressed in a cell.
- It is late in the project, but it would be nice to know (a) if the proposed design, with its more complicated manufacturing process and new materials set, would be more costly than that of state-of-the-art conventional stacks and (b) if the cost savings due to reduced use of bipolar plate material would be negated by increases in cost in these other areas.
- This project should look at doing a more detailed cost model for the system to show the benefits and the targets needed to reach them. It is not clear what the impact on the stresses on the material and MEA properties are; this should be correlated to work that is ongoing in other DOE projects. Perhaps this project should try reinforced and stiffer membranes. The project needs to think about water management issues and multiphase flow aspects in this structure where one could get water films and channeling where it would be detrimental.
- So far, the project has described a manifold configuration for single cells that is already much thicker than the convoluted structure. Manifolding the anode, cathode, and coolant flows along the two entrance and exit sides of the parallel channels in a stack will be very difficult without likewise thickening the unit cells appreciably, thus negating the benefit of the convoluted MEA. Provided the first successful convoluted cell is accomplished, the project should invest in an effort to develop a stack design that shows how the manifolding can be efficiently accommodated.

## Project # FC-091: Advanced Materials and Concepts for Portable Power Fuel Cells

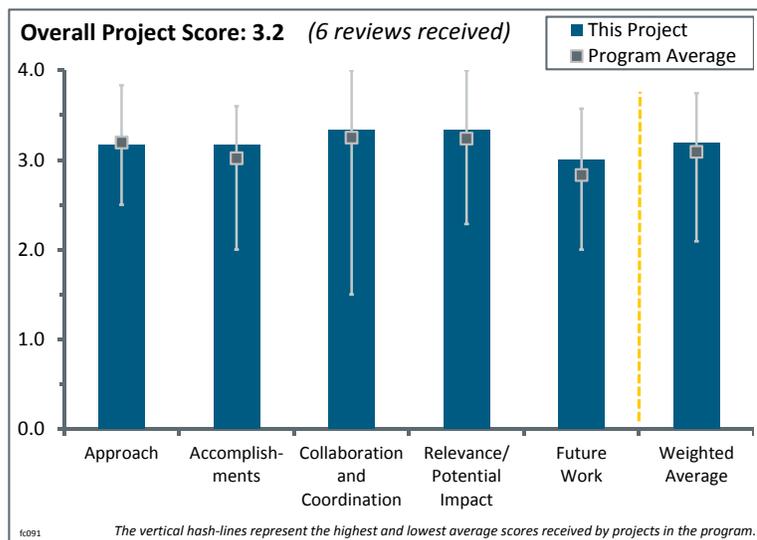
Piotr Zelenay; Los Alamos National Laboratory

### Brief Summary of Project:

The objectives of this project are to develop advanced materials (for catalysts, membranes, electrode structures, and membrane electrode assemblies [MEAs]) and fuel cell operating concepts capable of fulfilling cost, performance, and durability requirements established by the U.S. Department of Energy (DOE) for portable fuel cell systems. The project will also explore the development of a path to large-scale fabrication of the successful materials.

### Question 1: Approach to performing the work

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



- The approach is very reasoned and sensible. The team includes seven individual thrusts but the principal investigator (PI) holds it together. Despite some apparent isolation of the individual efforts, they are all of high quality and are focused on DOE milestones and barriers.
- The multi-directional approaches taken for the completion of all tasks are adequate. All the technical barriers had been addressed appropriately. The responsibilities for anode, membrane, alternative fuel development, and performance/durability testing were given to the research teams with significant experience and strength in respective areas of research.
- The approach is really a collection of small projects with no cohesion or overall focus. Interesting catalyst work is done, as is interesting alternative work, but there is no connection between the two, for example. This project has a large number of groups each going on their own way with no reason as to why they should be put together in one group. For example, ethanol and dimethyl ether (DME) will provide unique membrane challenges and it is unclear if the membrane group is targeting these. Doing durability measurements for 100 hours is not a good approach, and not much Ru dissolution should be expected. This short test does not prove the stability of a catalyst.
- The oxidation of small organic molecules on Pt-Ru-X (X = Sn, Pd etc.) electrodes has been an “attractive” research direction for decades. Therefore, it is surprising that in this proposal these systems are considered to be advanced catalysts. Although the PIs have mainly focused on activity, very little is presented about the stability of non-noble components (e.g., Sn and SnO<sub>2</sub>). It is also surprising that Cu-based nanowire (NW) has been used as a “support” for depositing Pt-Ru alloys. Having Cu in fuel cell environments is undesirable because even a trace level of Cu (from Cu underpotential deposition) would have a huge inhibiting effect in the electrocatalysis of small organic molecules. The computational approach the PIs used to find a new generation of catalysts is appreciated; however, the leading role of density functional theory still draws some skepticism. This is simply because, in addition to strain, which may or may not have a significant effect, the defects are usually playing a much bigger role, especially those created on thin metal films. The combination of FTIR with electrochemical experiments is good and is the right direction to go. In general, the approach is good, but could be improved.
- The overall approach in this effort is to develop advanced catalysts and materials concepts for direct oxidation fuel cells designed for portable power. It incorporates (1) advanced anode catalysts, (2) electrode structure, (3) hydrocarbon membranes, and (4) extending to more complex fuels, such as ethanol and dimethyl ether. The PIs identify a project success for direct methanol catalysts on the basis of ultra-thrified PtRuSn catalysts where 200 mA/mg Pt activity is claimed. This catalyst is not new and the performance

improvements in terms of lower loading, etc., are mostly a function of electrode structure and possibly the higher concentration methanol (2M) and elevated temperatures of 80°C. These systems have been extensively tried in several commercial entities with very limited success in terms of its sustainability. This aspect is manifest in the durability tests where, instead of a full cell cycling test, a DHE-based half cell is used with H<sub>2</sub>O (2M MeOH) at the working electrode and H<sub>2</sub> on the counter electrode. This does not provide a proper projection to cell operating conditions, wherein cycling and resultant effects at the interface cause severe losses. It is suggested that this approach to a durability test will never provide proper information on the stability of these systems in a working direct methanol fuel cell (DMFC). In addition, the use of Cu NWs is not without its problems, with issues related to its possible poisoning of the interface. No one in the commercial arena uses Cu as an additive in any form, including core materials, such as Cu NWs, due to their deleterious effect on the cathode.

## Question 2: Accomplishments and progress toward overall project and U.S. Department of Energy (DOE) goals

This project was rated **3.2** for its accomplishments and progress.

- In a short period of time, the PIs have made great progress towards the objectives. This is particularly true for lowering the amount of Pt without paying penalties in catalytic activity.
- Los Alamos National Laboratory has made good progress on increasing the anode activity; this is the most important contribution. The researchers do not properly address whether these materials can be made at a low cost. It is difficult to understand how the membrane work fits in here. The block copolymer work for DMFC has been looked at many times, including by McGrath. It is hard to see what is novel here.
- Significant developments were reported in lowering the catalyst loading at the interface, providing a pathway towards making these systems more viable. However, faulty use of durability tests provides no projection of understanding the sustainability of these systems for practical use. The steady state chronoamperometric (CA) results are a testament to quick poisoning of the catalysts, which are in direct contrast to pseudo steady-state polarization measurements. The PI should explain the differences between the CA results and those from polarization measurements.
- The team reported that the tetramethylbisphenol A (TM)-based, multi-block copolymer demonstrated a reduction in methanol crossover by 54%. However, the 54% decrease in methanol crossover resulted in only a 6% increase in power density. The polarization curve clearly shows that the MEA containing the TM-based, multi-block copolymer membrane suffers from mass transport limitations, which may be responsible for the lower performance increase. The team should focus on enhancing the mass transport gain and maximize the gain due to lower methanol crossover.
- The team achieved the methanol mass-activity target of 200 mA/mg Pt at less than 0.25 V (80°C) with an ultrathinned advanced anode catalyst (uTAAC), but obtained high DMFC performance with an advanced anode catalyst (AAC). The high mass activity of the uTAAC catalyst is not translating to high polarization performance due to its cathodic loss. Therefore, either of these two catalysts (uTAAC and AAC) may not be suitable to provide high performance at the system level. These two catalysts have individually achieved two different DOE performance goals; however, for constructing a high-performing DMFC power unit, only one anode catalyst with high methanol activity as well as polarization performance is needed. Having two different anode catalysts meeting two different goal targets is not practical.
- The work on “ultrathinned” Pt/Ru/C catalysts is outstanding, with the PI strongly focused on DOE goals and strongly committed to finding and mitigating potential problems. This is as might be expected for a national lab PI, but even so, he appears to be a good group leader. Other projects are all very good to excellent. In some cases (e.g., catalysts supported on Cu and on Au), there could be more work done to address durability; in other cases, early-stage work has not yet been translated into prototype power sources. There is more to be done, but overall this is a very strong effort with many accomplishments all at the cutting edge of fuel cells utilizing liquid fuels.
- Very good progress was made in anode catalyst research. On the membrane research, it would be very useful to check how the TM membrane/electrode interface changes in a durability test to validate the hypothesis that matching water uptake to Nafion can improve interface durability. Also, it is perhaps more useful to have the membrane swelling ratio data. The milestone for ethanol oxidation catalysts is delayed. The SnO<sub>2</sub>-modified catalyst made by micro-emulsion synthesis has much lower activity than the one made

by the Cu UPD method. No explanation was given. It is important to understand the cause, which can help further improve the catalyst. On the MEA durability test, the new results showed that catalyst-layer cracking has no major effect. The question still remains unanswered as to why MEA failed faster in a high-methanol concentration operation.

### Question 3: Collaboration and coordination with other institutions

This project was rated **3.3** for its collaboration and coordination.

- As in the past, the lead PI put together an outstanding team of researchers. The team consists of a good mix of university, national laboratory, and industrial partners. The collaboration with SFC Energy (SFC) and Oorja Protonics is very advantageous to the team since SFC has expertise in portable DMFC systems and Oorja has expertise in high-power DMFC systems. The team can obtain valuable information on the material/performance requirements for portable-power and high-power DMFC systems.
- The PI reports good collaborations among the partners in this effort. Some of the advanced concepts have yet to be incorporated into working fuel cells at SFC, however. All SFC results were with conventional catalysts and loadings. The highlighted advanced catalysts actually operating in an SFC cell will be proof of concept in this proposed effort.
- There are five focus areas and it is not at all clear how they are related or how these groups are working together.
- The individual efforts are all well executed, but there was not much synergy among them. They seem to hang together mostly because they are all funded by the same project.

### Question 4: Relevance/potential impact on advancing progress toward DOE research, development, and demonstration (RD&D) goals

This project was rated **3.3** for its relevance/potential impact.

- Most project aspects align with the Hydrogen and Fuel Cells Program RD&D objectives.
- This team has done excellent work addressing the key issues in DMFC and related liquid-fuel fuel cells for portable applications.
- Each of the project areas is relevant. Improving catalyst activity, developing better membranes, and using ethanol would all greatly help this field. It is not clear if any work was done on electrode structures. The ideas they wanted to pursue are not shown here.
- The potential impact of this effort is yet to be realized. As a practical fuel cell person, the proof of concept is yet to be shown with the new materials—be it the catalysts shown in this effort or the membrane. Most work in their limited half-cell environments, but these types of fuel cells are beset with best intentions gone unrealized. Two years on, we should be expecting some full cell results with the new materials shown in this effort.
- The project is relevant to the objectives of the DOE Hydrogen and Fuel Cells Program. This project is focused on the development of advanced materials, such as catalysts, membranes, electrodes, and membrane electrode assemblies for DMFC application, which is expected to be capable of fulfilling cost, performance, and durability requirements established by DOE and are very important for the commercialization of DMFC technology.

### Question 5: Proposed future work

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

- The future work described is aligned with the proposed work of the project.
- Proposed future work is a sensible extension of the prior work. This project is nothing unexpected, just a continuation of what has been started.
- The project is still about Pt-Ru (with some small addition of the third element). It would be good to see some design work on materials that are really novel.

- The researchers are proposing more of the same. This is a mature project and, in the final year, the team should be down-selecting, demonstrating scalability, and able to meet cost/performance targets and durability. None of these are discussed in the future work.
- There is a proper delineation of the future work. This reviewer recommends more tests in SFC hardware with proper, long-term, chronoamperometric data interspersed with start-stop conditions.

#### Project strengths:

- Catalyst work is very good, especially work on developing catalysts for ethanol and DME.
- This is an outstanding group of scientists. The catalysts are designed with a basis on a deep understanding of electrocatalysis, syntheses, and the transformation of fundamental science to real applications.
- The new materials concepts, including catalysts and membranes, are juxtaposed with characterization and a portable fuel cell partner (SFC). Good collaborations are shown. The results in some cases are promising, albeit in controlled, half-cell conditions.
- The team is well organized and capable of developing a DMFC membrane and MEAs. The team is composed of respectable research organizations with adequate expertise. Overall, the team is equipped with a necessary knowledge base, resources, and industry/academia/national lab mix that is required for the success of this project.
- New catalysts, and focus on high activity/low PGM is a strength. The team is cognizant of performance, cost, and durability issues. Low-risk work with methanol is balanced by high risk with ethanol and DME. Overall, this is a strong effort.
- The approach is good and involves experimentation and modeling guidance. The team is very strong and well assembled. This project has good planning, collaboration, and coordination. The results and progress are impressive and could have a significant impact on the portable power market using direct liquid fuel cells.

#### Project weaknesses:

- The combination of a large number of research organizations, which may be a management challenge for the prime organization, is a weakness.
- Coordination among the seven thrust areas could be better. It seems that each group works pretty much on its own.
- The catalyst concepts are not new or novel and suffer from the same issues described in literature dealing with their stability. The membrane effort is also not new and follows the same lines of previous efforts. Proof of a remarkable breakthrough awaits actual fuel cell results in SFC hardware.
- Oxidation of small organic molecules on PtRuX (X = Sn, Pd, etc.) electrodes has been an “attractive” research direction for decades. The PIs should go beyond PtRu systems; should avoid Cu; and, because of stability problems, should replace Sn/SnO<sub>2</sub> with more stable non-noble elements.
- The lack of cohesion among the different focus areas and lack of long-term testing (1,000 hours is only a 2-month test), is a weakness. This is the fourth year of the project and the testing should have been done for all of their promising catalysts. For ethanol and DME fuel cells, complete conversion to CO<sub>2</sub> is the most important/interesting thing, but that is not shown here. The goals at the beginning are given in terms of cost, efficiency, and energy density. These are the targets and none of the work is reflected back on these targets.
- On the membrane research, it would be very useful to check how the TM membrane/electrode interface changes in the durability test to validate the hypothesis that matching water uptake to Nafion® can improve interface durability. Also, perhaps it is more useful to have the membrane swelling ratio data. The milestone for the ethanol oxidation catalyst is delayed. A SnO<sub>2</sub>-modified catalyst made by microemulsion synthesis has a much lower activity than the one made by the Cu UPD method. No explanation was given. It is important to understand the cause, which can help further improve the catalyst. On the MEA durability test, the new results showed that catalyst layer cracking has no major effect. The question still remains unanswered as to why MEA failed faster in high methanol concentration operation.

**Recommendations for additions/deletions to project scope:**

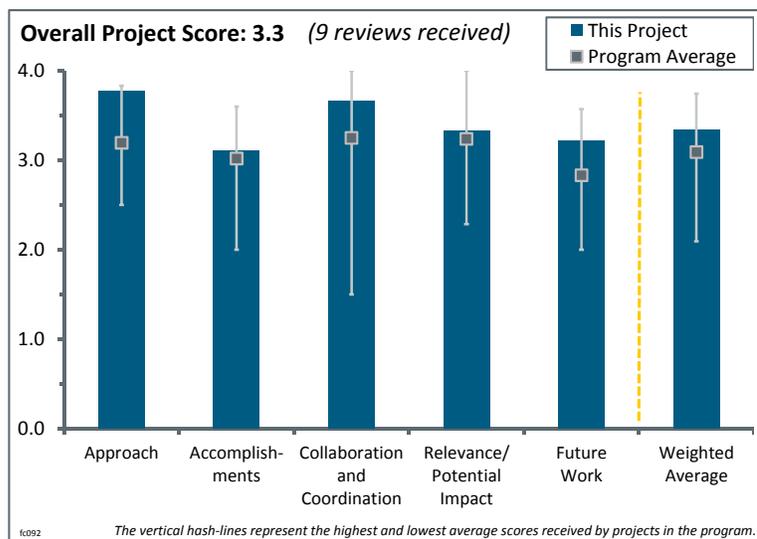
- One thing to add to this project is a cost analysis on the catalyst and membrane.
- Any use of Cu NWs should be avoided due to their well-known poisoning effect when dissolved. The proper choice of durability tests should be incorporated in this effort.
- Given the research team's strength in direct fuel systems, the team should drill down to the fundamentals of DME fuel systems and determine the viability of the success of DME technology as a competitive technology to DMFC.
- The membrane work should include a look at ethanol and DME crossover to bring it into the fold of the overall project. Efforts need to be done to show how this work moves toward DOE's goals for efficiency, power/energy density, and cost.

## Project # FC-092: Investigation of Micro- and Macro-Scale Transport Processes for Improved Fuel Cell Performance

Jon Owejan; General Motors

### Brief Summary of Project:

Expected outcomes of this project include (1) development of a validated transport model, including physical and chemical properties of all the fuel cell components; (2) public dissemination of the model and instructions for exercising the model through a project website that includes all data, statistics, observations, model code, and detailed instructions; (3) compilation of the data generated during model development and validation; and (4) identification of rate-limiting steps and recommendations for improvements to the plate-to-plate fuel cell package. Model validation with baseline and auto-competitive material sets will provide key performance limiting parameters.



### Question 1: Approach to performing the work

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

- This project has a wide-ranging analytical approach, which addresses major barriers.
- The project approach is logical in design and reasonable in scope. The project is well-balanced between practical in-situ characterization/diagnostic experiments and directly insightful modeling.
- This is an excellent project approach to improve the fundamental understanding of what limits state-of-the-art fuel cells and thereby enables commercially viable automotive fuel cells. Additionally, websites and publications ensure that understanding is available for others to access and use.
- This project has a very substantial and well-articulated, multi-scale approach that includes substantial diagnostics, methods development, and sensitivity studies. Unfortunately, there were no considerations for freezing conditions.
- The proposed model could be very useful; however, there are some doubts about the robustness of the model. With so many parameters, the physics is sometimes lost. It is not clear whether the team has done a sensitivity analysis to test how much the predictions of the model respond to changes in the parameters.
- The approach is great. It leverages General Motors' (GM's) work and keeps the project relevant to automotive applications. Making data available to the community in general via a website is a great strength of this project. One concern is that it is not clear if the baseline or the auto-competitive materials are available for other researchers to purchase. This might be needed if additional data on materials properties are required.
- This project has an outstanding modeling and experimental approach to understanding transport processes in polymer electric membrane fuel cell (PEMFC) membrane electrode assemblies (MEAs). It has contributed significantly to the knowledge of controlling factors in PEMFC performance and the design of improved electrodes.
- GM's approach combining ex-situ materials property measurements, multi-scale component level models, a 1+1D simplified transport model and extensive validation of the model with data from two material component sets would be difficult to improve on. The experimental effort is measuring the relevant parameters. The thin film measurements are now being attempted on relevant substrates.
- The principal investigator (PI) has done an excellent job of pulling together the approach to try and solve a complex modeling problem. As the project has evolved, the PI (with the research team) has been able to

link findings from the model development work to specific component attributes that have subsequently been employed to design new materials for fuel cell applications. The hallmark of any successful modeling effort is the application to and the improvement of real-world systems.

## Question 2: Accomplishments and progress toward overall project and U.S. Department of Energy (DOE) goals

This project was rated **3.1** for its accomplishments and progress.

- The overall progress is very good. Although details of the model are not provided, critical aspects seem to be included. The goal of using the model to identify critical components is excellent.
- While the progress has been slowed this past year by the reorganization and relocation of GM, the overall progress throughout the duration of the project and the dissemination of the progress has been very good.
- This project has made good progress over the past year; however, it seems like there is still a lot to finish with only 15% of the budget remaining. Additionally, this project has made significant contributions towards overcoming barriers, but there are no real game-changers here.
- The project almost completed all its objectives and has good model dissemination to the community. Due to the high impact of non-active transition areas, it would be useful to include the results averaged over the load profiles rather than at the steady states only. Also, transient responses would be valuable to present.
- The project has achieved several relevant accomplishments and has made good progress. Of particular note is the work to understand the O<sub>2</sub> transport losses at the ultra-low platinum group metal (PGM) levels, which is a key limitation for achieving DOE's PGM targets for 2017 and beyond for many catalyst systems.
- The project's progress is broadly on track. This project has demonstrated good correlation between models developed and experimental results. The project is a little behind (approximately six months), although this is not a significant issue since the models are developed and the extra time is required to do sensitivity analysis and make the information public.
- There were numerous accomplishments in all areas. One area that stood out was the collaboration with the National Institute of Standards and Technology on the use of the neutron imaging techniques to monitor water transport. These studies are critical to improving the designs of the fuel cell "plumbing," the anode and cathode outlets. Pore and slug flow issues were clearly identified by neutron imaging, and the GM team used these to modify designs, which is excellent.
- Good progress was made both in modeling and in experiments. The project leverages a lot of GM efforts in this area. There are concerns about the errors for the auto-competitive material. It is not clear if this is similar to the baseline material, and if any other data (other than voltage on a polarization curve) is used for model validation. For example, it is not clear if the model can predict the water balance in the various material sets, or if it can predict the water profiles (from inlet to outlet) obtained from the neutron imaging. More needs to be done to convince the community that the model has predictive power.
- The project has provided a useful, very complete dataset for baseline materials; has developed a second auto-competitive materials set showing performance and water content; and has made the dataset publicly available. The gas diffusion layer (GDL) characterization work is important. Measurements of thermal conductivity as a function of saturation and compression are useful. The work characterizing the effects of droplets and films on O<sub>2</sub> resistance, the transition from slug to film to mist flow, and the channel effects have been beneficial. The model does not perform as well at high current density, with more than 20 mV error for more than half the cases shown for the baseline materials set (slide 19). In particular, it appears to systematically over-predict voltage at low temperatures. In addition, the model does not do as well at predicting current density for the auto-competitive dataset. There appear to be issues dealing with liquid water or high water saturation. The component model appears to use interfacial resistances at the Pt-ionomer and ionomer-gas interfaces as fitting parameters, and it is not clear whether or how these interfacial resistances would be adjusted for other materials sets. The data presented, which have been interpreted as indicating interfacial resistance at the Pt and ionomer interface, is not conclusive. The data on slide 16 appears to fit a simple logarithmic dependence of the resistance on the ratio of the ionomer area to the Pt area and does not appear to have a minimum, as the model with the additional interfacial resistances would predict. The O<sub>2</sub> transport measurements did not show any interfacial resistance. Most of the thin film studies showing changes compared to the bulk material appear to be on SiO<sub>2</sub> substrates, though it is unclear whether the substrates are Si or SiO<sub>2</sub>. Thin film studies need to concentrate on films with representative

substrates. The project is moving in that direction, though it appears these studies may not be complete by the end of the project.

### Question 3: Collaboration and coordination with other institutions

This project was rated **3.7** for its collaboration and coordination.

- This project has good collaboration.
- Although many partners are involved, their specific participation is clear.
- This project has an impressive array of modeling and experimental experts.
- This is a large and diverse team that seems to have been well coordinated.
- The collaborators contributed significant material and data sets, including diagnostic analytical methods.
- The project appears to have managed collaborations between GM and its partners effectively.
- This project has good collaboration with other institutions, especially on more fundamental property measurements/characterization. It is not always clear from the presentation how relevant some of the items are (e.g., using TEM of thin films of an ionomer to elucidate transport characteristics and then inferring that this may be what happens in a catalyst layer).
- This project has great collaboration with various universities where the fundamental work is done at the universities and the modeling and validation is done at GM. This project has effectively used the transport modeling working group to foster collaborations.

### Question 4: Relevance/potential impact on advancing progress toward DOE research, development, and demonstration (RD&D) goals

This project was rated **3.3** for its relevance/potential impact.

- Posting a simple demonstration of the use of the model could be very interesting and useful to potential users.
- This project has made good contributions towards the DOE Hydrogen and Fuel Cells Program goals and objectives. The project has not made any breakthroughs though.
- The project addresses a key area for fuel cell understanding, namely, the impact that water production and its movement has on the operation of fuel cells (with a focus on the sub-component level).
- This project addresses transport processes that limit performance at full power. The performance at full power is instrumental in determining system size and cost. An effective transport model would help developers decrease transport losses and achieve higher power with smaller systems, decreasing the cost.
- Water transport is an important issue. The role of the ionomer in the catalyst layer, especially at the low loadings, is even more critical. The project is doing a great job in addressing these issues. Innovative ideas are lacking, but at least a good evaluation of the problem has been presented.
- The tools and knowledge developed in this project have the potential to impact the future direction of catalyst layer design and to guide the understanding of performance limitations in catalyst layers based on high specific activity catalysts with the ultimate goal of designing and fabricating high-performance electrodes to reduce PEMFC cost.
- The work is directly relevant to the Program's barriers of performance, water transport within the stack, system thermal and water management, and startup/shutdown. The results clearly indicate that the O<sub>2</sub> transport issue with low-PGM cathodes is a potentially significant barrier to achieving DOE's PGM targets.

### Question 5: Proposed future work

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

- The proposed tasks are appropriate and will complete the objectives.
- This project should focus on finding links from various ionomer studies.
- The proposed future work is appropriate based on the time left in the project.
- The project is in its final phase and looks as though it will conclude very successfully. Well done!
- The team primarily needs to complete documentation of the work that has already been done.

- The project is near its conclusion. The proposed work is what is needed to finish the model and complete the project.
- The project is ending and most of the GM people involved in the project have left, including the PI. GM should continue to engage with the various national laboratories and universities involved in the Program to address the problem of transport losses in low-loaded catalyst materials.
- The funded portion of this project has ended and it is currently in a no-cost extension for the few months left in the project. The future work is finalizing and disseminating the models, which is commensurate with the short time left in the project.

### **Project strengths:**

- This is a diverse team that provides open access to results and focuses on relevant issues.
- The model dissemination is very useful through the interactive website.
- This project's public distribution of the validation dataset has provided a valuable resource for the community.
- The experiments are integrated in a simple model, which will be useful to assess fuel cell performance and the role of the various components.
- Strengths of this project are the multiple-component approach to water management modeling (i.e., plate, GDL, and catalyst layer effects) and including the evaluation of an auto-competitive sample for longer term DOE targets.
- This project has excellent collaborations with universities and transport modeling working groups. The extensive data set was made public on the website and was shared with the community. This project sets a great standard for other DOE projects to follow.
- The project is well balanced between practical in-situ characterization/diagnostic experiments and directly insightful modeling. The project addresses the key barriers towards understanding and improving the transport issues for lower PGM MEAs. The publishing of all project data and models is of tremendous benefit to the PEMFC community at large.

### **Project weaknesses:**

- No real weaknesses are evident.
- The PI and several other project personnel have left GM.
- This project does not have a clear description of how the various components of the model may interfere with each other, thus making model results difficult to interpret.
- The model this project developed is somewhat specific to the architecture of the flow-field with the specific transitional areas studied, which limits its industrial applicability.

### **Recommendations for additions/deletions to project scope:**

- Since the project is near completion, no deletions/additions are suggested.
- This project should work on better model validation in addition to the needed voltages from polarization curves.
- It would be interesting to see the model predictions for the material sets developed with the gradient features, including through and in-plane direction, or for the project team to produce narratives on the model's outcome, if such material is developed.

## Project # FC-096: Power Generation from an Integrated Biomass Reformer and Solid Oxide Fuel Cell (SBIR Phase III Xlerator Program)

Quentin Ming; InnovaTek

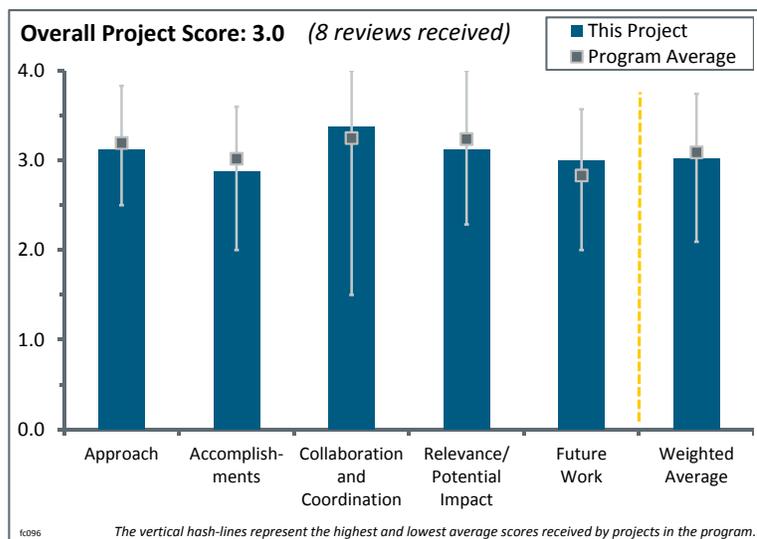
### Brief Summary of Project:

The goal of this project is to develop and demonstrate a fuel cell distributed energy system that operates with second-generation biofuels. The objectives are to establish a design to meet technical and operational needs for distributed energy production from renewable fuels; design, optimize, and integrate proprietary system components and balance-of-plant in a highly efficient design; and demonstrate the technical and commercial potential of the technology for energy production, emissions reduction, and process economics.

### Question 1: Approach to performing the work

This project was rated **3.1** for its approach.

- The approach, which is now focused on natural gas, makes sense.
- The project has been focusing on (1) improving system design and operating efficiency and (2) performing economic analysis.
- This project went well and reached all milestones. InnovaTek did a very good job on reforming technology development and system integration.
- It is difficult to independently validate how well the principal investigator (PI) is doing in meeting project goals and objectives. No data or performance metrics are really provided.
- The approach is to develop and demonstrate a fuel cell distributed energy system that operates with second-generation biofuels. The system is based on InnovaTek's steam reforming process and a Topsoe solid oxide fuel cell (SOFC). Non-food biofuels include pyrolysis oil and biokerosene, which is processed locally, and is to be demonstrated in Richland's renewable energy park and tied to the grid.
- This project is focused on developing the biomass reformer. The fuel cell stack is outsourced. Early market entry is assumed with natural gas fuel. There are other fuel cell developers who are also working on 5 kW systems. It is not clear what differentiates InnovaTek's product from others. The cost for 5-kW systems at the production rates mentioned in the study are very optimistic.
- The project develops technology for the production of fuel-cell power from renewable biofuels. Fuel cells yield more useful energy from a fuel and reduce CO<sub>2</sub> emissions and criteria pollutants. Bio-kerosene is a refined fuel and will likely be expensive. The analysis presented indicates that the fuel needs to be \$3.50 after taxes to be economically feasible or attractive.
- This project is targeting cost, durability, and performance and it appears that two of the three are addressed. Durability has not been addressed in the approach. A full bill of materials estimates, an analysis of the cost and design through modeling and simulation, and the cost of power versus financial benefits are all excellent pieces of this project's approach. The reviewer would like to see the improvements that contributed to taking the system from 37.5% efficient to 41%. It is not clear how much is attributed to advances in SOFC stack technology versus reformation improvements versus revised flow paths to enhance thermal energy.



**Question 2: Accomplishments and progress toward overall project and U.S. Department of Energy (DOE) goals**

This project was rated **2.9** for its accomplishments and progress.

- The project achieved the milestone of system efficiency greater than 40%. There are reduced part counts. Details on the system's operating characteristics are lacking.
- The accomplishments to date are very good. They have reduced the costs of various components that they are developing. The initial performance is promising.
- For the bio-kerosene reforming, the catalyst performance was very stable for more than 900 hours. The SOFC was operated at 750°C. Since the reformat had approximately 10% methane at 750°C, it is not clear if there is any carbon deposition on the fuel cell electrode.
- The reviewer would like to see the performance of the reformer for both bio-kerosene and natural gas, and would also like to understand the cost projections with variable volume. The production volume is not specified in the analysis; it is a key parameter. Efficiency values in the presentation did not specify what fuel was used.
- Thus far, the program has hit its milestones, met the go/no-go criteria, and addressed the performance barriers for this program. Achieving over 40% efficiency is important, especially when it is being accomplished on a bio-kerosene. The reduction of reformer complexity and optimized flow paths would take advantage of the heat created in the system and will bring the system closer to meeting the criteria and barriers set out to be reached through this project.
- InnovaTek's proprietary catalyst reforms bio-kerosene during long-term tests. It is an integrated system that produces power from bio-fuel. The measured efficiency needs to be higher to be attractive. A different SOFC may produce better results. It is not clear how many hours were actually measured, if the total system electrical efficiency was 27.49%, and if the test ran 200 hours. The test conditions, such as temperature, utilization, etc., were not specified. It was unclear if the stack showed degradation or coking.
- The stack was operated at 65% efficiency. The high efficiency was achieved by operating at a very high voltage and low current and power densities. The low power density will lead to higher stack costs. The reviewer suggested showing the results of a tradeoff analysis between capital cost and efficiency. The reformer has been operated for 900 hours and the reformat contains approximately 10% methane. While 4%–8% methane is desirable for stack cooling, the higher methane content may lead to excessive cooling at the entrance. The extent of stack cooling resulting from internal reforming in the anode is not clear. This data was not presented. Stack current density and durability have improved. Economic analysis is optimistic, assuming 45% net alternating current efficiency.

**Question 3: Collaboration and coordination with other institutions**

This project was rated **3.4** for its collaboration and coordination.

- The PI seems to have a capable team assembled.
- This project is collaborating with partners very well.
- InnovaTek has good cooperation with the fuel cell industry, national laboratories, and government.
- This project should pursue continued collaboration with the fuel cell developer (Topsøe Fuel Cells).
- InnovaTek is working with manufacturers and a national lab and is supporting students at universities.
- Leveraging regional advantages and a cost share with Impact Washington will help this program reach a larger audience. Leveraging the work of other DOE-funded projects increases the efficiency of DOE investment and prevents duplicative work. Collaborating with local businesses in creating H<sub>2</sub> from renewables is the best way to bring the cost down in this particular region.
- InnovaTek seems to be limiting its focus to fuel processing and systems integration. It should narrow further as total system manufacturing, warranty, etc., is going to be extremely challenging for such a small company. It would be better to see a systems integration partner that can help with some of the systems integration expertise and customer relationships/specs input that will be hard for a small company to develop.
- The strategic partners are well selected. Pacific Northwest National Laboratory and Washington State University-Bioproducts, Sciences & Engineering Laboratory provided bio-oil made from wood sawdust.

Boeing provided bio-kerosene made from camelina. The City of Richland Electric Utility provided the site for field demo. Mid-Columbia Energy Initiative is a strategic partner.

#### Question 4: Relevance/potential impact on advancing progress toward DOE research, development, and demonstration (RD&D) goals

This project was rated **3.1** for its relevance/potential impact.

- The project fully supports the objectives of the Hydrogen and Fuel Cells Program (the Program).
- The work is certainly relevant to and the Program's R&D goals. Bio-fuel is a renewable energy with a C effect. Completing this project is the way to advance technologies and generate jobs in the states.
- The critical work here is the biomass reformer. If InnovaTek can meet cost and performance goals on the biomass reformer, the project will be successful.
- This technology will help shift the primary energy source for H<sub>2</sub> from fossil fuels to renewable non-food biomass. Use less fuel through high-system efficiency by effective thermal integration and off-gas recycling. Provide an alternative method for distributed power generation near the source of the feedstock, enhancing grid stability.
- The technology for fuel processing and the stack is being advanced by this project. The progress in stack technology is good and needs continuing support to become competitive. The fuel processor and stack technologies need to address sulfur in fuels since most fuels, including natural gas, contain sulfur and without the broader fuel application it will be difficult to succeed commercially.
- One solution to utilizing bio-fuels is through the reformation of liquid fuels. They are easy to transport and store. This project has a high potential impact on proving that the efficiency and performance of using this resource is feasible. Making use of renewable, distributed, non-food-based biomass, demonstrating the feasibility and efficiency of it, and providing power has a large impact.
- If successful, the project could be relevant to DOE's goals of deploying stationary fuel cell systems for residential and light-commercial applications. It is a long road and will require significant extension of operating lifetime and extreme reliability (both of which will cost a lot of money), as well as a company with a balance sheet to service the customer with a warranty. The outcome of this project could show that a small SOFC system with a reformer might be a good concept to develop.

#### Question 5: Proposed future work

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

- The proposed future work is vague.
- The system testing in the next phase is very critical.
- The proposed future work is consistent with the project plan and the technical progress.
- For the for-profit company, the target is to make a profit. InnovaTek is on the right track to make products.
- The project appears to be partially funded with that assumption that the future work identified makes sense.
- A higher measured efficiency will be obtained in year two with better insulation and design improvements.
- The economic analysis is needed and will be valuable in guiding the path of this project towards commercial development. A continued effort toward improving efficiency and durability is needed, but the strategy is not clear. Methane conversion in the reformer needs to improve. It is not clear what is limiting the stack current density and how it will be improved.
- The proposed future work appears to be the next logical step; however, more clearly defining how durability is going to be addressed would strengthen the project. An accelerated stress test of some kind could provide insight into the prospect of reaching the 40,000-hour life predicted. Additionally, a reforming catalyst that lasts 40,000 hours has not been proven or predicted yet. It is not clear if there is an estimated number of hours of operation that would require a reformer overhaul. Partnering with a local business to provide a real-life, long-term demonstration of the system would also prove useful and provide an excellent learning opportunity.

**Project strengths:**

- Development of the biomass reformer is a strength of this project.
- Development of the fuel processor and system design and integration are strengths.
- The project has demonstrated improvements in durability and performance. More than 40% efficiency has been demonstrated. The economic analysis shows a path to commercialization.
- It is difficult to independently ascertain the project's strengths beyond the claims made by the PI. Very little data was presented that is specific to the technology.
- Achieving high efficiency from reforming biomass and producing power from non-food biomass are strengths of this project.
- The durability of the SOFC and reforming system is still an issue. Some long-term tests are needed. On/off tests with cycles are also needed for end users.
- This project has a good focus on natural gas as a bridge fuel. InnovaTek seems to have limited its scope to systems outside the stack. Limiting the scope and leveraging partnerships makes sense.

**Project weaknesses:**

- There are no weaknesses, just challenges for the commercialization.
- It is recommended that more emphasis be placed on evaluating the system's operating characteristics and the effects of key operating parameters on system performance.
- There should be more focus on durability and identifying the expected maintenance schedule and the cost and time associated with it, including the operational availability.
- Some weaknesses in the presentation were omissions of critical information. For example, efficiency was quoted without specifying what fuel was used. Another example was the capital estimates for the units were reported without referencing the production volume. Also, it would make sense to have even more partnerships in the system integration domain.
- The high efficiency has been demonstrated at the cost of low-current density and higher capital cost. The economic analysis is based on a very optimistic price of bio-kerosene and anticipated future efficiency values. The methane yield in the reformer is high. The presentation did not clearly distinguish between the actual experimental work from which data was obtained and the projected scenario that was used to estimate the performance and cost.
- Very little data was presented that was specific to the technology. No information was presented regarding the reformer technology, catalyst, and method of operation. It is not clear from the presentation materials how the system is to be used (continuous use, back-up, or stand-by). This information is important to know since the temperature cycling may significantly impact the SOFC, reformer durability, and long-term performance. A slide is given regarding catalyst durability, but these data appear to be for continuous operation. It was not clear if there was a concern with poisoning by the odorant levels in natural gas. The PI does not explain the source of performance decrease with time.

**Recommendations for additions/deletions to project scope:**

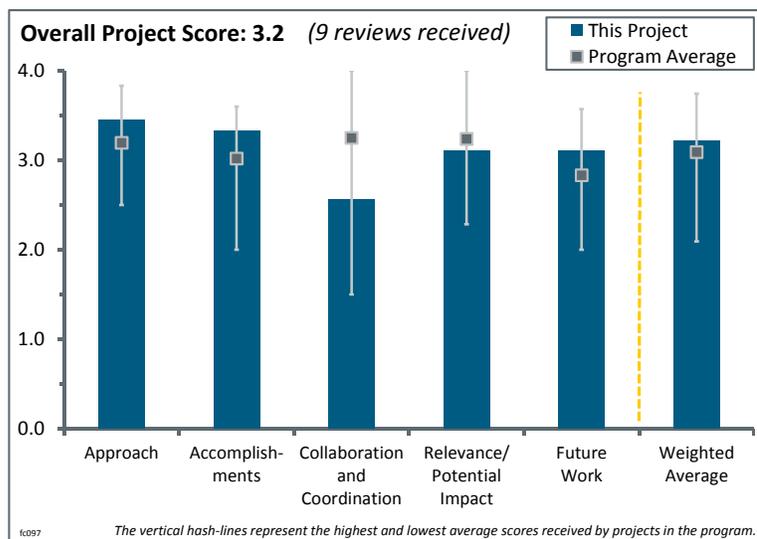
- The project should develop additional partnerships for system integration.
- The project should partner with FuelCell Energy in the SOFC area. Surely they can produce a 1 to 5kW SOFC stack.
- The PI should provide more technical details within the obvious constraints of protection of proprietary information.
- The project should focus on the performance and durability of the components and the integrated hardware in the laboratory. The researchers should investigate operations with sulfur in the feed to the reformer and the stack. They should also study the tradeoffs between efficiency, current density, and cost, and they should defer the field demonstration.

## Project # FC-097: Stationary and Emerging Market Fuel Cell System Cost Analysis – Material Handling Equipment

Kathya Mahadevan; Battelle (presented by Vince Contini)

### Brief Summary of Project:

The objective of this project is to assist the U.S. Department of Energy (DOE) in developing fuel cell systems for stationary and emerging markets by developing independent models and cost estimates. The applications modeled include primary power (including combined heat and power), backup power, auxiliary power units (APUs), and material handling equipment (MHE). Fuel cell types modeled included polymer electrolyte membrane (PEM) and solid oxide fuel cell (SOFC) technologies. Multiple production volumes and fuel cell sizes are modeled. The project also addresses cost reduction needs for non-automotive applications by performing cost analyses of fuel cell system designs.



### Question 1: Approach to performing the work

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

- The approach is systematic, thorough, and has focused in the last year on the MHE market. Gathering stakeholder input and feedback throughout the project is important for the success of the project.
- The methodology is excellent; however, as with any model, the accuracy of the inputs are critically important. Some of the cost inputs appear to be one to two generations old.
- The project directly targets cost and manufacturability barriers, which in turn will affect customer acceptance. Starting with fuel cell systems for MHE is appropriate, as are the assumptions about production volume and the bill of materials for the 10 kW and 25 kW systems.
- This is a good method for system costing; however, it is surprising that the cost estimates are two orders of magnitude higher than light-duty automotive cost estimates (as per Strategic Analysis, Inc. [SA]). It would be beneficial to benchmark the models against each other.
- Studying the cost at multiple production levels is a valuable step of this project. It seems like the process of gathering vendor quotes could be influenced by many factors. Some of the specifications were included, but the ranges of inputs (or number of inputs) from vendor quotes were not clear.
- The approach to estimating production costs appears to be consistent with other DOE-sponsored cost analyses, so results can be compared when differences in system configurations are taken into account. The costing methodology used by Battelle is used by SA and other companies and is a robust method for estimating manufacturing costs.
- The project is effective in addressing most of the stated barriers, but the project is very dependent on the design for manufacture and assembly (DFMA) software and many of its embedded assumptions, and it is using generic designs. The researchers could make more effective use of their industrial partners to explore the extent to which DFMA assumptions are not necessarily applicable, and the extent to which generic designs are not representative of what is or will be deployed.
- As identified in slide 5, the approach is systematic and appears to cover the relevant areas. This project has good validation from the industry. The balance of plant (BOP) is a difficult area for obtaining good cost data due to the breadth and variety of system components, and it represents a major cost driver. System

integrators understand this and are working to get the parts count down, but this will remain difficult for the project to address.

- This project takes a very detailed approach to determining the costs associated with manufacturing MHE fuel cell systems. Most of the modeling inputs seem reasonable. One exception is the assumed battery change time in the cost of ownership results. While there are certainly battery change times of 30 minutes, these are the exception, not the rule, in the high-productivity sites where fuel cells have a play. Since the re-charge time of fuel cells is one of their primary benefits, it may make fuel cells look more attractive than they really are.

## **Question 2: Accomplishments and progress toward overall project and U.S. Department of Energy (DOE) goals**

This project was rated **3.3** for its accomplishments and progress.

- The researchers appear to be making very solid progress toward meeting their stated project objectives.
- The team has made good progress representing system complexity and modeling completeness since last year. The detailed manufacturing cost and total cost of ownership results should be useful to industry. Also, the focus of the work has sharpened to include only relevant system sizes.
- This question is really not applicable since this is cost modeling. It is providing a projection of what the future cost might be, but really it is not doing anything to drive down the cost. Once again, the accuracy of the model is determined by the quality of the inputs to parameters.
- This project has done great work with PEM systems; however, it would be at least informative to examine the effects of current density and Pt loading. The accomplishments state that SOFC/APU work has been partially completed. It would be beneficial to have shown this data (stack level for example) in relationship to PEM.
- The progress is excellent. A thorough cost analysis for two different classes of PEM fuel cell forklifts has been completed at various production levels. The BOP manufacturing costs contain two high-cost items identified as additional work and other components. A high-level breakdown of these items would be beneficial.
- The comparison between the MHE and light duty vehicle fuel cell system costs was good. The systems are similar enough in scale and application that this comparison is a useful check on the assumptions and methodology in both DOE-funded studies. Overall, the approach used for the MHE fuel cell system should be applicable to the other systems that are studied in the future.
- Overall, the project has done a good job in developing its cost models and inputting data. The models have shown where R&D effort needs to be applied to lower costs (slide 23). In regard to the capital cost assumptions, there is a large variation between \$3 million and \$20 million in total capital cost. This appears to be for the Columbus, Ohio area. It is not clear if all this equipment can fit on one acre of real estate—real estate is very expensive at \$125,000 per acre. The project should take corporate overhead and profit margins out and stay with the hard costs. Each corporation is different and the competitive situation is a driver, particularly on the profit margin. For slide 21 on Pt cost, it was not clear if the values in brackets should be swapped and what the effect was on the bottom line number of \$3,423.
- Progress has been somewhat greater than was the case last year. The conclusion that systems that do not operate 24/7 result in a value proposition for the MHE market that is not favorable is consistent with general expectations and experience. The system schematic appears consistent with MHE, but it is unclear if the system schematic represents all of the MHE systems being deployed or if the system and operating conditions have been vetted with the MHE developers. There appears to be a significant discrepancy between the BOP cost estimate of Battelle and that of SA. It would be instructive to determine where the differences lie. The MHE analysis appears to include silicone gasket material. Other alternatives should be investigated due to the tendency of the material to migrate into areas of the cell that are detrimental to performance and durability. Progress in the SOFC APU area has not been as good as in the MHE area.
- It was unclear which were new analysis results when the current presentation results were compared to the 2012 DOE Hydrogen and Fuel Cells Program Annual Merit Review system selection chart. The 10,000-hour lifetime is too low for fuel cell MHE to provide savings when compared to battery MHE. It was unclear what the reason was for selecting a 10,000-hour lifetime, thus changing out the fuel cell system every 3 years, basically on the same schedule as batteries. It was also not clear how 10 kW and a 25 kW

MHE systems were identified for the base cases. It was expected that the final estimate, with a markup, would be a price number and not a cost number. Steel tanks have been used for a while in order to reduce the cost. Steel should thus be used as the baseline, not an opportunity for cost reduction. The PI did not mention if integration into the forklift was investigated as an opportunity to reduce cost. It is unclear where the life cycle cost assumption comes from. For instance, the battery change-out time and the hours of operation per year are on the high side. The time for fuel cell refueling is higher than the average identified in the National Renewable Energy Laboratory's reporting of the American Recovery and Reinvestment Act systems. The lifecycle cost analysis assumes \$8/kg for H<sub>2</sub>, but it does not look like a monthly service charge for H<sub>2</sub> infrastructure was included in the operating cost for fuel cell MHE. Assumptions for maintenance of batteries and fuel cell MHEs are not provided.

### Question 3: Collaboration and coordination with other institutions

This project was rated **2.6** for its collaboration and coordination.

- Input from industrial partners and their feedback ensures the success of this project.
- Collaboration appears extensive regarding fuel cell stack and system design. Numerous collaborators appear to be involved that have materials, stack components, and system design expertise.
- This project needs to partner with an OEM who can provide actual volume price quotes for BOP components. Of course, the OEM will have to remove the supplier information from the quotes.
- There is a broad group from the industry providing input; however, the only company still currently active in the MHE market is Plug Power. It is understandable that they may be less willing to contribute, since they are still trying to make a business of this market. Their absence, however, is notable.
- It can only be assumed that there has been collaboration. There were no slides describing the degree of collaboration, so this is difficult to judge. It would have been useful if the project presentation followed the format requested.
- The speaker referenced getting feedback from the industry, but the work to date appears to have been solely done by Battelle. The degree of industry participation is unclear, and it is therefore recommended that it be strengthened.
- It is positive that the number of collaborators significantly increased from the 2012 review, although a leading fuel cell MHE manufacturer is not included. It was expected that there would be some collaboration with a similar project at Lawrence Berkeley National Laboratory.
- The project has a well-selected list of collaborators in the industry; however, the presentation did not make clear the extent to which these collaborators were consulted to seek key inputs on model results, particularly regarding cost sensitivity assessments. Also, it is not clear whether or how the researchers made efforts to reach out to make comparisons and seek feedback from other DOE-funded national laboratory efforts that are conducting similar cost analyses.
- Plug Power is not on the list of collaborators. They are one of the leaders in forklift sales.

### Question 4: Relevance/potential impact on advancing progress toward DOE research, development, and demonstration (RD&D) goals

This project was rated **3.1** for its relevance/potential impact.

- The project is directly relevant to a growing area of fuel cell deployment.
- This project has no real impact. It might drive people to work on only more expensive components, but that is only a good thing if the inputs in the model are correct and it does not seem like they are.
- This is an important market segment for the DOE. Understanding the costs and potential areas of improvement can be accomplished through this type of analysis.
- The cost is a key barrier that needs to be overcome in order to achieve market acceptance of H<sub>2</sub> and fuel cells. Developing accurate cost models using industry data is very important to identifying where DOE program dollars need to be invested for the good of the overall program.
- The cost analysis of materials handling fuel cell systems is well aligned with the DOE objectives. It establishes a cost baseline for the current state-of-the-art systems and identifies key components for potential cost reduction.

- In general, the project aligns well with the needs of the Hydrogen and Fuel Cells Program; however, the system boundaries set up in the cost model tend to restrict the systems cost analysis somewhat and the focus on generic design and the use of DFMA assumptions could limit the ability of this project to anticipate a broader range of cost impacts in fuel cell deployment.
- It is important that the cost projections for non-automotive systems be at the same fidelity as that for automotive systems for the same reasons, namely to assist DOE in setting appropriate targets, particularly since there is no equivalent to the U.S. DRIVE Partnership in the non-automotive space. The project is very relevant and needs to achieve the same level of detail and fidelity as the SA work on the automotive system.
- The cost analyses from this project will provide a solid baseline and future estimates for the total cost of ownership for fuel cell systems. The analysis appears to be mostly from first principles. It is recommended that a teardown analysis of an existing system may provide a stronger case for the cost estimates than the informal industry survey approach, which appears to have been used. The team identified BOP as a significant factor in the cost of 10 kW and 25 kW systems. Input materials are also a significant factor in costs (75%–83% of the total system cost). This brings to light the fact that these costs need to be reduced in some way. For example, the lithium-ion battery, the H<sub>2</sub> storage tank, and the power electronics were identified as the top three cost items in both the 10 and 25 kW fuel cell systems. However, other than recommending a steel tank for H<sub>2</sub> storage, a choice that also has safety considerations, no recommendations were presented on pathways to lower cost.

### Question 5: Proposed future work

This project was rated **3.1** for its proposed future work.

- The future plans are adequate.
- This project needs to focus on getting more accurate cost inputs.
- The future work seems light, given that 90% of the APU assessment is already completed.
- The planned future work should be relevant to the fuel cell industry. The project methodology should be relevant to these other areas as well.
- The work done on other systems is important, but it is also important to continue to refine the MHE cost analysis for comparison with the automotive projections being developed by SA.
- The team needs to consider stronger recommendations for where future manufacturing R&D should be directed to address the manufacturing costs for fuel cell systems for the applications being studied. The team should also clearly identify what the barriers are to reducing component or sub-system costs.
- In spite of this reviewer's minor concerns about the relevance of this work to the Program, the researchers have been very effective in building their future plans on past progress and are focused on the barriers they have identified.

### Project strengths:

- The methodology is a strength of this project.
- The interaction with stakeholders at all levels of the analysis is a strength.
- This project includes a detailed analysis of the costs associated with this technology.
- This project has a good modeling effort and has identified the cost drivers and areas where R&D effort needs to be applied.
- The cost analysis appears to be using a straightforward approach to estimating fuel cell system costs. The results so far, and especially the level of detail provided, will be a useful resource for those in the industry.
- The estimates at various production levels and the details at the manufacturing and stack levels are both strengths of this project.
- The list of collaborators is extensive and can provide valuable insights into the assumptions and methodologies employed in this study.
- The researchers appear to be making very solid progress toward meeting their stated project objectives. The researchers have been very effective at building their future plans on past progress and are focused on the barriers they have identified.

**Project weaknesses:**

- This project needs to refine some cost models with better data or provide options analysis, particularly for capital costs. It looks like the data may have been from one source.
- A leading fuel cell MHE manufacturer is not a collaborator. The life cycle cost analysis is missing pieces (like maintenance assumptions) or has numbers that should be updated.
- The ability to get accurate costs is a weakness of this project. Companies do not want to share this information, so it is hard to predict costs at high volumes. The researchers need to present the future cost as a range and not an absolute number. It is not clear what the uncertainty is.
- Researchers should consider activities that could allow a broader range of cost assessments that address geographic and use variations. The researchers could make more effective use of their industrial partners to explore the extent to which DFMA assumptions are not necessarily applicable and the extent to which generic designs are not representative of what is or will be deployed.
- This project appears to be one of three proceeding in parallel that have strongly overlapping objectives. It was not clear what benefits this approach provides to DOE's program mission. It is unclear how the results from this project will be reconciled with each other as it concludes. The life cycle cost analysis for fuel cell MHE versus battery-powered MHE seems incomplete. There appear to be applications for which the value proposition favors fuel cell MHE already. It is not clear if the cost analysis assumptions need further input from the industry partners or, even better, from companies that are operating fuel cell MHE already.

**Recommendations for additions/deletions to project scope:**

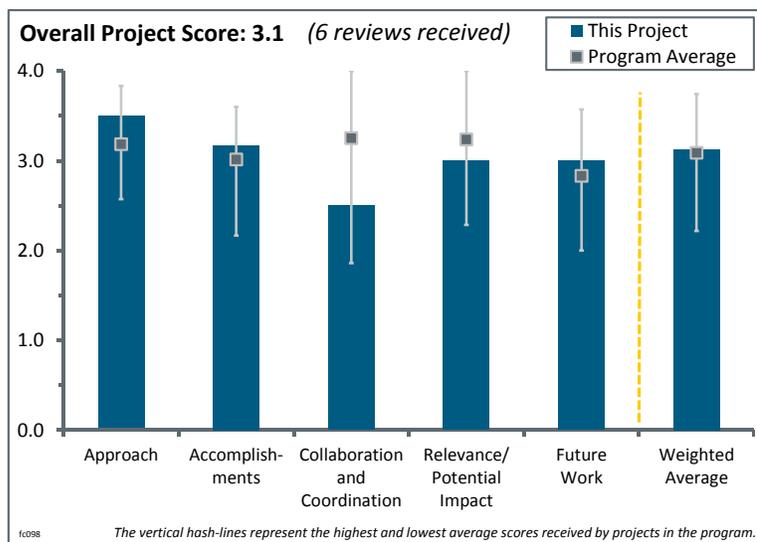
- This project should make more use of the model performance evaluation to set research priorities. It should also make more effective use of industrial partners in assessing results of the DFMA analyses.
- There are very different numbers from this analysis and its sister analysis by Strategic Analysis. It would be beneficial to benchmark the models to understand their agreements and differences.
- This project should solicit feedback from Plug Power, a key manufacturer of PEM fuel cell systems for forklifts. The researchers should also publish a report on PEM fuel cell MHE cost analysis.
- The project should take a more detailed look at battery swap times for the different classes and include these as a sensitivity in the life cycle cost analysis, as they are essential to making the business case for fuel cells in MHE work.
- It is recommended that the scope of this and the related projects be clearly defined so that each has a primary area of focus. Based on the presentations at the AMR, it seems like we are likely to get three answers to the same basic question, and it is not clear that the answers will be entirely compatible with each other.
- Since a dispersed catalyst system is being employed in the analysis, a comparison could be made between the system and the nanostructured thin film system used by SA. It would be necessary to ensure that both systems are modeled with the same fidelity to make the comparison meaningful. Alternatives to silicone gasket material should be investigated due to the tendency of the material to migrate into areas of the cell that are detrimental to performance and durability. The definition of overall plant efficiency should be explicit in the presentation. Every opportunity should be taken to compare the MHE system design and cost projections to that of SA for the automotive market. There is much to be learned from this exercise. Differences in the costing of BOP need to be examined.

## Project # FC-098: A Total Cost of Ownership Model for Design and Manufacturing Optimization of Fuel Cells in Stationary and Emerging Market Applications

Max Wei; Lawrence Berkeley National Laboratory

### Brief Summary of Project:

The objective of this project is to provide a comprehensive cost analysis for stationary and materials handling fuel cell systems in emerging markets, including ancillary financial benefits. The framework of the cost analysis includes life-cycle analysis and design for manufacturing and assembly (DFMA) analysis with additional data emerging on carbon credits, health and environmental externalities, end-of-life recycling, and reduced costs for building operation. System designs are explored to meet the lowest manufacturing cost and total cost of ownership goals as a function of application requirements, power capacity, and production volume.



### Question 1: Approach to performing the work

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

- The approach seems to be consistent with industry norms for cost analysis and the total cost of ownership models.
- The methodology is excellent; however, as with any model, the accuracy of the inputs are critically important. Some of the cost inputs are one to two generations old.
- It is not clear if the material handling equipment (MHE) was dropped off the task list or if it was completed prior to the 2013 Hydrogen and Fuel Cells Annual Merit Review (AMR).
- The proposed approach is correct and the tools seem to have been adapted to reach the objectives. The low-volume productions are well adapted for the start phase of the commercialization. The integration of regional impacts is well done.
- This project has a very good approach overall. The authors consider production volume as a primary variable and also go down to quite a low volume, which is important. The authors also look at what is procured and the different volume sensitivity of these procured items and stack parts. They also consider appropriately different system configurations for different applications. Considering externalities to the overall value proposition probably makes sense at this emerging state of the technology. The challenge is that the externalities can vary quite widely depending on where the product gets deployed and who the customer is.

### Question 2: Accomplishments and progress toward overall project and U.S. Department of Energy (DOE) goals

This project was rated **3.2** for its accomplishments and progress.

- This project has shown good overall progress to date. This is sort of a slow-paced program, which presumably is a function of the budget allocation. Hopefully, this effort can be maintained by DOE.
- The first key deliverables are only just becoming available now, making the accomplishments difficult to gauge. It appears that the project team is on track at this point.

- The manufacturing cost model that excludes many high-cost items, such as research and development (R&D) costs (especially at the low-production volume levels), is incomplete and could be misleading. The addition of the environmental/health impact is valuable.
- This question is really not applicable since this is cost modeling; it is providing a projection of what the future cost might be, but it really is not doing anything to drive down the cost. Once again, the accuracy of the model is determined by the quality of the inputs to parameters.
- Significant results are shown this year. The whole system is considered, including the tank. The stack and balance of plant (BOP) costs for different production rates are described well; however, some results are surprising, such as the BOP and reformer costs remaining almost constant regardless of production rate (100–10,000 units). This is not in accordance with other AMR-presented studies and is difficult to consider for components like compressors and humidifiers.

### Question 3: Collaboration and coordination with other institutions

This project was rated **2.5** for its collaboration and coordination.

- The collaboration appears very fair. The impression is that Lawrence Berkeley National Laboratory (LBNL) is working alone, with Ballard Power Systems (Ballard) bringing just the stack and system specifications.
- This project needs to work with an original equipment manufacturer (OEM) who can provide actual redacted cost quotes. It seems that some of the project's input costs are off.
- It seems that the LBNL group is making good use of capabilities elsewhere, including at the University of California (UC), Berkeley, and some fuel cell manufacturers. Getting a little more help from some of the stack part producers would be appropriate.
- The collaboration on this project seems to meet minimum standards. It is not clear how much support is coming from key partners at UC Berkeley or Ballard. The report suggests LBNL is doing most of the work on the program with some consultation from the named partners.
- Industry collaborations decreased since 2012 and no longer include a MHE system industry representative. Most of the results are focused on combined heat and power (CHP) but the collaboration with fuel cell CHP manufacturers is weak. Some collaboration with a similar project at Battelle was expected.

### Question 4: Relevance/potential impact on advancing progress toward DOE research, development, and demonstration (RD&D) goals

This project was rated **3.0** for its relevance/potential impact.

- Using a systematic and consistent approach to look at both production volume and application type makes a lot of sense. Making sense of various externalities will probably represent a bit of a challenge.
- The project team is developing a total cost of ownership model to help identify and address cost barriers. The team is also looking at a lifecycle carbon analysis to address CO<sub>2</sub> (or greenhouse gas) emissions issues.
- This project has no real impact. It might drive people to work on only more expensive components, but that is only a good thing if the inputs in the model are correct—and it does not appear that they are. This project cannot be used to suggest what to work on until the accuracy of the inputs are improved.
- The cost analysis used will contribute to determining key cost drivers and provide insight for the direction of R&D priorities. Fuel cell stationary systems, in particular with reformers, represent a very significant part of fuel cell commercialization. As the cost studies focused mainly on transportation in previous years, this study completes the cost panel.

### Question 5: Proposed future work

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

- The remaining scope of work seems commensurate with the budget remaining.
- Basically, the future work simply includes analyzing the systems yet to be completed and considering externalities. This makes sense.

- The proposed work is correct and monetizing health damage is a very good point. This parameter may have more impact in the near future than reducing CO<sub>2</sub> emissions. Mapping the effects for different regions should be useful to prioritize the fuel cell deployments.
- The researchers need to work with an OEM to get real quotes.
- It is unclear if the total cost of ownership model will only include the manufacturing costs.

#### Project strengths:

- This project is addressing critical needs.
- The methodology is a strength of this project.
- Strengths of this project include the life cycle cost analysis for different regions and the monetization of health damage.
- The consideration of different applications and volume production levels with one single modeling program is a strength of this project. The inclusion of a systematic DFMA model is meaningful and different.
- A great deal of background work has been completed, hopefully laying the ground work for many results in the coming year.
- It is appreciated that the cost analysis is being done at several production volumes. It looks like the large break in labor and amortized capital is between 100 and 1,000 units per year. The next break is going from 1,000 to 10,000 units per year, but with lower marginal benefit, as expected.

#### Project weaknesses:

- There are no major weaknesses identified.
- The lack of volume effect on the cost of BOP components is surprising and differs from other studies. It should have been detailed in the presentation. The parameters used for the parameter study are different from those used in Strategic Analysis and Battelle studies. Therefore, the comparison is more difficult.
- The ability to get accurate costs is a weakness as companies don't want to share this information. It is hard to predict cost at high volumes. This project should present the future costs as a range and not an absolute number. It is not clear what the uncertainty is.
- This project appears to have a high degree of overlap with two other projects currently funded by DOE. It is recommended that the scope of each be clearly defined to eliminate redundant work where possible. Also, please make sure that the results from these projects are being reconciled against each other so that when the final results are available they are consistent. The project team should more clearly identify the pathways to reducing manufactured cost besides increasing production volume. It is not clear how manufacturers can reduce the materials costs for these systems. The project touts CO<sub>2</sub> reduction benefits, but this benefit is not relevant to the national energy policy, as there is neither a carbon tax nor a cap-and-trade system in place at the federal level. As the research team is primarily based in California, it is understood why this is of interest, but it is not relevant to the DOE program currently. The team should review why the BOP cost does not scale strongly with production volume. This may be a result of the assumption that the BOP components used in the largest system essentially scale down to the smaller systems.

#### Recommendations for additions/deletions to project scope:

- An annual update of the existing models should be carried out: the update should not wait for the end of the project as presented in the planning.
- This project should consider a collaboration with project FC-083, Enlarging Potential National Penetration for Stationary Fuel Cells through System Design Optimization run by the National Renewable Energy Laboratory.
- It seems like there is the potential for overlap between this program and project FC-097 on the CHP cost estimates. It is not clear how DOE will make sure its funding is being used wisely for these analyses. DOE may be considering a teardown analysis to develop a fuel cell system bill of materials (BOM) and thereby generate manufactured costs. The current BOMs seem to be developed by surveying the literature and manufacturers, which seems less rigorous (or more open to manipulation). It is recommended to add an

analysis to identify the top 5 to 10 systems that contribute most heavily to the overall fuel cell system cost and then provide recommendations on how to mitigate their effects on fuel cell system cost.

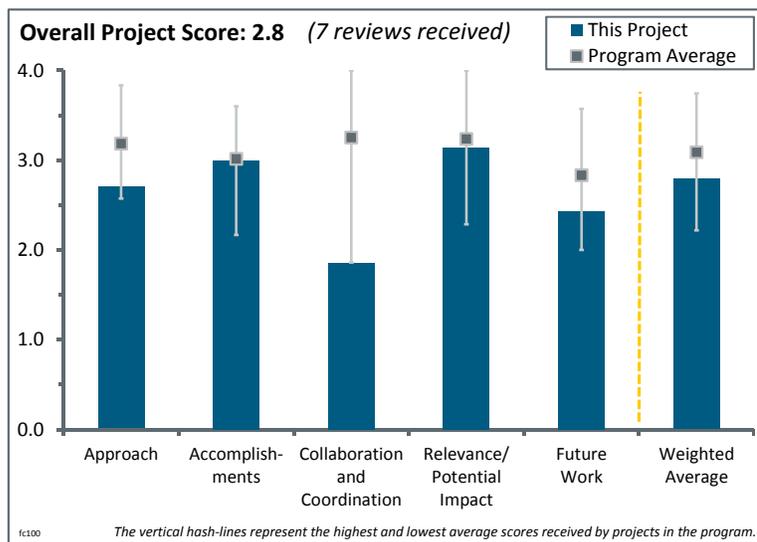
- The researchers should look at two things. First, some of the cost numbers, even at low volume, would portend that there should be some markets where fuel cells can break through. It is not clear what the barriers are that prevent adoption. The researchers should clarify if the cost numbers are right, or if there are other costs that swamp direct costs (i.e., assume that a company invested a couple hundred million dollars to make a product) and they make 33% gross margin on a 100 unit/year market, with a ramp of some rate. It is not clear when the investors will get paid. At least for their own purposes, this quick analysis should be done. Second, benchmarking to the Japanese New Energy and Industrial Technology Development Organization (NEDO) program for small stationary CHP should be done. Those systems were considerably more expensive than projected in this report (though they were quite small). What can be learned from those data to calibrate the “should-cost” here and the “does-cost” of the real world?

## Project # FC-100: High-Aspect-Ratio Fuel Cell Catalysts

Brian Larsen; National Renewable Energy Laboratory

### Brief Summary of Project:

The objective of this project is to produce novel, high-aspect-ratio, nanostructured, platinum (Pt)-based catalyst materials with increased activity and increased Pt utilization. The synthesis of Pt-alloy extended thin-film electrocatalyst structures (ETFECS) using three different alloying metals allows for maximization of Pt ETFECS specific activity. The development of methods to increase ETFECS surface area allows for increased mass activity of the Pt ETFECS. Finally, ETFECS are integrated in membrane electrode assemblies (MEAs) and evaluated for effectiveness.



### Question 1: Approach to performing the work

This project was rated **2.7** for its approach.

- This project was very straightforward and directly focused on the objective of reducing Pt loading.
- Novel, high-aspect-ratio Pt structures are being developed.
- The approach is sound, but it would have been good to include a pure Pt baseline for comparison. Maybe it was a 2012 objective, but no data was presented.
- Pt-alloy ETFECS is a reasonable approach to meet U.S. Department of Energy (DOE) cathode catalyst performance and durability targets; however, the National Renewable Energy Laboratory's (NREL's) approach for optimizing these materials was not explained.
- This work involves the fabrication of catalyst formulations and testing of these in the fuel cell environment. The approach is to address targets, numerical values set by DOE. The goals are to achieve performance by using the precious metals more fully, the result of additional dispersion.
- The approach described seemed to be disjointed; the continuity between the different preparative methods to enable a comparison between factors in catalyst and preparative procedure was discontinuous.
- This project created high-aspect fibers to reduce Pt loading in polymer electrolyte membrane fuel cell electrodes. However, it is not clear that this approach will actually reduce Pt loading versus creating a high dispersion of supported Pt nanoclusters, since reducing particle size for higher dispersion will only result in shorter fibers and, ultimately, high-aspect-ratio will no longer be a factor.

### Question 2: Accomplishments and progress toward overall project and U.S. Department of Energy (DOE) goals

This project was rated **3.0** for its accomplishments and progress.

- The project was completed on time and within budget with excellent results.
- The project has met most of the goals and the performance tests have been performed.
- This project has successfully made nanofibers and demonstrated catalytic activity.
- Progress is satisfactory. The idea was to make nanowires of Pt alloys—one set of Pt-Ni alloys and a second set of Pt-Co alloys. Successful alloy structures were prepared and the data show good results.
- The accomplishments are good, but there is no science. It is not clear why this works.

- The project was shown as 100% complete, but no durability testing was done. This testing is important because leaching transition metals from alloy catalysts is one of the limiting features of these types of catalysts. Beginning-of-life mass activities in MEAs and rotating disk electrodes (RDE) are still below DOE targets.
- Because the principal investigator (PI) has left, the work is in disarray and the plan to complete the effort and provide a high degree of technical understanding of the effect of alloying on catalyst performance seems doubtful. It was fortunate that Shyam Kocha was available to describe much of the work for which he was not responsible, as he defended the project. It is not clear what advantage ternary alloys would offer with the limited understanding provided on the alloys presented. It may be relevant to investigate other methods of characterizing the Pt catalyst to establish a correlation with the observed difference in performance relative to the baseline. It is also unclear what ratio of Pt to alloy metal is optimum relative to the preparative method used and how this is important.

### Question 3: Collaboration and coordination with other institutions

This project was rated **1.9** for its collaboration and coordination.

- It does not appear that any collaboration was required for this project. There should be an “N/A” category for this question so that the overall score is not affected.
- There was no collaboration with outside organizations.
- The presentation did not show much collaboration.
- There is no evidence of any collaboration with other institutions.
- There were no collaborations. Even if the project is a success (and, arguably, it is) there is no path forward.
- It was not clear that this was coordinated with any other effort, although the General Motors work certainly has some important parallels.
- The presentation showed no collaboration with other institutions, although clearly this omission is an oversight given that success is based on participation by a variety of outside vendors and colleagues. In this presentation, they were not described.

### Question 4: Relevance/potential impact on advancing progress toward DOE research, development, and demonstration (RD&D) goals

This project was rated **3.1** for its relevance/potential impact.

- The structures are unique and the performance significant.
- This project is aligned with critical areas of fuel cell cost and durability.
- Reducing the Pt content in fuel cells is critical to achieving cost reduction targets. By definition this project does that by developing and testing three different alloys.
- The project represents an interesting approach; however, galvanic displacement may be expensive and difficult to manufacture and handle for these materials.
- If the project had been carried out in a more systematic manner and details associated with the impact of the preparative procedure and catalyst involved were more cohesive, this effort could have provided a very valuable understanding of how preparative procedure variables can affect the activity and stability of the resultant catalyst.
- There has been considerable effort on achieving improved Pt electrode performance with a metric of the number of watts resulting from a certain mass of Pt. This work encompasses decades of effort. Because Pt has a high price, using less of the metal is one way to cut device costs. This work is clearly relevant. The result was that the Pt-Co alloy electrodes, utilizing the high dispersion afforded by this approach, resulted in superior performance.

**Question 5: Proposed future work**

This project was rated **2.4** for its proposed future work.

- Most of the proposed work has been accomplished.
- The suggested future work simply extends these tasks and includes looking at ternary (three element) alloys, along with a continued effort to incorporate these highly dispersed materials into usable electrode structures.
- The future work includes (1) “Synthesize ternary Pt-alloy ETFECS with sacrificial, ‘leachable’ metal (e.g., Fe, Mn)” and (2) “Increase performance at high current densities;” however, there are no specifics as to how NREL plans to do these two things. No durability tests are planned.
- There needs to be some focus on getting the in-situ performance to match the RDE data by structuring the catalyst layer. The project should not go into ternaries at this stage. The durability of these structures must be investigated in-situ. Characterization must go beyond microscopy. It is not clear what the crystal phase is or what the ratio of Pt to Co is. More work needs to be done here.
- Because the PI has left and the effort does not seem to have been carefully and systematically pursued, the balance of funding does not seem adequate to bring this effort to a meaningful conclusion.
- There are no comments on the proposed future work—the project is complete.

**Project strengths:**

- The project team has accomplished the objectives on time and within budget.
- This project has a novel approach for meeting DOE goals.
- This idea is great idea and has a neat synthesis route.
- NREL is studying potentially relevant materials.
- The experimental details of this synthesis process require a skill set of considerable ability. This success involves an excellent experimental team. That team makes the difference. Good people are the primary strength.
- The plan to investigate preparative procedure variations on the performance and character of different catalyst species is a worthwhile and valuable endeavor and would assist in understanding the importance of advancing the techniques of catalyst preparation. Combining catalyst preparative variations with electrochemical performance evaluation is the correct methodology.

**Project weaknesses:**

- This approach is a potentially expensive method to generate high activity.
- This project has no science, no partners or original equipment manufacturers, and no future work.
- This project lacks a systematic approach to design improved materials and durability testing.
- The project did not seem to be well organized in coordinating between preparative nuances and the various catalyst species being investigated. The amount of time spent on what was presented does not seem to allow for time to complete the work, unless another investigator can be assigned to finish the task.
- It is not clear that this work will really reduce Pt loading versus just resulting in a high dispersion of supported Pt nanoclusters. Reducing the particle size for higher dispersion will only result in shorter fibers and, ultimately, a high-aspect-ratio will no longer be a factor.
- There is a long history of Pt-Co alloys in fuel cell technology, but stability has been a previous problem. Depending on testing conditions, enhanced activity can show some endurance, maybe to 1,000 hours, but the Co slowly dissolves and activity loss occurs. If the test period is only a few hours, this result will not be apparent. However, when moving towards 30,000 hours of durability testing, this dissolution will usually result in the same performance that would have resulted with a pure Pt formulation. If that is the case, there is perhaps no advantage in alloying. It just does not pay. There has to be some longer term testing before this advance can be fully understood. The nanowires always look so fragile. Unfortunately, making fuel cell electrodes involves some pressure and fuel cell testing usually involves compression on the test fixture. While not a weakness really, the test results will be easily influenced by the test fixture design.

**Recommendations for additions/deletions to project scope:**

- Any continuation of this work should be rolled into Bryan Pivovar's ETFECs project.
- The project should do some durability testing. A great deal of work has to be done to get the catalyst layer to work with these materials. The next phase of funding should be used to sort this out.
- It was highly considerate of Shyam Kocha to present the task, considering that the PI had left and Shyam was only peripherally involved. Because of his background and understanding, it would seem appropriate that he help seek a qualified individual to bring the task to some logical and meaningful conclusion, perhaps with the assistance of others who have been working in this arena.
- It is smart to encourage skilled experimentalists to continue to explore ways to approach Pt fabrication that achieve more watts with less Pt. The next task here should be some replication, proving that the result can be obtained repeatedly. The other task of critical importance is building these complex micro wires into useful electrodes. There also needs to be some consideration of the amount of energy expended in spreading the Pt into a high dispersion contrasted to the amount of energy that investment will recover. Even at this early stage, it makes sense to ask that question, and perhaps think of less energetic approaches. In truth, today, the high-performance polymer electrolyte membrane electrodes have a cost well beyond the cost of Pt in those electrodes.
- There are no recommendations. The project has been completed.

## Project # FC-103: Roots Air Management System with Integrated Expander

Dale Stretch; Eaton Corporation

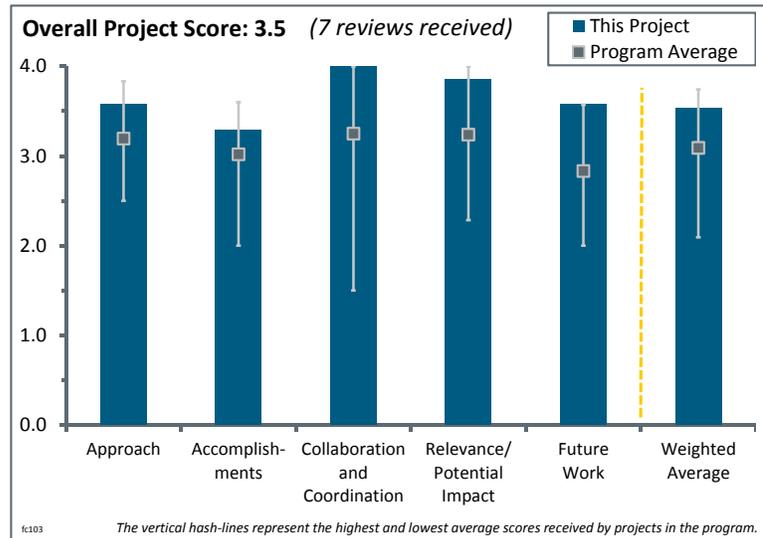
### Brief Summary of Project:

The primary objective of this project is to demonstrate key improvements to air management hardware efficiency, including compressor/expander efficiency greater than 65%/70% at 25% flow by 2017, combined motor/controller efficiency greater than 90% at full flow by 2017, and compressor/expander input power less than 8/14 kW at full flow by 2017. Secondary objectives include conducting a cost reduction analysis and achieving a fully tested and validated air management system capable of meeting 2017 project targets.

### Question 1: Approach to performing the work

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

- This project features a very clear approach, a good and clear list of deliverables, real-world validation, and good risk mitigation analysis. It is a well-managed project.
- This project features a highly focused systems engineering approach to improving air compressor technology.
- The approach is sound and offers an interesting alternative to high-speed centrifugal turbomachinery approaches. The researchers plan to reduce parts count and lower rotational speed (to allow conventional bearings and motors); application of near-net-shape rotors supports reduced system cost.
- The project approach is very good. It builds on Eaton's extensive experience with Roots blower technology and appears to be logical and comprehensive. Every subcomponent in Eaton's current technology is being looked at to determine where cost savings can be achieved while still meeting performance targets. The project is focusing on a lower speed alternative to turbo machinery, with its costly air bearing system for high-speed operation.
- Eaton presented a detailed discussion of its approach. The approach builds on the experience of Eaton and incorporates modeling methodology to develop designs at a greater rate. The researchers build on the experience of Argonne National Laboratory (ANL) to provide fuel cell performance data and fuel cell systems understanding that will accelerate the development of the compressor/expander. Eaton has coupled the modeling efforts with hardware manufacturing and systematic testing of the components. Eaton moves from component hardware development to prototype development and testing with a major fuel cell stack manufacturer.
- Eaton is aware of cost issues and how cost is affected by balance of plant component and system simplicity and integration. The single-shaft compressor expander motor configuration will reduce cost and efficiency losses. Modeling is being used to assess the impact of configurations without the need for multiple hardware builds. A roots blower "mule" is being used to cheaply and quickly test concepts ex situ.
- The project could be of value to developers if compressor costs are decreased. Investigators have done well in partnering with Strategic Analysis, Inc. (SA). Weight and volume targets are accounted for by the decision to go to plastic rotors, along with use of fewer bearings and a more integrated rotor design. Finite element analysis on the rotor has shown that there is a feasible solution.



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## Question 2: Accomplishments and progress toward overall project and U.S. Department of Energy (DOE) goals

This project was rated **3.3** for its accomplishments and progress.

- The project team has made excellent progress.
- The project has met all milestones to date and is on track to pass the June 2013 go/no-go decision point. The go/no-go criteria were not discussed quantitatively.
- The progress made in less than a year shows promising prospects. Major modifications/improvements of compressor-expander design have already been designed. There are very good complementary modeling and validation activities. The test stand is ready.
- Baseline compressor testing was conducted, showing fair/good results. Modeling of the expander and overhung rotor motor was conducted, but not completed. Substantial progress has been made, but there appears to be substantial additional work before the July milestone.
- The accomplishments during the first year are impressive. The team appears to have hit the ground running, so to speak, and both modeling and experimental results are very good. Trade-offs are being examined to achieve the most impact on system cost while meeting performance requirements. Despite the excellent progress, it is not clear if the project will meet the DOE 2017 targets even if completely successful. Increasing expander efficiency to 80% from the current 64% will be difficult, and the presentation does not provide a path forward that can ensure success.
- The project is new and test results are only just becoming available. Eaton appears to be systematically addressing each of the topic areas. Eaton is sharing data with ANL and is reporting compatibility of their own performance data with the ANL model. The data on expander experimental results were confusing; two of the three expanders were identified for additional testing, although only one of the two had tests described. It is unclear if the other one is not going to be tested. Compressor performance work is in the early stages without any conclusions available. The team is developing a model for compressor and expander computational fluid dynamics (CFD). The design of the overhung motor rotor analysis is underway. The test stand is under development and no data has been reported. The team has conducted expander plastic rotor analysis and has demonstrated 20,000 rpm, but materials properties may not be acceptable.
- It is unclear whether the plastic and aluminum materials would contribute to contamination. The project team needs to confirm noise, vibration, and harshness after new materials and design. More detail is needed on the test stand setup. This is especially true in understanding the accounting for the humidity inlet to the expander.

## Question 3: Collaboration and coordination with other institutions

This project was rated **4.0** for its collaboration and coordination.

- There is excellent collaboration with industry partners.
- The interaction between ANL and Eaton has been excellent and productive.
- The collaboration is excellent. Analytical support is being provided by ANL, SA, and Kettering University, and final prototype testing is planned with an 80-kW system at Ballard.
- A strong team was put together for making hardware, developing models that evaluate the performance of “real” hardware, and performing a detailed cost analysis. The team has a lot of capability.
- The project features a good mix of industry, institute, and university partners. The partners cover all of the necessary areas of know-how. The group is as big as necessary and as small as possible—it promises efficient and effective work.
- Simulation collaboration with ANL and cost modeling with SA are good. Collaboration with Ballard on inserting a real system between the compressor and the expander will be good. CFD with Kettering University should help with the rotor design.
- Partners include a national laboratory, a university, a stack system developer/supplier, and a cost analysis specialist.

**Question 4: Relevance/potential impact on advancing progress toward DOE research, development, and demonstration (RD&D) goals**

This project was rated **3.9** for its relevance/potential impact.

- Development of a low-cost, high-performance compressor/expander is critical for PEM fuel cell advancement.
- The project has high relevance to the DOE Hydrogen and Fuel Cells Program (the Program). The air handling system is a significant contributor to the system cost. Any means of reducing the cost should be investigated.
- Development of a new air intake system is critical to providing the weight, volume, and cost savings to commercialize fuel cells for many applications, particularly automotive. The technology has been overlooked until now, but it is now being studied. This is a long-overdue project.
- The single-shaft compressor/expander motor configuration will reduce costs and increase system efficiency.
- The parasitic losses in the air system of a fuel cell are a key issue. The project is addressing this in an excellent way.
- Eaton seeks to develop a robust, high-efficiency compressor/expander/motor unit optimized for fuel cell use. Because Eaton is an automotive industry supplier, it fully appreciates the need for reliability and has designed its system accordingly. Consequently, the potential impact of the project is substantial because there is a clear and strong need for a reliable (and low-cost) air system.

**Question 5: Proposed future work**

This project was rated **3.6** for its proposed future work.

- This project features well-organized future work with a schedule for the completion of activities.
- There is a very clear plan for the right activities. Validation in an 80-kW system is a real challenge; it is also proof of the confidence of the partners to achieve this goal, which is fully supported by the impression one gets from the presentation.
- The future work plan is very good. Prototypes will be fabricated and tested in year 2, and an updated cost analysis will be completed. If completed, these activities will enable DOE to determine if the concept will meet Program targets.
- The plan is concise, the go/no-go criteria are set right, and the project has identified the right tasks to do. The go/no-go decisions every July offer the capability to off-ramp if the technology does not work out, which is good.
- The plan is logical: Period 1 is designing; Period 2 is building and testing at Eaton; and Period 3 is testing with a fuel cell at Ballard.
- The proposed future work is in line with the project schedule and milestones, but the first budget period go/no-go criteria need to be quantified. More discussion of cost analysis would be helpful.

**Project strengths:**

- The experience and expertise of the team members will greatly help this project.
- This is a well-designed and managed project. It utilizes industry partners and has made excellent progress.
- An excellent team made excellent progress in year 1. Most projects with multiple collaborators and subcontractors take considerably longer to form a team and get the necessary paperwork in to DOE.
- Eaton knows how to produce technology and develop a product at significant cost savings. Targets have been well planned. Collaborations are with the right parties.
- The concept builds off of existing machinery for which much experience and technical detail is known. Eaton is a very credible developer and future manufacturer of the systems. Eaton knows the requirements very well.

**Project weaknesses:**

- More detail is needed on the laboratory setup (expander test stand). This will strongly influence “Period 2” in the work plan.
- Eaton is working on plastic expander housing. It does not seem that Eaton is aware of potential fuel contamination issues from the plastic component. The team should consult with the National Renewable Energy Laboratory on system-derived contamination.
- The project does not estimate the potential cost savings if the work is successful. This analysis probably exists and has been presented to DOE, but there is no indication in the presentation of the cost savings possible if the project is completely successful. Without this analysis, it cannot be determined if the proposed effort will result in a device that meets the DOE targets.
- Much work remains in Period II. Further results would be expected if the researchers are going to make the July design deadline. The expander efficiency is reported at only 64%—short of the 73% 2011 status and well short of the 75% 2015 target. It is unclear why efficiency went down and what the plan is to raise it. Compressor efficiency is reported at 74% at full flow, but the performance maps do not match this high level. An explanation of this discrepancy was not given. Much is made of reduced rotational speed to avoid “costly” bearings. However, foil bearings should not be considered costly. Thus, a driving element of the researchers’ design appears to be faulty. The overall pace of the project is a bit slow. One would think that a derivative product such as this could be developed in less than 3 years.

**Recommendations for additions/deletions to project scope:**

- The research team should keep up the good work.
- A cost analysis is planned. A preliminary cost analysis conducted during the design phase would have been useful input into the final design.
- The team should present an analysis that indicates the estimated cost savings for each individual change in component specifications. The sum should be a reasonably reliable indicator regarding the ability of the Roots technology to meet DOE performance and cost targets.

## Project # FC-104: High-Performance, Durable, Low-Cost Membrane Electrode Assemblies for Transportation Applications

Andrew Steinbach; 3M

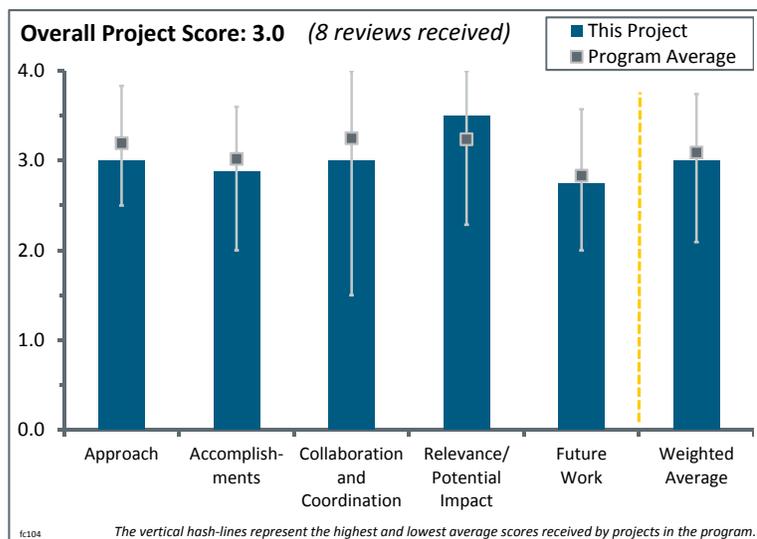
### Brief Summary of Project:

The objective of this project is to develop a durable, low-cost, robust, and high-performance membrane electrode assembly (MEA) for transportation applications. The project's approach will optimize integration of advanced anode and cathode catalysts, based on 3M's nanostructured thin-film (NSTF) catalyst technology platform, with next-generation perfluorosulfonic acid proton exchange membranes, gas diffusion media, and flow fields for best overall MEA performance, durability, robustness, and cost.

### Question 1: Approach to performing the work

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

- This novel approach both maximizes the performance and minimizes the amount (and consequently cost) of Pt in a fuel cell catalyst by maximizing Pt utilization.
- This project was exemplary in terms of the thoughtful plan and approach that was presented. It was clear that the strong research culture at 3M informed the systematic, but still creative, attack on the complex problems of electrode assembly properties and performance.
- This approach for developing an MEA that meets targets is well planned and comprehensive. The project uses an aggressive technological approach that is undoubtedly necessary to meet targets, particularly operating the cells at high temperatures (90°C) while using thin (<25 μm) and low equivalent weight membranes. Even if durability testing appears satisfactory, it is questionable that such a combination of temperature and materials provides a “safety factor” for avoiding membrane failure that is sufficient for commercial application.
- This project features a good balance of basic research and applied work that has led to a better understanding of the NSTF system and improvements in performance. Studies of the structure of NSTF catalysts before and after surface treatments, conditioning, and dealloying have been used to guide cathode catalyst improvements, leading to better peak power performance. Membrane studies have led to understanding how base metal leaching affects membrane and MEA performance. Water management work is integrated with the Lawrence Berkeley National Laboratory (LBNL) project. More of the effort and focus should be directed toward what appear to be the limiting factors for NSTF technology—water management and overcoming low-temperature operational issues.
- This project aims at further optimization of the NSTF format in the form of MEAs and with the use of bimetallic catalysts. The principal goal of this effort is to meet and exceed the U.S. Department of Energy (DOE) 2017 targets for MEA performance and loading, which include 0.44 A/mg of Pt at 0.9 V (iR free) and 0.720 μA/cm<sup>2</sup> MEA specific activity. In addition, the total metal loading target for the MEA is 0.2 mg/cm<sup>2</sup> or 0.2 gm/kW. Here, the primary focus is the NSTF cathode performance improvement via dealloying and annealing and electrode integration in an MEA format. The approach toward these goals follows the expected lines.
- The approach is very rigorous and the team is working very hard in a certain direction. The team should consider doing a full impedance analysis to better understand the results from the high-frequency resistance



tests to discern whether there is an impact from another effect in the MEA. The researchers might also look at a broader range of test conditions.

- Durability testing is shown to be completed by quarters 7 and 11, which is far too late in the project to be useful for informing major integration decisions. Given that the project is an integration project with no component development, it is curious to see a few slides on the continued Pt<sub>3</sub>Ni<sub>7</sub> cathode catalyst development. It is very likely that the project will have to revert to doing some component development in order to achieve integration goals. The success of many of the integration tasks will be dependent on cell design and assembly parameters (e.g., thermal mass, compression force, and channel geometry). The project needs to state how the results can be interpreted to be universal for developers.
- This project appears to essentially be a continuation of what 3M has historically been doing to develop NSTF-based MEAs. The NSTF catalyst architecture is very promising because it appears to offer a route to both high activity and improved stability relative to conventional dispersed catalysts. However, after more than a decade of development, there are still no commercially viable NSTF MEAs. The principal reason is that NSTF MEAs are extremely sensitive to both temperature and impurities relative to conventional MEAs. Therefore, it would seem that DOE's focus on thin-film catalyst architecture should be to determine if these fundamental barriers to the commercialization of NSTF can be overcome. Doing the same thing over and over again should not be expected to yield a different result. Again, this project is essentially just a continuation of what Mark Debe did for a decade; namely, continue to tweak the catalyst compositions and treatments (e.g., improve intrinsic activity), and change the membranes and/or gas diffusion layers (GDLs) (e.g., to alter the water management). However, 3M does not appear willing to actually change the catalyst-layer composition or architecture, which severely limits the probability of success here. In fact, the principal investigator (PI) states that this project is limited to "optimization of existing components and processes" and that there shall be "NO COMPONENT DEVELOPMENT." This limitation is very unfortunate because making NSTF successful requires much more than optimization; it requires a new catalyst layer architecture.

## Question 2: Accomplishments and progress toward overall project and DOE goals

This project was rated **2.9** for its accomplishments and progress.

- Good progress has been achieved over the relatively short duration of the project.
- The performance of 0.48 A/mg Pt at 0.9V for Pt<sub>3</sub>Ni<sub>7</sub>, as shown on slide 7, is impressive. There was a careful tracking of catalyst composition as a result of catalyst preparation, which helps make the results clear and understandable.
- Good progress has been made in the short time the project has been active. The project has already made improvements in decreasing platinum group metal (PGM) loading and increasing performance at high power.
- The mass activity is promising with SET processing of Pt<sub>3</sub>Ni<sub>7</sub>. A controversial point has arisen with regard to the assignment of ohmic resistances. Physical explanation needs to be provided for the "variable" cell area that is used to get iR-free curves to overlay each other. This may be due to protonic resistances that vary, but it is not accounted for in a high frequency resistance (HFR) measurement. The achievement of 20 μg/cm<sup>2</sup> Pt on the anode appears to be outside the context of adding an oxygen evolution reaction (OER) catalyst. Another 3M project shows that at least 29 μg/cm<sup>2</sup> is needed in the presence of an OER catalyst. The question exists then as to whether the two projects agree with each other. Proton pump data for the low-loaded anode would be interesting to see. It may also be good to see testing with H<sub>2</sub> dilution on the anode (40%–100% H<sub>2</sub>/N<sub>2</sub>).
- It appears that the properties that have been achieved are quite good, but the surprising, relatively low benefit of the SET on the Pt<sub>3</sub>Ni<sub>7</sub>/NSTF cathode activity was perplexing. The project is still relatively young, so perhaps the cause of this low benefit can be identified. Overall, the systematic and scientific approach instills confidence that the basic premise of the work will ultimately pay off with good results.
- The major barrier to commercialization of NSTF is the high sensitivity to operating conditions (as shown on slide 4 for Tasks 2 and 6), yet the progress on these tasks is delayed or has not even started. In addition, no real progress will be made in these key areas unless a different approach than what has already been tried is utilized, which does not appear to be in the plan. There does not appear to be a good fundamental

understanding of what is limiting the NSTF cells, as evident in slide 15, which does not explain the dominant mechanisms controlling the performance.

- The researchers have a long way to go on all of their metrics. It is not clear from the presentation which metrics are system-dependent and even flow field-dependent. The reported 67% loss of mass activity looks like a big concern, so while there are many passing metrics, it seems like it would be helpful to rank the importance of the various criteria. They should be ranked “good” because they seem to be progressing on so many fronts, but some of the results, while reported to three significant figures, might be misleading because of the use of optimal test conditions.
- The initial performance at this early stage is modest compared to the previous generation of work, especially the work conducted using SET. The principal difference appears to be related to grain boundaries, size, and morphology of the crystallites. In this context, some attention should be paid to the density of the resultant crystallites because it appears to be significantly lower than the bulk values and previous-generation SET-treated samples. Some background into the logic used to select the elements for cathode electrocatalysts should be specified. For example, it is unclear why PtCoMn was chosen as a ternary alloy. In addition, because the structure of the interface is very different from the conventionally supported electrode MEAs, some additional metrics on the activity at higher current density should be adopted. It is strange to see H<sub>2</sub>/air comparison at 0.9 V, where partial pressure of O<sub>2</sub> should not be a factor, and not have concomitant metrics at 0.65 V to see differences in the onset of mass transport. Because this work is aimed at MEAs and electrode structures, a He, N<sub>2</sub>, and O<sub>2</sub> study should be part of this effort. In addition, it is strongly recommended that the team pursue some semblance of transport modeling to see what elements of the electrode structure, ionomer content, equivalent weight, etc., are crucial.

### Question 3: Collaboration and coordination with other institutions

This project was rated **3.0** for its collaboration and coordination.

- The team includes many smart people who are investigating issues with the GDL, etc.
- The collaborators appear to be making meaningful contributions and working closely with 3M.
- The presentation was particularly effective in showing the multiple contributions and their value to trying to figure out how to better tune the SET approach for the lower-PGM-content MEAs.
- The industry (General Motors) and university (Johns Hopkins University [JHU]) team is lean and effective. This team has brought a new valuable approach and insight into development and optimization of precious metal and possible non-precious-metal catalysts.
- The collaborations within the project appear to be working well. The project is collaborating with a transport project at LBNL. Collaborations with original equipment manufacturers may be beneficial in elucidating what effects proposed changes may have on the fuel cell system (e.g., moving water out of the anode in a system with anode recirculation would probably lead to higher vent rates and lower efficiencies).
- While collaboration with Oak Ridge National Laboratory is evident from the transmission electron microscopy data, the corresponding collaborations with other institutions such as LBNL, Michigan Technological University (MTU), JHU, and Argonne National Laboratory (ANL) are not clear. Maybe it is too early; for example, work at JHU only started in February 2013, almost at the point when this presentation was requested.
- The PI needs to have more interaction with partners that can help to determine the root cause of the MEA performance issues and be open to suggestions on how to resolve these issues. The primary focus of the project should be on the development of a viable MEA, not continuing to make minor changes to the catalyst compositions and treatments.
- For an MEA project, it is extremely surprising to see that the list of collaborators does not include a stack developer (either automotive or otherwise). The three national laboratories and two universities will not have access to the operating conditions and cell designs needed for context. ANL is being tasked with hydrogen oxidation and hydrogen evolution reaction kinetics studies, but the slides refer to personnel associated with modeling. The question remains as to whether this is a modeling study. It appears that some of the collaborations are focused on dealloying Pt-Ni catalysts. Perhaps there are other parties that have already gone down the same path with other morphologies that could help. The list may include Nenad Markovic or some automotive developers.

#### Question 4: Relevance/potential impact on advancing progress toward DOE research, development, and demonstration (RD&D) goals

This project was rated **3.5** for its relevance/potential impact.

- The topic of the work is crucial to the long-term economic success of H<sub>2</sub> fuel cells, and it appears that the strategy being followed has a very good chance of significantly and positively impacting that topic.
- The project has strong relevance towards meeting DOE targets for low-PGM content and durability by improving electrode structures and mass manufacturability.
- As long as Pt is needed, this kind of approach is a valuable tool for lowering costs.
- The primary effort of meeting the 2017 targets is highly relevant and, if successful, the potential impact on the Program would be considerable.
- The project is apparently on the path to a high-performance catalyst.
- The goals of the project are well aligned with Program goals and objectives, which is why NSTF has deserved DOE's support for the past decade. However, the promise of NSTF will never be realized if the MEA performance issues are not resolved, and this will not be accomplished unless a different approach is undertaken.
- An optimized MEA with Pt<sub>3</sub>Ni<sub>7</sub> NSTF properly conditioned with thin, durable membranes could be very valuable to developers. There is some question here as to whether an MEA integration project is appropriate for public funding. Integration activities are usually pursued with developer funding because integration is often fairly particular to stack design and operating strategy.
- This project is focused on integrating NSTF catalysts into an MEA. NSTF has been the most active and most durable catalyst, but it has issues with integration in an MEA due to water management. This project addresses optimizing the rest of the MEA to integrate with NSTF and overcome the water management issues. If successful, it would allow for low-loading, low-cost, durable NSTF catalysts to be utilized effectively in fuel cell systems.

#### Question 5: Proposed future work

This project was rated **2.8** for its proposed future work.

- The proposed future work is in line with the aims and objectives of this effort.
- The proposed future work is consistent with the approach and the experimental plan already underway.
- The proposed future work addresses issues that were delayed in the program, and they are important to give attention to. These topics are noted on slide 4 of the presentation, and the PI clearly has these in focus and on the "to do list," so the proposed future work plan looks good.
- The proposed future work is appropriate. It was stated that transient response and water management will be the main focus for next year. Area should be the main focus of the project because it appears to be the limiting factor for NSTF technology.
- Test plans should be expanded to intermediate temperatures.
- The study needs to better prioritize durability. The full suite of DOE-prescribed stress tests should be done at the beginning of the project to understand the response to relative humidity (RH) cycling, base metal dissolution, and other possible concerns. It would be good in the future work section to see what stack formats and operating conditions will be used for the integration activities. The systematic study of land-channel characteristics needs to be outlined.
- The team has to make clear the effect of electrode area normalization. If the flow field is the same, then the area of the flow field should be the correct area of the fuel cell electrode. One way to see if this is true is to leave the linear activation zone and run the cells in the mixed transport activation region (until the curves bend) to see if the curves bend uniformly without and with area normalization. Dealloying offers another way to make effect catalysts through thin-film nanoporous supports; this should be explored for precious and non-precious metal catalyst work.
- The team must focus on the key barrier, which is the poor performance of the MEAs under realistic operating conditions. This reviewer was optimistic that having a new PI on 3M's NSTF program would also result in a new approach, but this does not appear to be the case. Instead, the plan appears to be to continue to tweak (or "optimize") the catalyst compositions, when the "elephant in the room" is the

unacceptable sensitivity of the resulting MEAs. The PI must be open to making substantial changes to the catalyst layer composition and/or architecture to resolve this key barrier. The team does not appear to understand the root cause of the MEA performance sensitivity. For example, it should be apparent that 3M's hypothesis on why changing the anode GDL somewhat helps the performance is flawed, because it states in a 2010 *ECS Transactions* paper, "While a significant and consistent performance difference was observed between two anode GDLs at both 30 and 50 C, no significant difference in product water distribution out the anode and cathode was observed." This paper does not agree with their stated hypothesis in the same paper that the performance improvements are due to "the amount of water leaving the cathode was also reduced and thereby the O<sub>2</sub> transport restrictions were reduced." Simply changing GDLs without actually understanding the mechanisms responsible for the change in performance is not an efficient way to address the key barrier. The root cause must be determined, and then truly effective mitigations may be efficiently developed. The root cause may be differences in saturation levels (not flux rates); this hypothesis would lead one to explore different GDL options. Additionally, the limitation may not be O<sub>2</sub> transport under some conditions, which may lead to an entirely different approach.

### Project strengths:

- This project features good teaming and innovation.
- This project features a strong, experienced, and productive team.
- The project is leveraging many years of DOE and 3M investment in catalyst improvement.
- This project features good collaboration and integration of the work at subcontractors and 3M—transferring basic knowledge and understanding of the system to the application in an MEA.
- The highly systematic approach was particularly impressive and is a clear strong point.
- The main strengths are in the NSTF morphology and performance. The scalability and potential to surpass the DOE 2017 targets for performance and durability are strong.
- The project team is working on one of the most promising catalyst architectures to date for PEMFC MEAs with high activity and good inherent stability. The project lead is also an MEA supplier, so the development of successful technology should also result in commercial products. The lead is a polymer company, which is the competency required to develop and manufacture viable MEAs (i.e., much more likely than a company that specializes in making catalysts).
- The investigators have years of experience developing a high-specific-activity catalyst that avoids support corrosion. 3M has shown the ability to generate the data needed to complete the project. 3M fabrication processes have the ability to generate the materials needed to complete the project. MTU is the right party to have on the project for water management modeling, especially with regard to pore network modeling.

### Project weaknesses:

- Although the routine characterization work is being very well handled, the area normalization is cause for some concern. A little more thought needs to go into the data analysis.
- It seems that some of the tasks have not been achieved as planned and were delayed. It was not completely clear why this happened, but there was some mention of an equipment or facility availability problem. In any case, it seems that the team is committed to achieving the various tasks in a timely manner, so this should not be seen as a serious problem.
- The main weakness is that this effort may not surpass the previous generation's NSTF, multicomponent, Pt-based catalysts. There is no clear approach, either computationally or in improving electrode structure through a scalable transport model. In short, the novelty of this project is unclear.
- The project results will be sensitive to cell design and operating conditions. Being an integration project, it overlaps with activities usually pursued by a stack developer. However, no stack developer was listed among the collaborators. The future work plan focuses first on beginning-of-life characteristics and later on durability.
- The relevance and effects of RH are glossed over. Lower HFRs are needed to achieve targets; yet, where noted, the cells are operated relatively dry. Because it would be difficult to avoid saturation at the anode, these conditions would seem to have significant stack and system ramifications.
- The team is doing the same thing over and over again and expecting a different result. The project is not focused on the primary issue that is preventing the commercialization of NSTF technology, namely,

unacceptable MEA performance sensitivity. There is an apparent lack of expertise in diagnosing what limits the performance of an MEA under various operating conditions.

- This project is a cause for concern. While all of the data looks really good, it is well known that 3M has a history of showing great laboratory results that do not translate well to practical stacks. The question is really whether they are carrying out the “right” tests. The MEA performance is all evaluated under “standard” test conditions, but such tests were really only validated in stacks for carbon-supported Pt nanoparticles. There is no assurance that the MEA test conditions for the 3M catalysts are best assured by the methods developed for Pt/C due to the significant differences in the catalyst layer structures. It would just be a shame to do all of this development and then fool everyone (including themselves) by testing in the wrong conditions. The path looks excellent, but it might be too test dependent. This criticism goes beyond just 3M; it seems to be a problem for the whole fuel cell community that standard tests unravel once off the path for Pt/C and related alloys.

### Recommendations for additions/deletions to project scope:

- The project should better prioritize durability. The project team should add a stack developer as a collaborator. The team should also seek to incorporate realistic cell design and conditions and to understand how results can be made universal for various designs and conditions.
- Fairly high operating temperatures (>88°C) are needed to meet targets. However, most testing, where noted, is performed at 80°C. In anticipation that the higher temperature affects longevity, particularly of the membrane, at least some of the durability testing should be done at the higher temperature.
- A clear modeling approach to understanding transport in the electrode structure is required. A fundamental effort needs to be applied to better choose the alloying elements. At the moment, this looks like a serendipitous route to selection.
- The project scope is reasonable and should lead to the desired goals. The academic team member, Ehlebacher, has published a dealloying process for making nanoporous supports to support Pt or Pt alloys (also formed dealloying). An electrode made with the nanoporous support and dealloyed catalyst as an electrode in an MEA should be examined for performance and durability while this team is still intact.
- The research team should focus the project on developing an MEA that performs as well as conventional MEAs under various operating conditions (i.e., performance is not severely degraded at 25°C relative to 65°C). The team should also be open to making substantial changes to the catalyst layers, as required to resolve the MEA performance issue (e.g., add ionomer and/or carbon to the catalyst layers, if needed). It should also quit working on “tweaks” to the catalyst composition until the MEA performance issue has been resolved. It should also include more interaction with partners that can help diagnose and/or model the MEA performance and determine the root cause, as well as propose mitigations.
- The team should perhaps carry out MEA testing beyond cold start-up and 80°C conditions—perhaps some intermediate conditions, such as 30°C, would be helpful to catch problems early. Some thought needs to be given to whether the tests developed for Pt/C in standard catalyst layers are relevant to the 3M catalyst layers, and the team should probably confirm the tests in a high-performance stack. While validating the test in a stack would be very time consuming, and might even be flow field dependent, it might save everyone a lot of grief early and allow 3M to make required changes while it still has time. While 3M is marching along to the DOE-approved methods, it might be worthwhile to question this overall approach.

## 2013 — Manufacturing Research and Development (R&D) Summary of Annual Merit Review of the Manufacturing R&D Program

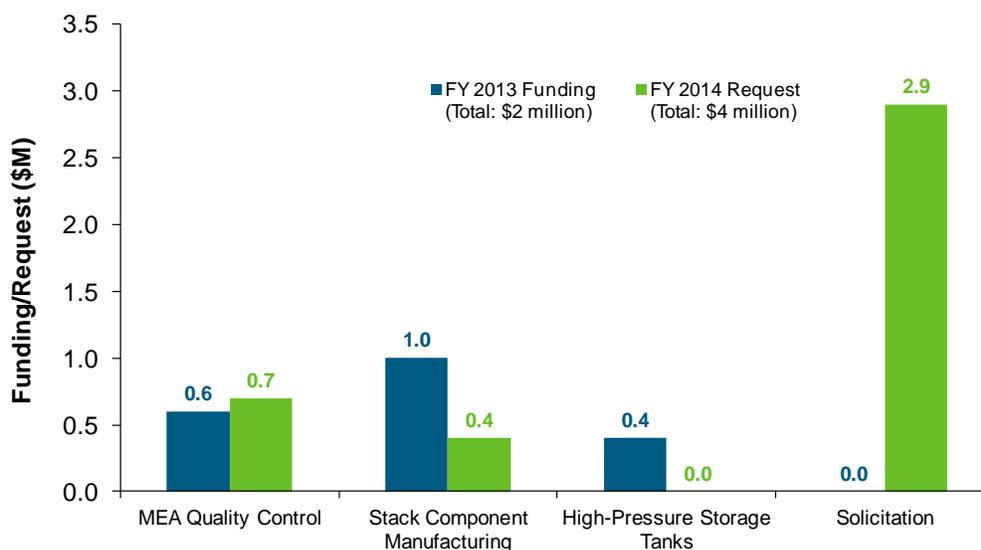
### Summary of Reviewer Comments on the Manufacturing R&D Program:

According to the reviewers, the objectives and progress of the Manufacturing R&D program were clearly presented and prior successes were described. The program appears to be focused, well managed, and effective in addressing the U.S. Department of Energy (DOE) Hydrogen and Fuel Cells Program needs. The reviewers suggested that DOE consider adding support for design for manufacturing and assembly relevant to polymer electrolyte membrane (PEM) and solid oxide fuel cell (SOFC) stacks as well as advanced stack assembly. In fiscal year (FY) 2013, four manufacturing projects were reviewed. These projects addressed fuel cell membrane electrode assembly (MEA) manufacturing, fabrication of catalyst-coated membranes, fuel cell stack in-line testing, and manufacturing of high-pressure vessels for hydrogen storage.

### Manufacturing R&D Funding:

Funding for the Manufacturing R&D program was \$2 million for FY 2013, and \$4 million was requested for FY 2014. The FY 2014 request-level funding will continue existing Manufacturing R&D projects and provide funding for new projects through a competitive solicitation, subject to appropriations.

**Manufacturing R&D Funding**



### Majority of Reviewer Comments and Recommendations:

Four Manufacturing R&D projects were reviewed and the maximum, minimum, and average scores for the projects were 3.6, 3.0, and 3.3, respectively. All projects were judged to be highly relevant to the DOE Hydrogen and Fuel Cells Program activities, with very good technical approaches. Project progress and accomplishments were judged to be extremely good. Project teams were judged to be strong; participation and contribution from industry partners were judged to be useful and coordinated. For most of the projects, reviewers felt that more details needed to be presented for future work.

The highest-ranked project (3.6) was considered by the reviewers to be highly relevant, with an excellent approach, outstanding accomplishments, and strong technology transfer and collaborations. Reviewers noted that the benefits of the technique developed in the project with the lowest score (3.0) were not clear compared to XRF and were possibly not compelling.

**Fuel Cell MEA Manufacturing:** Three projects were reviewed in the area of fuel cell MEA manufacturing, with an average score of 3.4. Reviewers noted that the approach for each of these projects was good and commended coordination with industry to improve manufacturing methods. The projects yielded performance gains and cost savings. The reviewers recommended that sensitivity be improved for all techniques and applications and recommended that the techniques developed be licensed/transferred to other organizations.

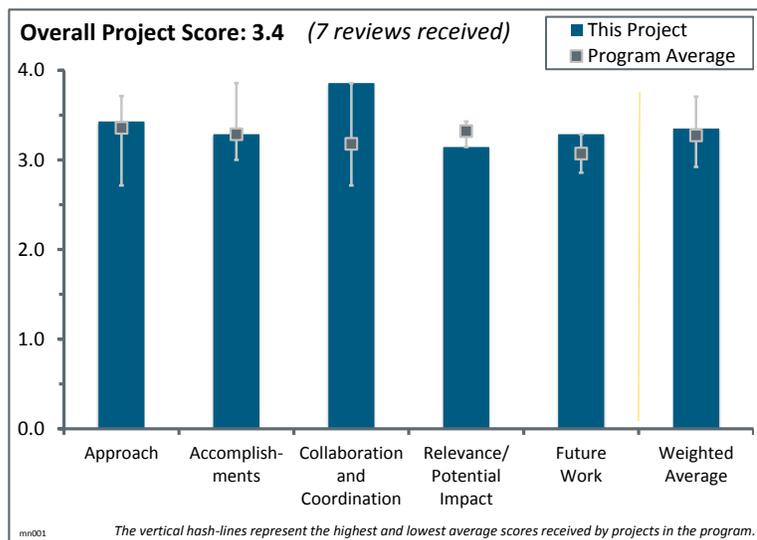
**Metrology for Fuel Cell Manufacturing:** The one project reviewed regarding metrology for fuel cell manufacturing received a score of 3.0. Reviewers approved of the general approach to this project but noted that it was unclear how surface changes due to normal manufacturing variation will impact measurement, and whether this variation can be accommodated in the processing. It was recommended that the researchers look into Mie scattering and some acousto- and electro-optical methods for flexibility.

## Project # MN-001: Fuel Cell MEA Manufacturing R&D

Michael Ulsh; National Renewable Energy Laboratory

### Brief Summary of Project:

The aim of this project is to develop the capabilities and acquire the knowledge for in-line quality control during fuel cell manufacturing. Industry partners and forums provide input to understand quality control needs. The project has highlighted the relevance of crosscutting quality control development by estimating the cost of poor quality analysis. Research in the past year focused on exploratory studies to improve the sensitivity of current techniques, expand techniques to new materials, explore the feasibility of new diagnostic concepts, and develop new in situ techniques and capabilities.



### Question 1: Approach to performing the work

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

- The approach is good; the principal investigators are developing techniques based on various excitation methods to detect defects in the fuel cell assembly process.
- The National Renewable Energy Laboratory (NREL) employs a good combination of input from industry and modeling to direct experimental efforts.
- NREL coordinates with industry to develop and improve diagnostics that are critical to fuel cell membrane electrode assembly (MEA) and gas diffusion layers (GDL) manufacturing.
- The first step taken is to understand suppliers' diagnostic and quality control (QC) needs. Early involvement of different component suppliers for different fuel cell types is a strong point. The approach covers identification of needs and possible solutions, development of techniques, and in-line validation. The intent to transfer the technology to industry is positive. Study of the effects of defects on cell performance will guide diagnostic development and define the defect envelope needing detection.
- There is a new approach planned that will focus more on exploratory studies; however, the researchers should continue to do "field evaluation" on other already "developed" techniques, such as optical observation of defects (such as GDLs, black on black, etc.).
- The approach is relatively broad based and covers a number of defects that can occur in MEA manufacturing processes. Input from component developers has helped shape the project objectives. Installing successful diagnostics on actual manufacturing lines, such as at Ion Power, is necessary to confirm the promise of these techniques to detect defects in industrial settings. There is still a need to demonstrate that these techniques can detect defects that occur during actual manufacturing runs rather than just detect defects in samples known to include them. This may be difficult to accomplish without detailed knowledge of the manufacturing processes in use by component suppliers.

### Question 2: Accomplishments and progress toward overall project and U.S. Department of Energy (DOE) goals

This project was rated **3.3** for its accomplishments and progress.

- Development of methods to detect electrode coatings on GDLs has been very encouraging. Further detection of local membrane failures is also encouraging.

- The optical diagnostic technique was demonstrated on polymer electrolyte membrane fuel cell (PEMFC) gas diffusion electrodes (GDEs) and solid oxide fuel cell tubes. However, sensitivity needs significant improvement in all cases.
- The project changed focus somewhat this year and the new areas of investigation are showing some promising results. NREL should examine the need for variable or multiple non-uniform applications of the non-uniform GDL/catalyst coated membrane (CCM) electrical excitation.
- The optical diagnostic (mainly reflectance), IR/DC, and IR/RFT are all performing very well, and suggested improvements will increase their value. Using IR/RFT with higher hydrogen should prove to be very valuable. It is not clear whether the “gas knife” design is optimum for measurement in an open environment for that process. There are many configuration choices available for that version of IR/RFT.
- Reasonable progress has been made since the last DOE Hydrogen and Fuel Cells Program Annual Merit Review. However, optical detection of defects on CCMs and GDEs was difficult for black surfaces typical of fuel cell MEAs; defects of approximately 1 mm were detected. It is not clear if these defects had a significant effect on performance. The IR/DC diagnostic is the furthest along in development in terms of detecting surface cuts and scratches. Even so, GDL/CCM cracks in line with the electric field were difficult to detect using the technique. Lawrence Berkeley National Laboratory (LBNL) modeling was used to good effect to optimize excitation geometry, and the diagnostic will be installed on an Ion Power commercial coating line. The other techniques presented need further development before their usefulness can be established. A new diagnostic to measure the ionomer/carbon ratio was described. It was unclear what variations can be detected and how they impact performance. The presentation did not indicate a strong industry need for this diagnostic.
- The project continues to make progress related to QC of MEA manufacturing. This year, the researchers have an agreement with Ion Power to deploy on their catalyst coating line. The team also developed a dual light source to improve sensitivity to low-emissivity materials, as well as demonstrated IR/RFT in an open environment. The next step is to demonstrate with a moving substrate and a dry-open air environment to measure I:C ratio – electronic capacitance.

### Question 3: Collaboration and coordination with other institutions

This project was rated **3.9** for its collaboration and coordination.

- This project features excellent collaboration with relevant industry partners.
- This project is well coordinated, from gleaning industry needs for measurements to deploying early developed diagnostic systems with industry partners.
- Collaborators from industry are essential for the nature of this work. This project has a good mix of these collaborations in addition to laboratory and academic partners.
- The agreement for deployment with Ion Power is excellent; one suggestion is that it should include recording of other experimental conditions, including relative humidity (RH), temperature, etc.
- Reasonable collaborations are evident with a number of the DOE manufacturing projects. LBNL modeling has been used to optimize the IR/DC and IR/RFT diagnostics.
- A formal collaboration with a manufacturer of fuel cell components, such as GDLs or MEAs, would strengthen the team. This small weakness is mitigated by testing materials provided by component suppliers and the early involvement of components suppliers in project planning and prioritization as well as diagnostics development and validation.

### Question 4: Relevance/potential impact on advancing progress toward DOE research, development, and demonstration (RD&D) goals

This project was rated **3.1** for its relevance/potential impact.

- The development of crosscutting component QC diagnostics is cost effective. Very high defect-free manufacturing yields are needed for fuel cell operation and durability. This project addresses this issue.
- The output of this project when implemented will have a significant impact toward addressing the highlighted barriers. While identification of defects is good, the project should focus on permitting the quantification of these defects to have a higher impact.

- All of the measurement methods developed in this project have value in aiding in fuel cell manufacture; some have significant value.
- MEA quality improvements (leading to cost reduction) offer opportunities for PEMFC cost reduction.
- It is worthwhile to develop improved diagnostics to detect defects in MEAs and GDLs that can be implemented on actual manufacturing coating lines. NREL has developed several techniques; the most successful is IR/DC, which can detect known pre-fabricated defects down to around 1 mm size at realistic line speeds. Because this technique will be installed on an Ion Power coating line, researchers will be able to determine the usefulness of the technique for detecting unknown defects on a full-scale line. The other techniques being investigated at NREL require further development before their usefulness can be assessed. Perception of relevance would be enhanced if there were clearer indications that the NREL project closely aligned with component suppliers' recommendations on diagnostic development needs.
- The potential impact could be good; however, it is dependent on whether the manufacturing developers are willing to use these techniques. Thus, a substantial portion of this project's future efforts should ensure that manufacturers are deploying the techniques or are willing to do so.

### Question 5: Proposed future work

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

- All of the future plans are important to fuel cell manufacturing. Deployment of the diagnostics in industry to ensure valuable feedback for optimization is very good. Hopefully there will be a chance to deploy the IR/RFT in a real in-line manufacturing arrangement.
- The overall plans for future work are well thought out. Deployment efforts and partner studies should yield valuable information regarding the ultimate usefulness for industry.
- The proposed future work features a logical progression of efforts. Important work on improving sensitivity is planned.
- The future work plans are good—the project team should continue developing these techniques to improve their performance in real-world applications. Schedule information and go/no-go decision points for the various diagnostics would be helpful. Decision metrics based on the expected impacts of various defects on performance are important and should be presented.
- The next steps appear reasonable, given the progress to date.
- The proposed future work lacks details on quantification; i.e., how these techniques can be used in a feedback process loop control. Further, the impact of these strategies on cost reduction is unclear.
- Much more can potentially be done with the capacitance measurement; the project should expand beyond I/C ratios. Work on deployment looks to be initiated with Ion Power. This work should demonstrate whether the industry developers are willing to incorporate the measurements into their lines. The value in the spatial failure studies in relation to MEA defects is unclear. This is not really a manufacturing/QC methodology, and it is probably not likely to be beneficial in relation to the goals of this project.

### Project strengths:

- A strength of this project is the manner in which NREL applies new techniques to solve production process controls in fuel cell manufacturing.
- This project features a strong collaborative team.
- The project is making good progress on multiple approaches and is working well with industry for guidance and deployment.
- NREL is using commercially available hardware from other industries and adapting the hardware for use in fuel cell manufacturing processes that occur at high line speeds. There is good synergy between NREL and the other DOE manufacturing projects in terms of developing and implementing these diagnostic techniques.

### Project weaknesses:

- Improved sensitivity is strongly required for all techniques and applications.
- The value of the segmented cell operation to detect MEA defects is not clear in terms of QC.

- This project seems more qualitative; it is not quantitative enough.
- Still to be resolved is the correlation between the prearranged defects that are used to develop the diagnostics and the defects encountered on high-speed production lines.

#### Recommendations for additions/deletions to project scope:

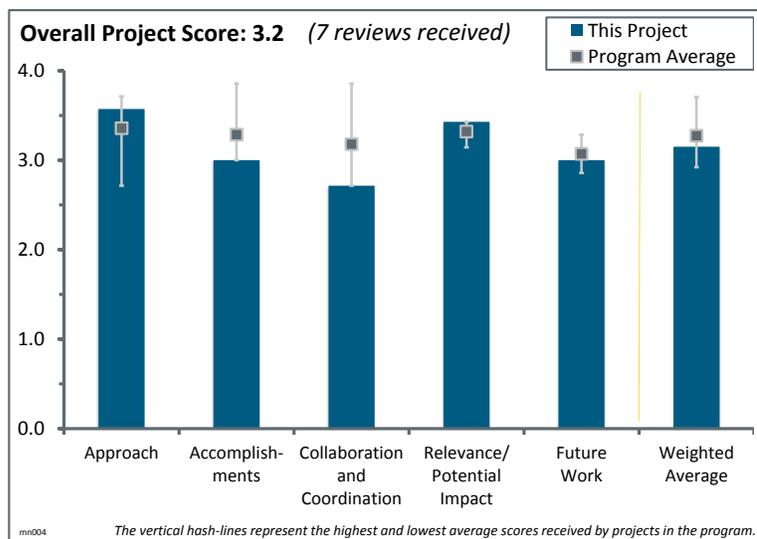
- Researchers should develop methods to quantify catalyst loading on the GDL after electrode coating application.
- Researchers need to further develop the relationships between defects and failures and cost.
- The project team should focus on diagnostics for manufacturing processes that have potential for implementation. For instance, segmented cell studies are not likely to be used in actual manufacturing environments. Decision points and go/no-go points should be established for each diagnostic along with decision metrics.
- The project team should consider other image processing algorithms to enhance information and increase signal to noise. For the reflectance, new information could be produced from these techniques with the same raw data. Suggestions may be two-dimensional auto correlations and cross correlations, among other software methods.
- The capacitance measurement could be interesting and useful. For the catalyst layers, researchers should refine this to reasonable carbon/ionomer ratios to see if they can distinguish anything for the small variations expected in manufacturing. They should also evaluate this as a function of RH; while RH does not vary at NREL, it certainly does in other places, such as Delaware, for example. The researchers should also evaluate the use of capacitance as a quick QC method for catalysts and catalyst supports. For example, they could compare MEAs with carbon black and graphitized carbon and vary the platinum loading on these. This technique might be more useful for catalyst QC (including Pt/C loading, carbon surface area, and catalyst loading on the MEA) than for I/C ratio monitoring. The modeling from LBNL looks interesting in terms of further utilizing the data and improving capabilities; however, it is unclear if and how this is being used. This analysis should be included in the demonstrations (such as at Ion Power). The researchers are concentrating on the visible spectrum of light for low-emissivity materials. They should try other wavelengths, such as ultraviolet.

## Project # MN-004: Manufacturing of Low-Cost, Durable Membrane Electrode Assemblies Engineered for Rapid Conditioning

Colin Busby; W.L. Gore

### 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, five-layer membrane electrode assemblies (MEAs) that minimize stack conditioning. Manufacturing processes must be scalable to fuel cell industry MEA volumes of at least 500,000 systems/year and must be consistent with achieving the U.S. Department of Energy (DOE) 2017 automotive MEA cost target. The products manufactured should be at least as durable as the MEAs produced using current manufacturing processes for relevant automotive duty cycling test protocols and must demonstrate power density greater or equal to that of MEAs made using the current processes.



### Question 1: Approach to performing the work

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

- W.L. Gore is using a well-designed combination of modeling, experiments, and in-situ validation in the effort.
- The project is well organized with objectives to reduce MEA and stack costs, as well as increase the durability and power density of the fuel cell stack. The approach combines component, manufacturing optimization, and manufacturing process development with mechanical modeling. The very systematic and directed approach increases the probability for success.
- The approach is good. W.L. Gore is developing methods to produce fuel cell MEAs in volume. Little attention has been given to the integration of the gas diffusion layer with the MEA from W.L. Gore. It is unclear whether this will be a significant cost adder. W.L. Gore should also focus on roll-to-roll lamination and integration of all layers.
- W.L. Gore is developing a direct-coating process to reduce the cost of MEA fabrication. The W.L. Gore project addresses one of the critical barriers to fuel cell introduction—cost. The approach is logical and, if successful, is expected to lower the cost of MEA fabrication to the DOE target of \$9/kW by 2017.
- The manufacture of low-cost, durable MEAs for high-volume processes is an important objective for DOE. The 2009 Process Waste Map helped inform efforts and project that up to a 25% reduction in MEA cost could be achieved. W.L. Gore identified six very relevant sub-objectives for this effort, including scalable manufacturing processes, reduction in stack break-in time, maintaining or improving power density for relevant automotive operating conditions, and making progress toward achieving DOE's 2017 cost target of \$9/kW MEA.

### Question 2: Accomplishments and progress toward overall project and U.S. Department of Energy (DOE) goals

This project was rated **3.0** for its accomplishments and progress.

- The project appears to be on track to achieve its overall goal of reducing MEA cost by 25%.

- The accomplishments have been very good; W.L. Gore has met and/or completed the majority of the project milestones. New 5  $\mu$  and 10  $\mu$  reinforced membranes have been incorporated into the primary development path. Previously modeled process improvements have been incorporated that indicate a potential 25% reduction in high-volume, three-layer (3-L) MEA cost. There is good potential to meet automotive power density and durability targets. W.L. Gore is seeking a new partner for stack testing; UTC Power is no longer the test partner after its sale to ClearEdge Power, Inc.
- Process and material improvement work with identified cost reductions appears to be on track to exceed original targets. The cost analysis support from Strategic Analysis, Inc. (SA) is a helpful addition to the team.
- The project passed its go/no-go decision. The University of Delaware (UD) work on parametric analysis went from 50% to 80% complete. The fatigue analysis work went from 0% to 30% complete and will be finished this summer. The low-cost backer task is 100% complete this period. Cathode layer work is 95% complete this period and the principal investigator stated it “is as good as or better than current MEA.” The reinforced membrane layer was demonstrated on a roll-to-roll process. Cost analysis went from 0% to 100% complete this period. Improvements have contributed to W.L. Gore going from 18  $\mu$  to developing a 5–10  $\mu$  MEA.
- W.L. Gore reports success in the development of low-cost backer material. W.L. Gore’s data on direct-coated cathodes demonstrates performance consistent with control materials. W.L. Gore developed a state-of-the-art thin, durable, reinforced membrane that has enhanced performance at high current density characteristics. The thickness has been reduced by up to 75%. The membrane was operated more than 80,000 cycles in the relative humidity (RH) cycling test. UD has successfully modeled the strains in the single cell associated with RH cycling. The model allows selective evaluation of RH effects on either the anode or the cathode and can separate those factors. Working with SA, W.L. Gore has established a cost model for a 3-L MEA manufacturing process. W.L. Gore’s analyses identify the three top cost uncertainties for the MEA: ePTFE cost, maximum coating speed, and ionomer cost. The analyses did not include the cost of the platinum group metal (PGM) catalyst and it must be assumed (and should be confirmed) that the cost of PGM was considered to be identical for all modeling conditions. The W.L. Gore/SA model predicts similar costs for the W.L. Gore MEAs and the 3M nanostructured thin film/membrane catalyst coated membrane. This is a surprising input and the catalyst loading for the two MEA structures was not identified.
- It is unclear what progress has been made since last year other than selecting a low-cost backer. The cost sensitivity shows the highest uncertainty due to ePTFE cost; it is not clear why this was not the focus. Further, there is no quantification of defect and fallout rates and their impact on cost sensitivity.
- This was, in essence, a repeat of the fiscal year (FY) 2012 presentation. It featured almost all of the same slides as FY 2012. The presenter showed the SA slides, which really feature SA modeling and not work from this project; otherwise, only two slides were new: slide 14 and slide 17. Even the summary slides were essentially exactly the same as last year. In addition, no modeling results were shown from the University of Tennessee, Knoxville, (UTK) and there was no indication of how these modeling results are being incorporated into this project.

### Question 3: Collaboration and coordination with other institutions

This project was rated **2.7** for its collaboration and coordination.

- The team would have been outstanding had not UTC Power withdrawn from the fuel cell activity. Depending on the replacement, the team could be rated outstanding.
- Appropriate collaborations are in place, albeit the project needs a new partner for stack testing.
- Losing UTC Power is a concern and replacing it will be important to the overall success of project.
- The project is making good use of outside cost analysis and academic modeling inputs. A replacement needs to be identified for UTC Power for stack testing.
- Collaboration among the remaining partners has been focused on modeling process improvements as well as a manufacturing cost analysis of the new process. Once the roll-to-roll process for the 3-L MEA has been demonstrated, the modeling focus will shift to the optimization of the process. Interaction among the partners appears to be effective.

- W.L. Gore has provided data to SA, which has clearly used the data in its project. This is a benefit to the DOE Hydrogen and Fuel Cell Technologies Program (the Program); however, it appears that this was a one-way transfer of information. The presenter discussed modeling from UD and UTK; no results from UTK are evident. There is no evidence that the UD modeling results are being used in this project, aside from it being a stand-alone modeling project at UD.
- UD completed its mechanical model work and it appears W.L. Gore will utilize this model once the new process is stabilized. It will be validated with in-situ nitrogen cycling testing. UTK heat and water management modeling work is complete. The UD/UTK publication of modeling work can inform the general public/industry/academia beyond just W.L. Gore, which no longer has UTRC as a partner for stack testing. W.L. Gore is looking for a new partner. UD work identified integral response as a critical parameter for fatigue life of the MEA. The National Renewable Energy Laboratory (NREL) is working with W.L. Gore on in-line quality control (QC). This will help W.L. Gore and also provide NREL with another industry partner from which to evaluate the efficacy of the in-line QC tools being demonstrated.

#### **Question 4: Relevance/potential impact on advancing progress toward DOE research, development, and demonstration (RD&D) goals**

This project was rated **3.4** for its relevance/potential impact.

- The project addresses one of the key barriers in the Program—cost in high-volume manufacturing. If successful, the project is expected to meet the DOE target of \$9/kW for a 3-L MEA product.
- The project is addressing a number of important barriers to meeting the Program’s objectives.
- The development of a low-cost, high-performance MEA is critical for the polymer electrolyte membrane fuel cell system. The reduction of the stack break-in time to 4 hours would be a significant improvement.
- The new 3-L MEA process exploration is “leading the charge.” W.L. Gore will utilize UTK/UD models during the future process optimization phase. New raw material formulations have been developed for the 3-L MEA process; it is not clear how these process improvements will translate beyond W.L. Gore. The cost model developed jointly with SA may help other U.S. MEA firms better understand cost drivers (e.g., 3M). This model identified the top three cost uncertainties as being ePTFE cost, maximum coating speed, and ionomer cost.
- The stated objectives are relevant; however, the approach and progress suggest that minimal impact has been made on addressing the barriers, contrary to the researchers’ claim. The project goal was to reduce the cost of MEA manufacturing, not the material cost that would have been used in the MEA.

#### **Question 5: Proposed future work**

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

- The proposed future work seems partially relevant.
- The remaining activities are appropriate and important (particularly scale-up and stack validation) to complete the project.
- The proposed future work is organized and consistent with the progress of the project. The schedule for the future work is reasonable and consistent with the capability of the team.
- Future work plans include optimization of the process once roll-to-roll fabrication is demonstrated and stack testing of the MEA package is performed. A new stack testing partner needs to be identified in short order to meet the project timeline.
- The proposed future work is consistent with what is appropriate, given the time and funding left on this project. Stack testing is important to validate results of this effort; however, W.L. Gore no longer has UTC Power to do this function.
- Future work includes MEA conditioning, process scale-up, and stack validation, which are all good tasks. However, no details were given on how the conditioning methodology will be conducted. Stack validation is probably straightforward and being conducted at UTC Power. It is unclear at what point in time the modeling at UD and UTK will be incorporated into this project; it does not seem to really appear in the project plans.

**Project strengths:**

- This is a well-designed effort that is exceeding expectations.
- This project features a strong project lead and partners.
- W.L. Gore's expertise and innovation are strengths of this project. The project also features great modeling support by the partners.
- W.L. Gore's experience and knowledge of membrane and MEA processing is the strength of this project. UD and UTK modeling expertise has been a significant help in predicting the impact of potential modifications to the manufacturing process.
- The strength of this project is the quality of experience W.L. Gore brings to the project. The MEA manufacturing capability of W.L. Gore is world class. The cost analysis capability of SA is well recognized.
- MEA costs are a large fuel cell cost driver and this effort addressed a multiple-percent cost reduction. The 3-L MEA process was informed by this effort, and when transitioned to production, it should provide significant cost and durability benefits. Inclusion of two academic institutions and NREL provides a greater degree of transparency, at least for the modeling and in-line QC efforts. MEA cost reduction efforts have made significant progress in recent years and this well-thought-out and well-executed effort has certainly been one of the key contributions.

**Project weaknesses:**

- There is a lack of focus on the areas of highest impact.
- There were not any visible inputs from NREL.
- The manufacturing improvements that W.L. Gore realizes from this project will likely apply only to W.L. Gore and not have any general applicability to the larger fuel cell developer community.
- It is not clear if the 25% reduction in high-volume 3-L MEA manufacturing costs will in fact be achieved. W.L. Gore has only indicated the potential for these reductions. In its defense, W.L. Gore is still in lab-scaled development of the 3-L MEA process.
- This project showed limited-to-no progress from FY 2012 to FY 2013; the cause of this is unclear. It featured almost all of the same slides as FY 2012. Even the summary slides were essentially exactly the same. For example, the 2012 Key Accomplishments include "lab scale development of the new 3-L MEA process is nearing completion," whereas the 2013 Key Accomplishments include "Lab scale development of the new 3-L MEA process is nearing completion."

**Recommendations for additions/deletions to project scope:**

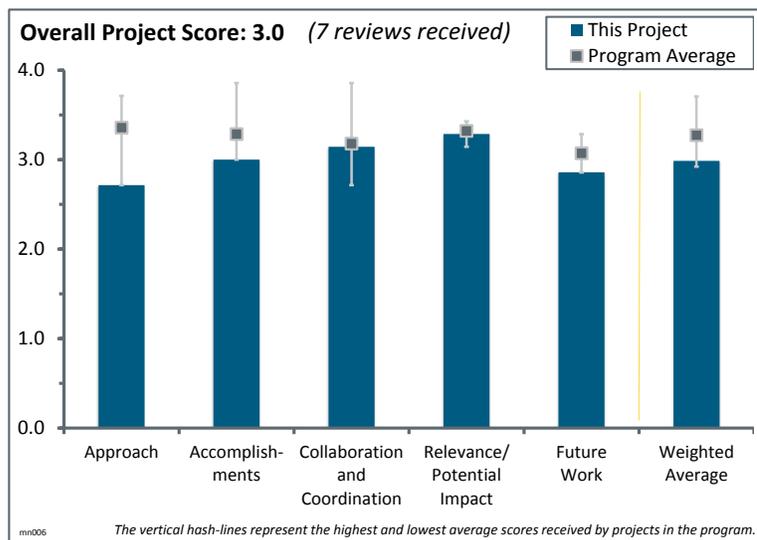
- The project team should conduct a cost model analysis of manufacturing MEAs through electrode coating on diffusion media approach.
- Researchers should seek to make the results of the project more broadly applicable to other MEA manufacturers.
- A "major" portion of the cost reduction of this project is moving to low-cost backing materials for the MEA. The project team should explore a reusable backing material instead of a replaceable, low-cost backing material. That would make for more substantial cost reductions. More clarity is needed on how the UD modeling and UTK modeling will actually be used. It is hard to know how the MEA/stack conditioning is going to work with no details. The researchers should show a comparison of performance direct coating versus the previous coating methodology.

## Project # MN-006: Metrology for Fuel Cell Manufacturing

Michael Stocker; National Institute of Standards and Technology

### Brief Summary of Project:

This project is focused on developing high-throughput optical process control methods to develop an accurate optical metrology infrastructure for semiconductors and nanomanufacturing. Using catalyst-coated samples provided by manufacturers with variations in critical parameters (e.g., platinum and platinum alloy catalyst loading) and including various types of defects characterized using standard methods, this project evaluates the sensitivity of optical scatterfield metrology to these parameters. A custom optical metrology tool, the Large Aperture Projection Scatterometer (LAPS), was designed and built to further understand the underlying measurement science and develop the necessary rigor.



### Question 1: Approach to performing the work

This project was rated **2.7** for its approach.

- The general approach to the effort was appropriate. Additional input from other researchers at laboratories or in academia may have been useful.
- This year's effort was primarily focused on the LAPS. The approach was direct in that the LAPS was used as it would normally be used for many material surfaces.
- The approach so far appears to have concentrated on samples with different nominal values. Researchers need to understand how the technique responds to spatial variability within a sample. Testing the LAPS under motion of the substrate is good to see, though 4 ft/min is quite slow. Researchers need to understand performance at higher speeds. Also, there does not appear to have been studies on gas diffusion electrodes (GDEs), though applicability is stated.
- The product is just now coming online, so it is difficult to fully assess the quality of the effort. The process it took to get to this stage is reasonable in regard to the approach.
- The project seeks to adapt existing equipment and procedures from semiconductors to fuel cell components and the development of new equipment. Some of the techniques do not appear useful on rough surfaces, such as 3M's nanostructured thin-film (NSTF) materials. More discussion of the applicability and capability of the techniques would be beneficial.
- The development of optical scatterfield metrology for determination of fuel cell catalyst layer properties is well focused on proving that the technique measures real catalyst properties, adapting the technique from a small sample measurement to larger sample-size measurements, and expanding the capability of the technique to "high-speed" production lines. The project approach addresses the first two of these issues. The third issue, high-speed production applications, was not addressed in this presentation— even though it is a critical component to success. The researchers introduce spectroscopic ellipsometry to the project. Ellipsometry is a well-known methodology used by industry (measuring the protective coating on metal used in the manufacture of soup cans), and it is not clear why the project team incorporated an existing technology. This incorporation needs a better explanation.
- The project approach appears to be "trial and error," as three iterations of instrumentation have been evaluated. A priori modeling, calculations, or other analysis on similar substrates may have helped narrow the choices.

## Question 2: Accomplishments and progress toward overall project and U.S. Department of Energy (DOE) goals

This project was rated **3.0** for its accomplishments and progress.

- When this equipment is finally tested, this project's progress could be upgraded to outstanding.
- The project team has achieved a good proof-of-principle on 3M NSTF and W.L. Gore catalyst coated membranes (CCMs).
- The LAPS device has some potential, but there still seem to be some process control issues to resolve, particularly samples that are not perfectly flat. Additional work is required to develop a full array and there will certainly be unanticipated hurdles bringing several of these devices together in a coordinated way.
- The development of LAPS appears to provide a strong advance over the original optical scatterfield system. LAPS has larger spot size—approximately 10 mm wide and at least that long (the spot is an ellipse, with length dependent on the illumination beam angle of incidence with the sample). It is unclear how this will enable detection of small defects. Also, it would appear that this large of a spot size, unless the response time of the measurement is extremely fast, would lead to significant smearing of the data as the substrate is moving, in process.
- The success of increasing the spot size for large data averaging is very impressive. However, the size of the spot is still very small compared to the width/length of a membrane electrode assembly (MEA) manufactured in a continuous manner. Researchers need to explain how to use the “larger” spot. The demonstration of platinum in real samples is impressive. Still, the technique is limited to a local, albeit larger, spot. Measurement of the diffraction pattern is impressive and the need to develop the technique for a greater understanding of how to apply the diffraction pattern measurement is important.
- The LAPS diffraction pattern (slide 10) contains information corresponding to the platinum loading, but it also looks like a possible forward Mie scatter pattern with intensity lobes. The Mie scattering would correspond to particle size, shape, and diameter ratio with laser wavelength. The measurement shown is likely diffraction with a correlation to loading ( $\text{mg}/\text{cm}^2$ ); however, it may be worthwhile to double check that the measurement is not also Mie scattering, indicating particle dimensions that could also correlate to Pt mass loading. Judging by the optics horsepower within the team, however, the presented conclusions are correct. The principal investigator is correct (summary slide) in that significant work remains, but other than time, there should be few showstoppers.
- The relatively low budget precludes major advances. Most of this year's progress has been equipment building and procedure development. Some preliminary data have been obtained on W.L. Gore (at line velocity) and 3M samples.

## Question 3: Collaboration and coordination with other institutions

This project was rated **3.1** for its collaboration and coordination.

- The project team is working with leading fuel cell MEA manufacturers that could most benefit from this technique.
- W.L. Gore and 3M are providing samples and insights into possible defects and their characteristics.
- The selection of the two CCM partners to represent the range of materials expected for measurement was very astute.
- This project features good collaboration with industry in test samples and measurement needs. The addition of research and development with a metrology toolmaker could prove to be very valuable in this field, which is rich in nuances in optical techniques.
- Current collaborators consist of sample suppliers. Additional collaborators may be helpful in moving along the characterization and validation of novel measurement techniques.
- The level of involvement from 3M and W.L. Gore is not clear. Also, there does not appear to be any involvement by a GDE company, though the applicability of the technique to GDEs is stated.

**Question 4: Relevance/potential impact on advancing progress toward DOE research, development, and demonstration (RD&D) goals**

This project was rated **3.3** for its relevance/potential impact.

- This project fits directly with DOE's directive for advanced quality control (QC) analytical methods. Measuring Pt on both sides of the MEA independently is a great accomplishment.
- If proven, the techniques developed in this project are very important to fuel cell manufacturing.
- In-line, real-time measurement of fuel cell component properties will definitely facilitate commercialization.
- This reviewer hopes that the testing of this product is successful.
- There could be potential for in-line Pt loading measurement to lead to cost savings, but the linkage is not clear.
- The technique(s) need to be demonstrated to cover the full width of a continuous MEA manufacturing process. The technique provides a local spot on the moving MEA.
- Uniformity of the catalyst layer is of high importance to scale up and reduce costs of MEAs. However, other than the benefit of being able to measure two-sided coated membranes (which has not been shown), it is not clear how this technique offers significant benefits over X-ray fluorescence (XRF) technique, which has already been funded and demonstrated under another DOE manufacturing project. Also, the widespread applicability of this benefit is not clear; all GDE structures are one-sided, and this reviewer is not aware of any simultaneous two-sided coatings, although it is a possible direction.

**Question 5: Proposed future work**

This project was rated **2.9** for its proposed future work.

- The proposed future work is a logical progression of what has been done so far. Measurements on large formats at web-line speed will be attempted.
- Researchers have identified considerable work to reach the project's goals, and it seems appropriate.
- The proposed future work builds well on prior discoveries/shortcomings, but it is unclear whether the current third path will work. The presenter noted that 3M NSTFs act as an optical grating, which may present issues.
- The "robust model" that permits flexibility and normalization among different measurement samples is a good idea. The multiple-beam LAPS is a necessity. Perhaps there are acousto-optical or electro-optical methods for scanning that could do the same as the multiple-beam approach.
- Until researchers establish the applicability of the technique to different types of electrodes, higher rates of motion, and samples with spatial variability, the value of spending a lot of effort on modeling is unclear. The objective of measuring membranes is unclear; it is not clear whether this is part of understanding the electrode measurement or a new measurement. The need for membrane measurement is also unclear—other techniques have been developed and demonstrated under DOE manufacturing funding. The plan to look at higher speeds is a good direction to pursue.
- The researchers are missing the application point and are more concerned with the development of a robust model for analysis. The researchers should consider how they can apply this technique, assuming the analytical methodology is complete (which it is not). They want to answer the analytical methodology question without addressing the application question.

**Project strengths:**

- The team is persistent in overcoming issues, able to measure both sides of CCM independently, and can meet the target data acquisition rate.
- Strengths of this project include NIST's expertise and the high-quality skills of the people working on this project.
- The project seeks to address a key QC need: Pt loading. The metrology capabilities at NIST are world class.

- This project features a great capability in advanced optical methodology; probably one of the top two or three in the world.

**Project weaknesses:**

- The slides are too dense.
- It is unclear how surface changes due to normal manufacturing variation will impact measurement, and whether this variation can be accommodated in the processing.
- The potential cost savings resulting from the techniques under development are not clear. There does not seem to be sufficient time before the project ends to complete the identified future work.
- The researchers need to get better input from industry. The question of how to apply the technique needs to be answered. If the technique cannot be applied, it is not clear why it should be developed.
- Overall, the benefits of this technique compared to XRF are not clear and possibly not compelling. The ability to measure two-sided coatings simultaneously is definitely something XRF cannot easily do, but the need for this benefit—i.e., how many companies actually will need a simultaneous measurement—is not clear and does not appear to be very widespread. The project team has not looked at defects yet.

**Recommendations for additions/deletions to project scope:**

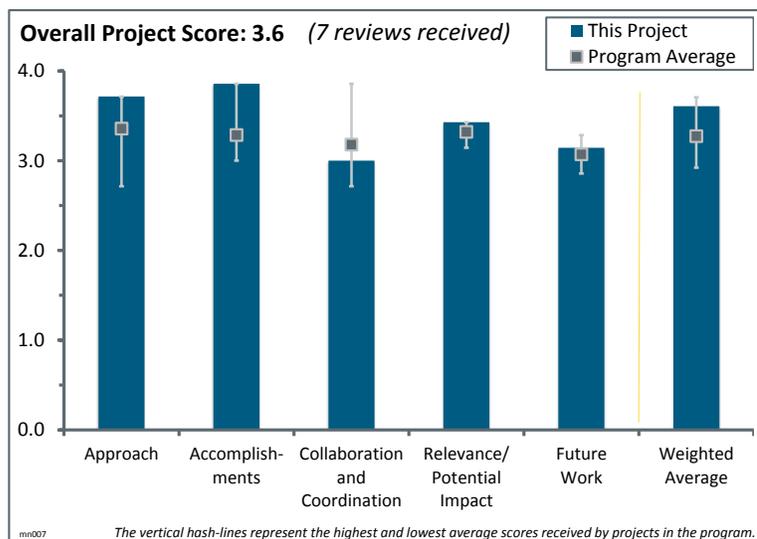
- Researchers should look into Mie scattering and some acousto- and electro-optical methods for flexibility.
- The future work should include testing of GDE samples.
- The project team needs to add a strong modeling component to understand whether the commonly found range of morphological differences will impact the signal/noise ratio. The team may have to focus on fixturing to keep moving web in a flat orientation to avoid spurious signals.

## Project # MN-007: High-Speed, Low-Cost Fabrication of Gas Diffusion Electrodes for Membrane Electrode Assemblies

Emory De Castro; BASF

### Brief Summary of Project:

The objectives of this project are to (1) reduce costs in fabricating gas diffusion electrodes (GDEs), focusing on GDEs used for combined heat and power (CHP) generation; (2) relate manufacturing variations to actual fuel cell performance to establish a cost-effective product specification within six-sigma guidelines; and (3) develop advanced quality control (QC) methods to guide realization of these two objectives. BASF also strives to further decrease costs with paper substrates, single-pass applications, and by exploiting stable links to promote platinum thrift.



### Question 1: Approach to performing the work

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

- The project systematically addresses the barriers to GDE production by building on past accomplishments and progress.
- The project has been making steady progress since 2009. The awardee laid out and implemented a methodical approach to addressing the problems in the statement of work (SOW). The approach was well thought out to achieve the goals, and the methodology has allowed the researchers to perform thorough root cause analysis for identifying issues for improvement of the GDE. An additional task was even added in 2012 and the awardee has been making progress on this task. Goals have been set and achieved throughout the project.
- Membrane electrode assemblies (MEAs) are a big cost driver in the production of affordable fuel cells. The GDE represents an important part of the MEA, and as stated, there is a lack of existing high-volume MEA processes. This approach is aimed directly at improving GDE production so that it is high speed and low cost. Having a GDE supplier (BASF) leading this effort makes it more likely that the resulting technology will transition. This effort has already led to new product development. The objective during this period of further decreasing cost with paper substrates and single-pass applications—including exploiting stable inks to promote platinum thrift—is considered a sound approach for this stage of the project. Specifically, BASF hoped to increase the solids content of ink without a loss of stability.
- This project is working to develop online diagnostics for QC that have good speed and are non-destructive.
- This project concentrates on the various aspects of throughput improvement—ink formulation, ink coating, maintaining quality, increasing width, and the effects of substrate.
- The only information presented on the approach was a list of milestones. It is assumed that the approach was valid because all of the milestones were met.

## Question 2: Accomplishments and progress toward overall project and U.S. Department of Energy (DOE) goals

This project was rated **3.9** for its accomplishments and progress.

- Milestones were met. Throughput (line speed) was significantly increased; the paper gas diffusion layer (GDL) cost goal was met; and variability now meets an acceptable level.
- This project has developed a technique that has led to a reduction in manufacturing variability.
- This project features impressive improvement in platinum variation, reducing costs and improving performance.
- The awardee has made significant progress on all of the goals of the project. Researchers have met many of the goals to reduce the costs of the GDE. They have accomplished ink cost savings and obtained performance gain of the GDE. They have worked with stabilizing the ink and switched from carbon cloth to carbon paper for cost savings. The project has reduced the base material costs. A new task was added in 2012 to achieve performance gain and reduce precious metal (PM) content, and both of these goals are being accomplished.
- Researchers have met or exceeded project throughput targets, leading to reduction in labor costs by 75%. It would be useful to see the cost breakdown between labor, machinery, and materials. Although a reduction in platinum loading was not an objective of the project, new inks, processes, and QC allowed less platinum to be coated and resulted in greater performance.
- The creation of a six-sigma specification for the production of GDEs will reduce the variability and minimize yield loss. This develops a control zone for the manufacturing process by carefully monitoring properties of manufacturing lots and results in performance enhancement. The use of carbon paper substrates with the development of a controlled micro-porous layer (MPL) increases the performance characteristics of the fuel cell. For a high-temperature membrane system, the MPL flattens the catalyst layer, but the high temperature precludes the benefits of water removal. The presenter did not report whether the MPL influences acid transport out of the high-temperature membrane. The catalyst thrift program of less than one year demonstrated savings in the catalyst. This is an outstanding result for a small effort.
- Task 2, subtask 2.2, creating six-sigma specification, was largely met. Reaching six-sigma in one year was considered a “stretch goal.” BASF is currently at approximately three sigma, which is much further along than it was in the past, when high-performing material was hand selected or “cherry picked.” The fact that this new method accounts for variability as well as performance, is a key accomplishment. The principal investigator (PI) gave an example of variability differences detected that led to the discovery of a heating coil that was failing and causing the excess variability. For Task 5, carbon paper substrates, BASF scaled single-pass MPL to production coating machining at 1/2 width. This is a 28% cost improvement compared to using carbon cloth (based on 3,000 5-kW systems). For the new task, exploring PM thrift, BASF successfully demonstrated a 30% cost reduction of PM at the anode with materials made on a production-scale coating machine. The PI commented that “this was impossible with pre-program inks.” The PI in 2012, however, had stated that this new task would address both anode and cathode coating. It does not appear any progress was made on the cathode. The levels of platinum used in this effort were significantly more than what would be anticipated in production.

## Question 3: Collaboration and coordination with other institutions

This project was rated **3.0** for its collaboration and coordination.

- BASF is working with a leader in high-temperature membrane fuel cells, which is a great benefit. The National Renewable Energy Laboratory (NREL) collaboration can benefit manufacturing QC.
- BASF shows good collaboration with NREL on GDE defect detection (see project MN-001). ClearEdge Power will evaluate materials for use in micro-combined-heat-and-power (micro-CHP) applications at the full stack level. This project is applicable to a minimal number of U.S. firms, namely BASF and its customer base.

- The project partners have been working together to meet the goals. NREL provided GDEs for part of the research. Currently, ClearEdge Power is evaluating the PM levels to accomplish the new goal established in 2012. There is good coordination and teamwork throughout the project.
- This appears to be mostly a BASF effort.
- A national laboratory provided samples with known defects to aid in the development of advanced defect detection techniques. MEA samples with thrifed platinum were sent to a micro-CHP stack integrator for stack testing. Results were not presented on the slides.
- The main collaboration in this project appears to be XOS; otherwise, there are limited collaborations.
- Case Western Reserve University (CWRU) and XOS are listed as partners, but not mentioned at all in the presentation. The XOS X-ray fluorescence (XRF) system has already been installed—it is unclear if there are any relevant improvements or future work. The status of the CWRU modeling work is unclear. NREL and ClearEdge Power were listed as collaborators, but nothing was shown regarding outputs from their collaboration. There are no stack results yet.

#### **Question 4: Relevance/potential impact on advancing progress toward DOE research, development, and demonstration (RD&D) goals**

This project was rated **3.4** for its relevance/potential impact.

- This research is important for the fuel cell community and aligns very well with the DOE Hydrogen and Fuel Cell Technologies Program goals. Because of this research, a new product was brought to market, supporting DOE's goal to help the U.S. economy/industry.
- Reducing PM content is key to the cost competitiveness of fuel cells.
- A new MEA product was released (March 2012), demonstrating the positive impact of this project. High-temperature fuel cells are an important part of the fuel cell portfolio and are critical to micro-CHP applications. ClearEdge Power is the only U.S.-based micro-CHP manufacturer. This effort will directly impact its systems. The XRF automated defect detection technique will provide for greater throughput at a larger scale of MEA manufacturing, and with NREL involvement, it could lead to industry-wide adoption.
- The project is very beneficial to micro-CHP and other high-temperature polymer electrolyte membrane (HTPEM) applications. In general, HTPEM has not been a strong focus of the DOE Fuel Cell Technologies Office, but it is work that is beneficial to the industry and overall market development/cost reduction.
- This is an important project for demonstrating manufacturing cost reductions for fuel cells. DOE should test to determine if the techniques developed in this project translate to low-temperature polymer electrolyte membrane manufacturing.
- This project works to improve the manufacturing and quality of GDEs for CHP. There are, however, only a limited number of developers who are looking to manufacture GDEs. If this project could be expanded beyond GDEs, it would have a greater impact in the fuel cell community.
- The presenter said very little about the applicability of the techniques to other fuel cell types.

#### **Question 5: Proposed future work**

This project was rated **3.1** for its proposed future work.

- The proposed work of scaling the catalyst coating to production level demonstrates efforts to build on work that was accomplished. Gains made at the pilot scale will be translated to actual systems. New work beyond this effort will include improvement toward more corrosion-resistant carbons.
- The project shut down is well organized. The researchers are not trying to push the project beyond reasonable limits.
- The presenter only briefly touched on future work, but the results seem to indicate that more development of these products could be achieved in the future. The project is closing out in June 2013.
- The project is virtually over. Scaling to production level is planned. After the project is completed, the knowledge should be applied to corrosion-resistant carbons.
- This project is essentially over; therefore, the future work does not seem relevant for much discussion.
- There are only a few months left in the project.

- The proposed next steps are in line with the discussed project pathway; i.e., applying advancements made on non-woven substrates to woven substrates, for potential additional cost savings. It would be useful to see the projected cost breakdown/savings of going to woven and an expected performance/durability comparison. Also, it is unclear whether the process will need to be modified to handle woven, which is more brittle and typically thinner.

#### Project strengths:

- This was a strong effort from start to finish.
- BASF is the major leader in HTPEM GDL manufacturing. The team brings in many years of experience in manufacturing.
- This project addresses key areas of MEA fabrication. Significant (30%) cost reductions have been achieved. The effort to move from expensive carbon cloth to paper-based materials appears to have been successful.
- The very structured nature of this project allowed it to meet the goals laid out in the SOW. This is a well-performed research project with strong results. There was good collaboration with partners. Overall, it was a very good project that was well run and well executed.
- The project addresses key process variables in a structured way to improve throughput. Advancements leveraged corporate BASF competencies beyond the fuel cell group. BASF is a leader in HTPEM MEA production, so it is valuable for DOE to support the advancement of this technology.

#### Project weaknesses:

- The results and benefits of collaborations (other than XOS) are not very clear. Neither the stack data validating performance nor the modeling results were shown.
- Researchers did not address the major issue of acid movement and how to manufacture components to control acid movement.
- It appears that the project team's technique shows +/- 0.4 g Pt/m<sup>2</sup>, which is 0.04 mg Pt/cm<sup>2</sup>. This is still a rather large variation, considering that the DOE target loadings are moving toward 0.125 mg Pt/cm<sup>2</sup> (i.e., this would be a 33% error in loading). The technique has a large depth of penetration; therefore, it appears that it is only applicable to one-sided MEAs or GDEs.

#### Recommendations for additions/deletions to project scope:

- It would be nice to see that the results of this project help the overall community more.
- The project is wrapping up in June 2013 and is on track.

## 2013 — Technology Validation

### Summary of Annual Merit Review of the Technology Validation Program

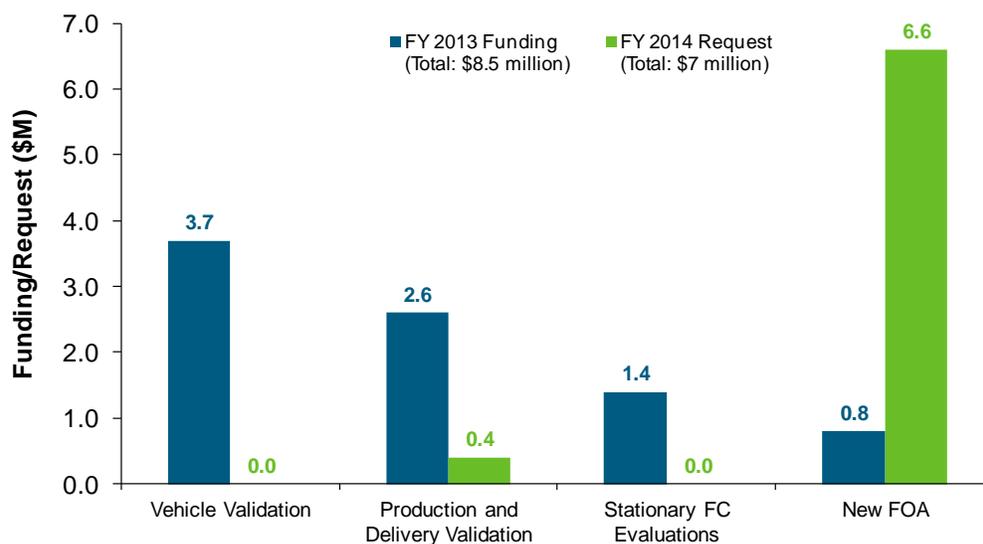
#### Summary of Reviewer Comments on the Technology Validation Program:

In general, the reviewers believed the program area was adequately covered. The role of the Technology Validation program within the structure of the Fuel Cell Technologies Office was clearly identified. Progress relating to projects was clearly presented and plans were identified for addressing issues and challenges. The partnership with the National Renewable Energy Laboratory's (NREL's) data collection/analysis team was seen as key to the success of the program's efforts, and to achieving its goals and objectives. Given the high failure rate observed with compressors, reviewers suggested that further attention should be given to their validation. Suggestions were also made for the program to consider the evaluation of 700-bar dispensing, along with related components such as gas pre-cooling refrigeration systems and flow meters. Reviewers also recommended that the program's funding decisions should reflect analysis that identifies technologies capable of providing a significant portion of the demand for hydrogen and that address a robust market for fuel cells.

#### Technology Validation Funding by Technology:

The Technology Validation program's funding portfolio will enable it to continue to collect and analyze data from fuel cells operating in transportation and stationary applications, as well as from hydrogen production and delivery technologies. Analysis of several new hydrogen refueling stations and fuel cell vehicles in California and the Northeast will be the main focus of the data collection activities. Data from fuel cell buses, forklifts, and backup power systems will continue to be evaluated. The fiscal year (FY) 2013 appropriation was \$8.5 million. The majority of the FY 2014 funding is likely to be focused on projects resulting from proposals submitted in response to a funding opportunity announcement that was issued for a variety of application areas. The FY 2014 request of \$7 million is subject to congressional appropriations.

#### Technology Validation R&D Funding



#### Majority of Reviewer Comments and Recommendations:

The reviewer scores for the six Technology Validation program projects that were reviewed had a maximum of 3.8, a minimum of 3.3, and an average of 3.5. A key strength identified by reviewers in all of the Technology Validation projects was the excellent participation from collaborators—this has been critically important to the success of the

projects. Reviewers also observed that NREL's approach for collecting, securing, and analyzing data is well established and trusted by project collaborators.

It was noted that the fuel cell bus data collection project is critical to the wide-scale adoption of fuel-cell-powered buses, providing valuable insights for both U.S. Department of Energy (DOE) project managers and transit fleet operators. It was suggested that performance and reliability comparisons with previous-generation buses, as well as bus deployments already performed or underway in Europe, should also be considered. Reviewers remarked that the results of the stationary fuel cell evaluations should be compared not only to DOE targets, but also to results for other conventional and emerging prime power technologies. In addition, reviewers suggested that it would be valuable to evaluate stationary fuel cell deployments in other states, even if it included only those that provide incentives for stationary fuel cells.

While recycling of hydrogen could be an attractive business proposition for a subset of industrial hydrogen users, uncertainties exist regarding how much of the future demand for hydrogen could be met by this method, and reviewers felt that the potential is limited.

The electrolyzer hydrogen station evaluation project was seen as having the potential to significantly reduce costs for small hydrogen stations utilizing renewable hydrogen via electrolysis. Evaluation of components by NREL was seen as needing more aggressive marketing to industry so that component developers may take advantage of NREL's testing prior to demonstrating their new products with customers in order to assess performance under "real-world" operating environments.

The reviewers believe that NREL's business case analysis of the economic and operating performance of fuel cell forklifts and backup power systems has contributed to the commercial ramp-up of these systems, delivering high value and impact to fuel cell system suppliers and DOE. Reviewers recommended the continuation of the data collection and analysis activities for early market fuel cell (forklifts and backup power) projects, with the purpose of establishing a long-term performance record for these systems and to portray trends over several years.

## Project # TV-008: Technology Validation: Fuel Cell Bus Evaluations

Leslie Eudy; National Renewable Energy Laboratory

### Brief Summary of Project:

The objectives of this project are to validate fuel cell electric bus (FCEB) performance and costs and to document progress and lessons learned on implementing fuel cell systems in transit operations to address barriers to market acceptance. The project collects data from transit partners to develop reports on individual site performance and annual FCEB status reports, including crosscutting analysis and projections for continued success.

### Question 1: Approach to performing the work

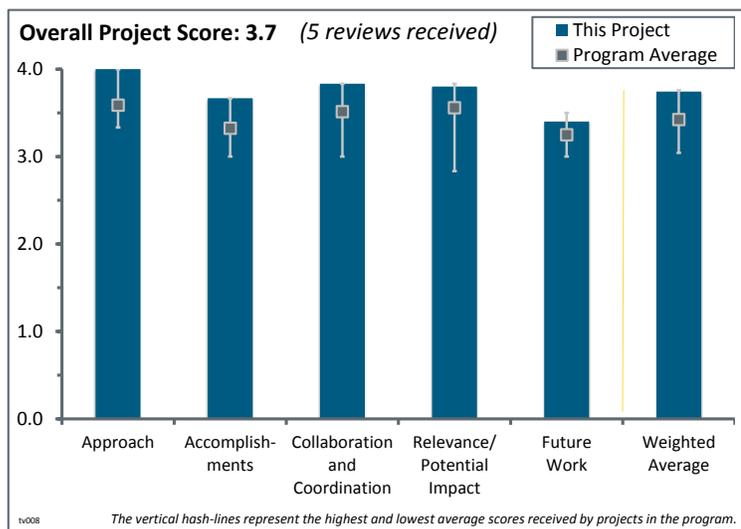
This project was rated **4.0** for its approach.

- The data collection project is well designed and organized.
- The National Renewable Energy Laboratory's (NREL's) data collection and reporting are of high importance to the bus program.
- This project is well focused on the key technology validation issues for FCEBs.
- This project has done a nice job of comparing current technology to project work. This is well-balanced work that is well thought out, especially in terms of the inclusion of technology readiness levels (TRLs).
- The approach, as summarized in slide 4, is straightforward and time-tested. It has evolved and proven successful during the years of NREL's working with transit partners to collect data, conduct analysis, and document progress.

### Question 2: Accomplishments and progress toward overall project and U.S. Department of Energy (DOE) goals

This project was rated **3.7** for its accomplishments and progress.

- Bringing credible TRL levels is a good additional step in terms of the data included in the reporting.
- The principal investigator should consider performing comparisons with past data in order to show the technology's progress.
- This project has made a significant amount of progress in the past year. The fuel economy numbers for the FCEBs are impressive in comparison to the diesel bus numbers. It is unclear why the AC Transit buses are not running in the 2012–2013 timeframe.
- This project has made good progress. If possible, NREL should identify the cause of the large increase in fuel economy and higher availability of the American FCEBs at Sunline Transit (SL AFCB) compared to the earlier bus (SLAT).
- This project has done an outstanding job tracking progress. There are real problems with reliability when first discussing availability; the justification for why FCEB reliability rates were so low did not seem to fully address the problem. If the average availability is 57%, and 47% of the non-availability problem is fuel cell-related, there are some real reliability issues that need further, more open discussion, and not doing so does not help the case for FCEBs.
- Slide 3 provides metrics, targets, and the current status for the performance and cost of FCEBs. These can be understood, and progress toward targets can be determined, at a glance. Slide 21 summarizes progress toward the targets as of 2013. With slides 5–16, an exceptional job was done conveying information about



the bus fleet, for which data have been (and will be) collected and analyzed. Displays and graphs, such as those on slides 8–16, are packed with information. The results during the year since the previous DOE Hydrogen and Fuel Cells Program Annual Merit Review are clearly identified. For relevant metrics, the performance of buses and transit fleets is compared to targets. The reasons for unavailability of FCEBs are detailed and provide valuable insights for both DOE project managers and transit fleet operators. The performance of FCEBs is compared to that of other bus types, including conventional, those with diesel hybrid propulsion, and ones fueled by natural gas. The conclusion stated on slide 14, a 56% increase in fuel cell system miles between road call (MBRC), is a bit misleading. The MBRC for April through August 2011 were evidently higher than that for January 2013 (the most recent month on the chart). An explanation of this apparent anomaly would have been helpful.

### Question 3: Collaboration and coordination with other institutions

This project was rated **3.8** for its collaboration and coordination.

- The key collaborations are in place.
- This project has outstanding team collaboration.
- There appear to be strong working relationships among the stakeholders and NREL.
- NREL's project managers maintain continuous communication with transit agency management, FCEB manufacturers, state and local government agencies, universities, and other organizations with an interest in bus fuel economy and emissions. The project managers maintain contacts both nationally and internationally. NREL's work and approach have enabled it to earn the confidence of many organizations with an interest in advanced bus technology. NREL acquires data, analyzes the data, and provides reports on all fuel cell buses operating in the United States.

### Question 4: Relevance/potential impact on advancing progress toward DOE research, development, and demonstration (RD&D) goals

This project was rated **3.8** for its relevance/potential impact.

- This information is critical to the wide-scale adoption of FCEB and will help to accelerate the adoption process.
- The data collected and presented by NREL should be a major selling point to convince other transit agencies to convert to FCEBs.
- The principal investigator has done a great job coalescing the data from various bus deployments. As mentioned previously, the investigator should consider performing performance comparisons with past bus deployments in order to show technology progress.
- For 20 years, since the start of DOE's support for vehicle fuel cell research and development (R&D), transit buses have been an important target opportunity for fuel cells. Given the focus on FCEB development, both in the United States and internationally, and the public resources devoted to buses, tracking the performance and cost is key to determining progress and making decisions about the merits of further development.
- The availability reports provide great data in terms of understanding the performance and identifying components that require improvement, especially since the failures appear to be caused by components other than the fuel cells. It is recommended that more be done to compare the different technologies and, if applicable, also compare new generations of vehicle technology with the previous generation of vehicle technology. This would provide data that show to what extent the technologies are improving from one generation to the next.

### Question 5: Proposed future work

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

- The future work is well planned.
- It is essential to keep recording these data to provide a long history of FCEB performance.

- Consider comparing performance and reliability data with other bus deployments already performed or under way in Europe, such as the past Clean Urban Transport for Europe (CUTE) program or the current Clean Hydrogen in European Cities (CHIC) program.
- Slide 19 clearly displays the future plans, which include technology validation for a variety of FCEB types operated by transit agencies in Illinois, Texas, Alabama, New York, Ohio, and Massachusetts, in addition to California and Connecticut. Slide 20 highlights the work to be done during the remainder of fiscal year 2013 and fiscal year 2014. The products will be consistent with the pattern that has been established in prior years.
- It would be helpful if the reporting discussed in more detail the differences in generations of buses to better inform the direction in the performance of the products. It appears the newer generations are performing better than the previous generations. It is recommended that more be done to compare the different technologies and, if applicable, also compare new generations of vehicle technology with the previous generation of vehicle technology. This would provide data that showed to what extent the technologies are improving from one generation to the next.

**Project strengths:**

- The level of detail in the reports is a strength.
- This is a very well-planned and executed project. This is an excellent set of results.
- As indicated above, buses have been an important target for fuel cell R&D for 20 years, both in the United States and internationally. NREL's approach to data collection, analysis, and reporting has steadily resulted in building solid, productive working relationships with all parties having an interest in advancing bus technology. The bottom line is that NREL's people and systems are the foundation of this project's success. There are multiple reports, publications, and presentations by NREL on the results of FCEB data collection and analyses. Both DOE and the U.S. Department of Transportation's Federal Transit Administration support this project.

**Project weaknesses:**

- The inability of NREL to access warranty costs continues to be an issue affecting the assessment of progress in reducing the operating cost of FCEBs. This limitation was noted during the presentation.
- The lack of discussion on performance of the newer-generation buses versus the previous-generation buses is a weakness. There should also be data analysis to compare the different technologies among the buses.

**Recommendations for additions/deletions to project scope:**

- There are no recommendations. This is a vital contribution to DOE's support of FCEB, and NREL is doing an outstanding job. NREL should just keep it up.
- This project should have generation-versus-generation comparisons of performance and technology comparisons.
- One reviewer did not have any recommendations at this time.

## Project # TV-016: Stationary Fuel Cell Evaluation

Chris Ainscough; National Renewable Energy Laboratory

### Brief Summary of Project:

The objectives of this project are to independently assess, validate, and report stationary fuel cell system performance under real operating conditions.

Validating the performance and cost of technologies in stationary fuel cell systems under real-world conditions supports market growth, product awareness, and technology growth. This project addresses a gap in data for stationary fuel cell systems, leveraging capabilities established through previous research activities.

### Question 1: Approach to performing the work

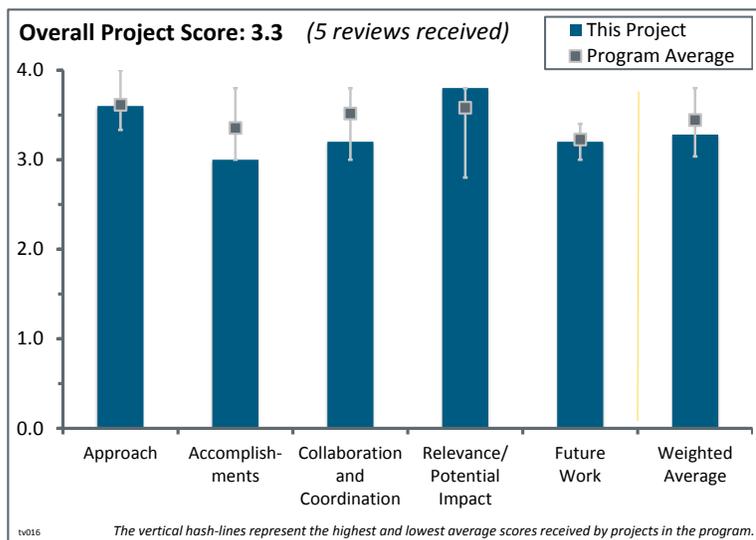
This project was rated **3.6** for its approach.

- The approach appears to be solid with technical data products, analysis of operation and maintenance data, and close collaboration with system vendors. It would be helpful to split out data by fuel cell technology type, but perhaps the number of installations is too low.
- The technologies have finally moved from pre-commercial to commercial stages of technology readiness. Accordingly, these stationary fuel cells will need to compete on price and value with heat engines and the grid. The availability of data and the reporting of economic and operating performance data should help boost the pace of commercialization for stationary fuel cells.
- The National Renewable Energy Laboratory's (NREL) approach to evaluating stationary fuel cells builds on the systems established, and experience gained, during implementation of similar projects for other fuel cell applications. As shown in slide 6, the approach includes analyses, which resulted in detailed data products and composite data products. Data are received by and processed in NREL's Hydrogen Secure Data Center. Thus, this relatively new addition to the Technology Validation (TV) portfolio takes advantage of previously developed elements of similar projects.
- There seems to be a little more emphasis on how to analyze the study data, as compared to actually acquiring the study data.

### Question 2: Accomplishments and progress toward overall project and U.S. Department of Energy (DOE) goals

This project was rated **3.0** for its accomplishments and progress.

- An extensive set of accomplishments is portrayed and documented in slides 9–21. Two types of accomplishments are identified: (1) installation, operation, and results for stationary fuel cells in California and (2) NREL's accomplishments in collecting data and analyzing and reporting the results. Except for slide 19 on installation costs, there is no reference to DOE goals or targets. Thus, the accomplishments generally do not include reporting on progress relative to targets. This is the first review year for this project on systems providing prime power, so it is expected that progress toward performance targets (reliability, durability, availability) will be documented in future reviews. This observation is supported by slide 23's indication of intent to expand project analysis to include maintenance and degradation data. NREL has disseminated results through publications and a website.



- Data have been obtained on the different types of fuels that power stationary fuel cell systems. However, few data are given about the operations of the systems themselves.
- There is a lack of data on stationary fuel cell systems in real-world applications being addressed. There was not much talk about codes and standards. Perhaps the technology is not sufficiently mature or in high-enough volume to make useful inputs for this. The data span a large set of power levels, combined heat and power (CHP)/non-CHP and other various technologies, so it is a bit hard to see trends, draw conclusions, etc. It is not clear if there is any reliability data. This could be a critical barrier/concern and cost issue.
- The data are limited to California. It would be good to bring in other states, even if it included only those that provide incentives for stationary fuel cells. The data also need to be better interpreted because the substantial changes in regulations could have an impact on the cost of the fuel cell deployments. As an example, if the regulations changed from allowing directed biogas to not allowing directed biogas, this change alone could have a substantive impact on the cost of the deployments. This could explain, at least partly, why the costs have been increasing.

### Question 3: Collaboration and coordination with other institutions

This project was rated **3.2** for its collaboration and coordination.

- This project appears to have a solid set of partners including California, vendors, and research support.
- To date, work on this project has been focused on installations in California. More characterization of the interactions and communications with partners would enhance the presentation. It seems that NREL is still in the process of establishing the working relationships needed to achieve robust collaboration and the desired benefits of a stationary fuel cell validation data project. This is supported by slide 22, which indicates that communications are under way with other organizations about agreements for sharing data.
- It would be good to bring in more states as collaborators.
- This project would benefit from more collaboration on the acquisition of the data it needs to analyze. For example, there is no mention of the Bloom solid oxide stationary generation systems that are in place and operational.

### Question 4: Relevance/potential impact on advancing progress toward DOE research, development, and demonstration (RD&D) goals

This project was rated **3.8** for its relevance/potential impact.

- There is a need for assessment data on stationary fuel cell power generation.
- Economic and performance data are very important, and this effort should be expanded. The pre-commercial days are over, so stationary fuel cells will need to compete with heat engines and the grid on cost and value.
- The real-world data collection is essential to understanding barriers to greater commercialization, deployment issues, and technical limitations. Thus, high value and impact is delivered to fuel cell system suppliers and to DOE.
- Fuel cell manufacturers and the government have made, and continue to make, substantial investments in the development of fuel cell systems for stationary applications. Customers of fuel cell power systems, supported by government incentives, are investing in installations. Hydrogen infrastructure is not an issue. Given this situation, data collection and analysis of stationary fuel cell installations are vital components of a complete TV portfolio. The DOE Hydrogen and Fuel Cells Program Annual Merit Review (AMR) presentation could include more emphasis on the importance of this work and address DOE's goals and objectives for stationary fuel cell power.

### Question 5: Proposed future work

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

- This project should bring in comparisons with heat engines and data from other states.

- This project needs to put more emphasis on developing more sources of stationary fuel cell operational data.
- It would be good to be more specific in terms of the partnerships being pursued/the plans for collecting maintenance and degradation data.
- Slide 23 provides general statements about future plans. Expanding analysis to include fuel cell maintenance and degradation data is key to a completely successful project. In future AMRs, more details on future work plans with some selected milestones and targets for expansion of data sources would make the presentation more complete.

#### Project strengths:

- NREL's deep skills in data collection, analysis, and reporting are a strength of this project.
- This is the first assessment of installed and functioning stationary fuel cell industrial systems.
- This project explores an important emerging market application area and samples a wide range of system sizes and technologies. This project presents time-trend data, which is very informative.
- The ability to leverage the capabilities established by NREL for its implementation of other technology validation projects is a strength of this project. These instances include the Hydrogen Secure Data Center and the NREL Fleet Analysis Toolkit. The experience of NREL's management and staff in creating and implementing similar data collection, analysis, and technology validation projects is also a plus.

#### Project weaknesses:

- This project is in the early stages of completion, and there is much more work to be done.
- There are not a lot of data generated yet on stationary fuel cell industrial systems.
- The presentation does not include a listing or summary of DOE's metrics and related targets for stationary fuel cell systems. The performance and cost targets should be identified so they are readily understood and can be compared to the results achieved by current installations. If metrics and targets have not been sufficiently developed, that should be done in collaboration with those responsible for this project.
- It is hard to draw conclusions from the data shown. There is a mix of different technologies and end-use deployments. In slide 18, it is unclear which are CHP installations and if this confounds the data. The other presentation from NREL on forklifts seems to have a greater scope of data collection. It is unclear if this is because of less forthcoming vendors or different data collection methodology. More information on uptime, reasons for delayed starts, and operational issues/limiters would be helpful.

#### Recommendations for additions/deletions to project scope:

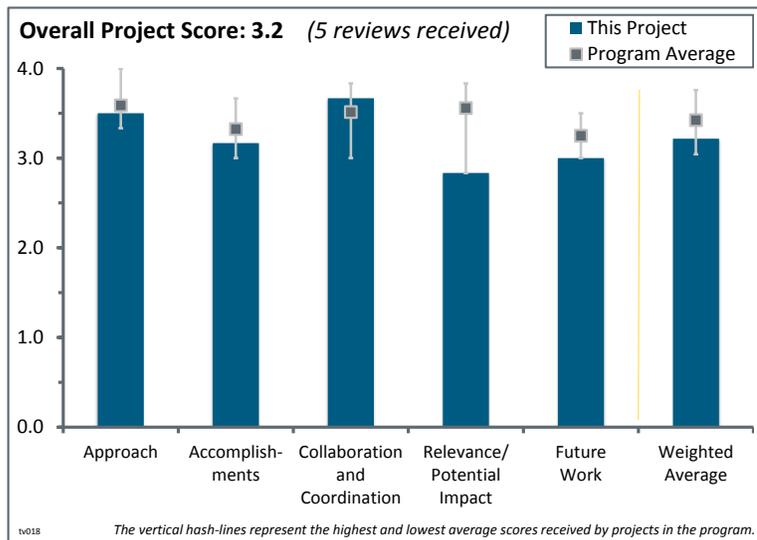
- There are no recommendations.
- This project should bring in other states and other stationary distributed generation technologies.
- Maintenance/operation/performance degradation data are needed for this type of study. Since this project scope of system sizes and technology types is large, it might make sense to focus on deeper data collection on a smaller emerging market segment (e.g., system sizes below 500 kW).
- NREL, in conjunction with fuel cell interests such as the Fuel Cell & Hydrogen Energy Association (FCHEA), should strive to expand this project to include coverage of all stationary fuel cell installations throughout the country. Sufficient funds for this should be provided by the TV program. This project should have an increase in funding (e.g., from \$200,000 to \$300,000 annually). This project should have a higher priority than activities contemplated in the funding opportunity announcement discussed during the TV overview presentation. NREL should aggressively work to acquire, analyze, and report on fuel cell system performance, maintenance, durability, operating costs, etc. (as indicated in slide 23 on proposed future work). The fuel cell system analysis results could be compared not only to DOE targets but also to results for other conventional and emerging prime power technologies.

## Project # TV-018: Hydrogen Recycling System Evaluation and Data Collection

Rhonda Staudt; H2Pump

### Brief Summary of Project:

The objectives of this project are to demonstrate the product readiness and quantify the benefits of H2Pump's Hydrogen Recycling System (HRS-100™) by installing and analyzing the operation of eight pre-commercial 100 kilograms per day systems in real-world customer locations. H2Pump will install, track, and report on multiple field demonstration systems in industrial heat treating, light-emitting diode (LED) fabrications, and semiconductor applications. The demonstrations will be used to develop case studies and showcase the benefits of the technology to drive market adoption.



### Question 1: Approach to performing the work

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

- The approach is sound and follows logical progression.
- This project just started, but it is off to a good start. It is on time and within budget.
- This is a very good approach for the demonstration of their hydrogen recycling system under real-world industrial conditions.
- A creative approach was described to utilize waste stream hydrogen. The pilot approach and corresponding data collection and analysis are appropriate.
- The approach to the project, as depicted in slides 10 and 11, is straightforward and logical. The discussion of the approach could be enhanced by augmenting it with a chart that shows the time period (from project start or calendar month) during which each task/work element will be accomplished.
- Further developing a system that will reclaim hydrogen from industrial waste is a technology that warrants validation. This project is starting with metal processing industries before moving to the more lucrative, but perhaps more complex, semi-conductor and LED processing industries. Utilizing multiple metal processing industries with various gas components reduces risk by ensuring the H2Pump system has wide utility. It is not clear how sharply focused this effort is on critical barriers. The industrial processes do not appear to be negatively affected by the price of hydrogen. The source development of renewable hydrogen is an important U.S. Department of Energy (DOE) goal. The barrier this effort seeks to overcome (hydrogen infrastructure) does not appear to be much of an issue in the applications it is addressing. A question was raised about whether online monitoring of CO was taking place at the installation sites. The principal investigator (PI) said no. This may or may not be needed. The sequential approach of site visits for gas sampling, system build, installing and commissioning, data collection, and monitoring and operation/maintenance is sound.

### Question 2: Accomplishments and progress toward overall project and U.S. Department of Energy (DOE) goals

This project was rated **3.2** for its accomplishments and progress.

- The project has figured out where to deploy the system and is on schedule.
- The project began in January 2013, and three site installations have already been established.

- The progress to date is good, especially considering this is a new project that began a few months ago.
- This project would be outstanding, but the go/no-go in April is past due, and data collection is behind schedule. The range of installations is impressive, from LED fabrications to reduction furnaces and specialty mills. This adds weight and credibility to the technology pilot.
- After only four months since the start date, it is difficult to render an opinion on progress, but the project appears to be off to a good start with Ulbrich Systems almost in place and systems three and four 100% complete. The data collection has begun, and the PI stated that the H2Pump system has had difficulty getting data automatically.
- The installation and commissioning of three systems, within four months of the official project start date, is impressive. With the benefit of funding from other sources, H2Pump was evidently prepared to move quickly on accomplishing project tasks. It would have been preferable for Task 1, data collection and reporting tool, to progress as expeditiously as equipment installation and start-up. The data plan, and collection of data from operating units, is on the critical path in terms of achieving Technology Validation (TV) program objectives. Providing background information on H2Pump's history and its technology, at the beginning of the presentation, was helpful for the reviewer.

### Question 3: Collaboration and coordination with other institutions

This project was rated **3.7** for its collaboration and coordination.

- There are very good collaborations with the industrial partners.
- There appears to be a solid team with analysis, engineering, and customer hosts in place.
- The collaborations with demonstration sites are very good. This is critical for completing work and collecting data needed for assessment.
- This project has great collaboration with its partners. They already know where they will be deploying all eight systems, and they know why they need to install two in Rome, because the system demand is huge.
- The working relationships with the metals industry host sites seem to be well established and productive. Cooperation and commitment of the host site companies are key to the project's success. The roles of the engineering firms listed on slide 17 were not discussed or identified during the presentation. Slide 12 states "select a supplier" in the context of Task 1. The involvement and roles of those associated with Task 1 were not sufficiently clear from the slides or presentation.
- The New York State Energy Research and Development Authority (NYSERDA) involvement is important. This could encourage the use of more reclaimed hydrogen processes. National Renewable Energy Laboratory (NREL) involvement in data collection will ensure it is an objective and intellectual-property-protected data dissemination product. Twelve to eighteen months of data collection appears sufficient. Because this is a single supplier of a single application, it is questionable how much information NREL will be able to share without giving away the source. The industrial partners cover multiple industries.

### Question 4: Relevance/potential impact on advancing progress toward DOE research, development, and demonstration (RD&D) goals

This project was rated **2.8** for its relevance/potential impact.

- This project needs to do a better job of explaining the cost per kilogram of hydrogen supplied.
- This project is aligned with DOE's goal of reducing hydrogen costs and using renewable sources. This appears to apply to industrial use only. It is unclear how the lower cost for this use will affect the cost of hydrogen overall.
- The recycling of waste hydrogen from various industrial operations can have a significant impact on the cost of hydrogen for fuel cell applications, provided that enough waste hydrogen is recovered economically.
- It would be good to try to quantify or estimate what kind of overall impact this could have, estimating the number of sites and some percentage of penetration, for example. It is not clear if there is any possibility of integrating the hydrogen stream into an onsite fuel cell system.
- The principal investigator estimated annual projected customer savings of about \$40,000, but based on the responses to reviewer questions, this appears to be a very rough estimate and will need to be validated as

part of this effort. Given the significant need for electricity to conduct this hydrogen reclamation process, this may have limited utility in areas of high electricity costs (e.g., California). The local area is home to a growing semiconductor industry, a significant user of industrial hydrogen, and success in this effort could lead to large sales of this application. There may be other renewable hydrogen reclamation technologies informed by this effort.

- Recycling hydrogen could be an attractive business proposition for a subset of industrial hydrogen users. However, no information was provided on how much of our future demand for hydrogen could be met by recycling hydrogen-rich exhaust/waste streams. The reviewer estimates that the potential is limited. This is not a criticism of the project and how it is being conducted, but an issue about whether the technology's potential as a source of hydrogen is sufficient to justify priority in terms of DOE support over other projects. It would be helpful to have information on the cost per kilogram of pure hydrogen produced by H2Pump's technology. This is a common metric used by DOE's Fuel Cell Technologies Office.

### Question 5: Proposed future work

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

- This is a good plan that follows a logical progression with checks in place.
- The researchers have just begun on the project, and they need to complete this before this question becomes relevant beyond the current scope of work.
- The proposed future work looks reasonable. There should be a better description of the new sites to be established, and also a more detailed account of the future timeline.
- It is assumed that there will be a fuller and more detailed cost-of-ownership model and a fuller description of what type of pre-treatment or site-specific engineering work or costs are required in next year's update.
- There seems to be an inconsistency between the information on slide 10 (Task 1 is 30% complete) and that on slide 16 (database online in April 2013). During the presentation, the reviewer concluded that the months shown on slide 16 are not accurate, and that the work cited on the slide will be completed later than shown. For example, the statement was made that the go/no-go decision meeting has not yet occurred.
- This question is not applicable, as this project is just getting under way.

### Project strengths:

- This is a very well-focused project.
- There is good project management and oversight.
- This project addresses renewable hydrogen and creates it onsite. It is too early to discuss the strengths of the project execution effort.
- The goal of lowering hydrogen cost using a renewable source could facilitate adoption of hydrogen technology.
- This is an innovative technique that appears to be cost-effective. This project has diverse pilot sites and good partnerships in place.
- This project involves a contractor (H2Pump) with an entrepreneurial team committed to development and commercialization of a technology that represents a different and possibly unique approach to providing hydrogen for industrial customers. Other strengths include the willingness of companies to provide host sites for installation of H2Pump's equipment and to participate in data collection; participation of NREL, with its expertise in data collection, handling and analysis; cost share and support from NYSERDA; acquisition of "real-world" operating data; and use of those data in preparing case studies for reference by companies that could benefit from the H2Pump technology.

### Project weaknesses:

- There are no weaknesses.
- The cost data need to be more transparent.
- It is too early to evaluate project execution impact.
- It would be good to see how this source of hydrogen could be used for other applications.

- This project is a bit behind schedule, and this was acknowledged. Some plan to recover the schedule is needed.
- Ideally, a data collection plan should have been completed and approved prior to a go/no-go decision on proceeding with the expense of site preparation and installing equipment at multiple sites. (The validity of this comment could be influenced by a better understanding of the extent to which particular tasks are being funded by DOE, and whether tasks other than data collection would be done solely with funding from other sources.) Insufficient information on data collection plans, data elements, and related metrics was provided, suggesting that significant work remains to be done on Task 1, which is vital to project success.

**Recommendations for additions/deletions to project scope:**

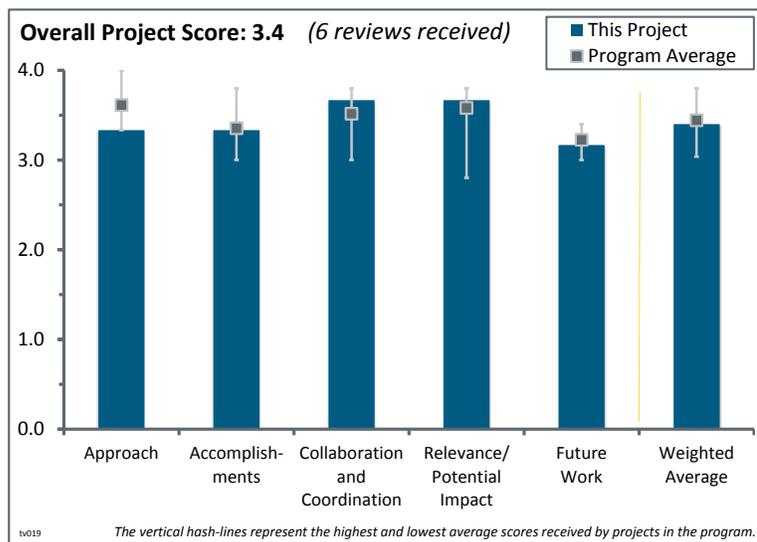
- The cost per kilogram for hydrogen should be supplemented by each system.
- More non-proprietary descriptive information about the hydrogen recycling system would be useful.
- The addressable size of this segment in industry or volume of hydrogen recovery is unclear. It would be very good to get detailed customer feedback and impressions next year; the PI is probably planning to do this.
- It is unclear if DOE has analyzed how much hydrogen could potentially be recycled/re-used. It is assumed that the amount is small compared to the current hydrogen demand and very small compared to the projected demand in a “hydrogen economy.” If this analysis has not been done, it should be considered for inclusion in the analysis program and accomplished before more funds are committed to hydrogen recycling projects. While H2Pump’s technology is interesting and has a possible benefit for a niche industrial market, DOE’s funding decisions should reflect analysis that identifies technologies capable of providing a significant portion of the potential demand for hydrogen.

## Project # TV-019: Hydrogen Component Validation

Kevin Harrison; National Renewable Energy Laboratory

### Brief Summary of Project:

This project provides fully integrated system-level testing to address barriers that include a lack of performance data, instrumentation, sensor accuracy, technology transfer, and integration with renewable sources including wind and solar. The project performs operational reliability and performance testing, advances instrumentation and technology transfer, and focuses on system integration and advanced grid integration. The National Renewable Energy Laboratory (NREL) works closely with industry to understand and improve compressor reliability and hydrogen mass flow limitations and to exercise NREL's existing test platform.



### Question 1: Approach to performing the work

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

- This project has utilized its funding well. These technologies are being tested and moving closer to market reality. Keeping the costs down on new compressors and running electrolyzers through rigorous testing and data collection are essential. It is a first-come–first-served basis in terms of what equipment is tested. Readiness safety and hazard operations on reliability are important to this project.
- The approach enables equipment, such as compressors and electrolyzers, to be tested while operating within an integrated hydrogen production, storage, and dispensing facility. The integrated facility allows the National Renewable Energy Laboratory (NREL) to efficiently test selected components and gather data on their performance at a relatively low cost.
- The approach is very good; it appears to be very customer-focused, flexible, and highly capable of testing and validation. The capability to provide unique testing is a real highlight. It is not clear how much the approach is going to support incoming requests versus building capacity for key or emerging test validation areas. Doing more of the latter with U.S. Department of Energy and stakeholder input could perhaps be a further enhancement of the capacity.
- The strategic direction or focus of the project needs to be clearly defined and articulated. The overall effectiveness could be significantly improved if results and efforts were coordinated with data from existing deployments.
- It would be helpful to know more specifically what work at the integrated test facility is funded by the Technology Validation program. The presentation and responses to questions did not address sources and the total amount of funds associated with the various activities identified in slides 4 and 5. That information would provide better awareness about the leveraging of the DOE contribution.
- The strategic value of this effort to the DOE Hydrogen and Fuel Cells Program is indirect but valuable. The funding provided by the Program to NREL enables this facility to be used to do testing for the fuel cell and hydrogen industry. NREL's testing and analysis is a valuable service to the companies that provide their near-commercial products to NREL for testing. This service should accelerate commercialization and the robustness of commercialized products. All this being said, it would have been good to have seen more cooperative research and development agreements (CRADAs) with companies to test their products. This is the primary reason for a “good” rating versus an “outstanding” rating. As a suggestion, NREL testing could

be a strategic step prior to the products being demonstrated in real-world operating environments by the customers.

### Question 2: Accomplishments and progress toward overall project and U.S. Department of Energy (DOE) goals

This project was rated **3.3** for its accomplishments and progress.

- More CRADAs would have been good.
- This project is collecting data on equipment performance. Compressor reliability is an issue. The researchers are running electrolyzers in variable modes. They are running a variety of electrolyzers and comparing their performance and reliability.
- This project has very good flexibility and capability. It appears to be somewhat unique in this output. Technical capability and the span of various components being tested appear very strong. The output of this work can be an essential part of market validation and perhaps the basis for a larger effort for flexible and responsive testing and validation.
- Slides 6 through 12 provide evidence of excellent results and the ability of the test facility to generate useful data and test results. Accomplishments include lots of data and the results of data analysis. While slides 6, 10, and 11 provide a sense of progress in achieving test results, for this reviewer, complete understanding of the information contained in the slides requires more than a 30-minute session. Discussion in response to a question on slide 6 highlighted the need for work on simplifying/clarifying the message. On slide 11, a succinct statement on the practical conclusions and implications of the work accomplished would be useful. The reviewer assumes that not all the accomplishments presented (e.g., slide 12) have resulted from the \$265,000 provided to the project by the Technology Validation program. If this is correct, it would be nice to identify the specific accomplishments linked with the DOE project being reviewed. In preparing for the next review, attention should be given to comparing results (for example, on compressor reliability and performance) with DOE goals and addressing indicators of performance progress.

### Question 3: Collaboration and coordination with other institutions

This project was rated **3.7** for its collaboration and coordination.

- The collaborations are good; it would be good to see more of them.
- The project has good collaboration with various electrolyzer companies and compressor manufacturers.
- It is amazing to see how many CRADAs are involved; it is excellent. There should be more of these.
- NREL could expand components to other manufacturers and types; for example, they should seek to test conventional piston compressors.
- Again, the flexibility of collaboration and the demonstrated partnership with industry, utilities, universities, and CRADAs are impressive.
- Collaborations that have been established provide evidence that some manufacturers of key hydrogen system components have confidence in working with NREL. They have determined that using NREL's facility, testing capability, and analytical expertise is beneficial and cost-effective. Giner Electrochemical Systems is mentioned as a partner in slide 2, but it is not shown on slide 13. Providing summary information on the value of equipment donated and time committed by collaborators could move the mark for this criterion to "outstanding."

### Question 4: Relevance/potential impact on advancing progress toward DOE research, development, and demonstration (RD&D) goals

This project was rated **3.7** for its relevance/potential impact.

- NREL's component validation is a highly valuable strategic tool.
- The potential impact on early market adoption for these technologies is significant. Only through testing will anyone know the potential market application.

- The potential impact and relevance can be significant since few of this type of capability exist, and this type of CRADA agreement can certainly be a model for public–private partnership moving forward.
- The work around improving compressor reliability is important to improving the growing number of hydrogen fueling stations. It would be great to see more linkage with stations deployed in both problem analysis and problem resolution.
- For a relatively small expenditure, this project provides valuable information leading to better understanding of issues related to the performance of hydrogen system components. A particular focus is on compressors. Acquiring and analyzing test data on compressors can help determine progress toward related objectives, as well as priorities for research and development attention. The slides/presentation should include a few relevant DOE goals that are associated with the project’s validation activities.

### Question 5: Proposed future work

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

- Having large-scale electrolysis up to 1 MW is a great idea.
- Compressor reliability is a key area and appropriate to highlight for future work.
- Testing and validation of compressor technology, design, and materials seem to be an appropriate target on which to focus future efforts supported by the Technology Validation program. This is consistent with the information in slide 14.
- It appears that future work is driven by customer requests. A more proactive approach could be to develop a strategic plan and identify focus areas; this would make future planning easier. This would also make decision making easier.
- It would seem that an aggressive recruiting effort aimed at industry would bring in more CRADAs. The recruiting could target companies with products in the near-commercial stage of the pipeline. It could also target products or components where improvements of performance are critical to the successful implementation of the project plan. It may be desirable to more aggressively market to industry so that industry can take advantage of NREL’s testing prior to demonstrating the new products or components with customers in order to assess performance under “real world” operating environments.

### Project strengths:

- NREL’s testing and reporting capabilities are a strength.
- This project has good collaboration and excellent partners.
- This project has great facilities and experience with renewable hydrogen equipment.
- Uniqueness, flexibility, potential to scale up scope, and the number of components under testing are good. The fully integrated system-level testing is also a strength.
- NREL’s fully integrated hydrogen system test facility, which enables efficient testing of components with multiple types and designs, is a strength. NREL has significant experience in utilizing mechanisms, such as CRADAs, to structure and implement agreements with industry for the testing of equipment. NREL has built credibility with equipment manufacturers through its operation of the integrated test facility, as well as its capability to handle and protect data.

### Project weaknesses:

- This project has no weaknesses.
- This is not necessarily a weakness, but it would be helpful to poll stakeholders or have an industry listening session to better focus key activities and capabilities for testing and validation.
- This project needs to better position NREL testing as a strategic step toward product commercialization. The concept would be a “pre-commercial” demonstration in a controlled environment as an intermediate step prior to a demonstration at a customer site.
- No evidence was provided to show that project results are being used to track the progress of hydrogen system components in terms of achieving specific DOE goals and objectives. This is likely being done, but the linkage should be clear as part of the DOE Hydrogen and Fuel Cell Program Annual Merit Review. If the objectives are not a focus of the project, they should be.

**Recommendations for additions/deletions to project scope:**

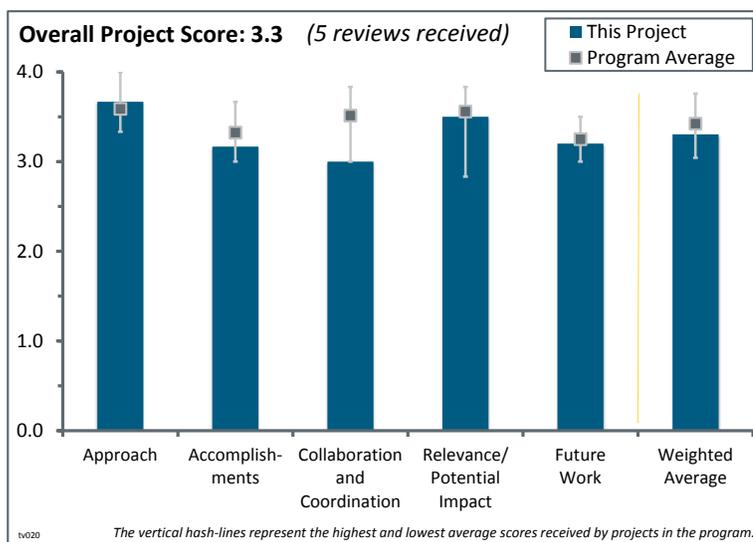
- This project should publish the results widely.
- Accelerated testing at the component/systems level and/or related data collection or development of testing methodology is critical and an area of focus.
- If possible, NREL should seek to test the Linde ionic compressor, which might significantly reduce the compression energy required and possibly achieve lower cost and higher reliability, which is the main motivation to get third-party validation of ionic compressor reliability.
- In the reviewer-only slide on publications, it was noted that the most recent publication listed was done in 2010. If there have been no publications on work related to this project since 2010, attention should be devoted to disseminating information on results of the testing/validation work. If there have been publications since 2010, the list should be updated.

## Project # TV-020: Validation of an Advanced High-Pressure PEM Electrolyzer and Composite Hydrogen Storage, with Data Reporting, for SunHydro Stations

Larry Moulthrop; Proton OnSite

### Brief Summary of Project:

This project seeks to validate an advanced high-pressure polymer electrolyte membrane (PEM) electrolyzer and composite hydrogen storage for SunHydro hydrogen stations, addressing costs, hydrogen storage, codes, and lack of hydrogen refueling station performance data. The project validates hydrogen fueling infrastructure performance gains of an advanced 57 bar PEM water electrolyzer, next-generation 87 MPa composite storage tanks, and skid-mounted compact refueling component arrangements with an updated SunHydro #1 station and a fully containerized SunHydro #2 station.



### Question 1: Approach to performing the work

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

- The approach for each task is solid.
- The project is utilizing storage vessels, compressors, and fuel cell stacks that the project has worked on at a smaller scale. The researchers are trying to keep the footprint small and create a container with the goal of making it portable. SunHydro #1 has been successful. They hope to increase the efficiency of the PEM stack. They also have composite storage tanks they are validating from 280 to 870 bar. The compressor is also being tested. Their unit, the SunHydro #1, looks good. They are going to instrument the system and start collecting data up to 24 months, which will include reliability data. Sunhydro #2 will be installed in 2013 in Massachusetts.
- The potential to save up to 12 kWh/kg by utilizing 57 bar (vs. 30 bar) pressure and doubling the usable storage per unit volume could help lead to competitively priced hydrogen utilizing electrolysis. The advanced composite hydrogen storage that has been identified by DOE is a key enabler. The effort provides two years' worth of station data that can inform codes and standards as well as performance. Novel component arrangements enable a maximum location of equipment away from the classified zone with firewalls in between. This effort will validate voltage reduction at full scale. Part of this effort includes participating in NFPA 2 revisions and "bringing authorities having jurisdiction (AHJs) onboard" throughout the process to inform codes and standards and speed the permitting process.
- The investigator should assess cost and determine what cost reductions are needed to meet hydrogen cost targets.

### Question 2: Accomplishments and progress toward overall project and U.S. Department of Energy (DOE) goals

This project was rated **3.2** for its accomplishments and progress.

- Progress is as expected, considering it is a new project that began a few months ago. The tasks appear to be on schedule.
- The project has been recording data for two years and hopefully will publish these data in the future. The researchers are building a new cell stack, and they have an ambitious goal for the next-generation fuel cell stack.

- Cost is probably the main obstacle in deploying electrolyzer-based fueling stations. More emphasis needs to be placed on cost-reduction efforts.
- The project is only 12% complete, so it is difficult to ascertain progress this early in the effort. Combining the two projects into one is a good idea and will eliminate administrative redundancies. Long-lead-time materials have been ordered. Ten fuel cell electric vehicles (FCEVs) have been secured from Toyota and will be used as part of the demonstration.

### Question 3: Collaboration and coordination with other institutions

This project was rated **3.0** for its collaboration and coordination.

- This project has good collaborations with component suppliers and users.
- For SunHydro, Toyota has provided 10 FCEVs. Air Products is providing some components also.
- Ideally, this evaluation should be expanded to include other fueling stations, organizations, and technologies.
- Working with Air Products brings expertise on hydrogen storage and dispensing technology to the project. Partnering with Toyota, which has a planned FCEV commercialization launch in 2015, increases the chances of a successful implementation. SunHydro LLC, a builder of hydrogen fueling stations, rounds out the project team nicely.
- SunHydro LLC and Proton OnSite share the same ownership. This could restrict the transfer of technology to other electrolyzer and hydrogen station original equipment manufacturers (OEMs). Data will be sent to the National Renewable Energy Laboratory (NREL) Secure Data Center. Having NREL be part of the team will enhance objectivity and transparency in reporting of results.

### Question 4: Relevance/potential impact on advancing progress toward DOE research, development, and demonstration (RD&D) goals

This project was rated **3.5** for its relevance/potential impact.

- This project is trying to address hydrogen costs and reduce energy usage with some measured success.
- This project fits well with DOE's goals and is expected to lower costs with improved and more efficient components. Data will go into existing DOE analysis for hydrogen stations, which builds on the current body of knowledge and allows further comparison to other sites. A station with a smaller footprint is good and could speed up the process of installation and approvals at multiple sites.
- The potential of this effort is to speed up AHJ approvals by packaging a fueling station in an ISO container with 24 months of data to validate its safe operation. The potential is for significant reduced costs for small hydrogen stations utilizing renewable hydrogen via electrolysis. With only a 50% increase in hydrogen tubes, Task 3.0 (composite storage) could realize dispensing capacity increases from 16 kg/hr to 30 kg/hr. This would allow more vehicles to be refueled at a single station and lower the cost of hydrogen.
- The cost and price need greater emphasis.
- The relevance and impact are limited since this project evaluates one design and one set of components (e.g., just one type of hydraulic compressor and one electrolyzer).

### Question 5: Proposed future work

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

- This project is on schedule.
- The future plans are sound and well outlined.
- This question is not applicable, as this project has been underway for only approximately five months. It is premature to discuss future work.

### Project strengths:

- This project has solid project partners.

- This project improves efficiency to lower the cost of hydrogen. A station with a smaller footprint could be useful in multiple locations where space might be an issue. This will help with the ability to increase the adoption of the technology.
- This project is renewable hydrogen-oriented and addresses technology barriers with a logical plan to overcome them. All the barriers appear to have a solid technical approach toward achievement. It is too early to make a judgment on project execution. The emphasis on involving AHJs from the start is indicative of an OEM (SunHydro LLC) that wants to commercialize the results of this technology immediately upon completion of the effort.

**Project weaknesses:**

- There are no apparent weaknesses, but the project is too new to determine this at this point.
- It is too early to make a judgment on project execution.

**Recommendations for additions/deletions to project scope:**

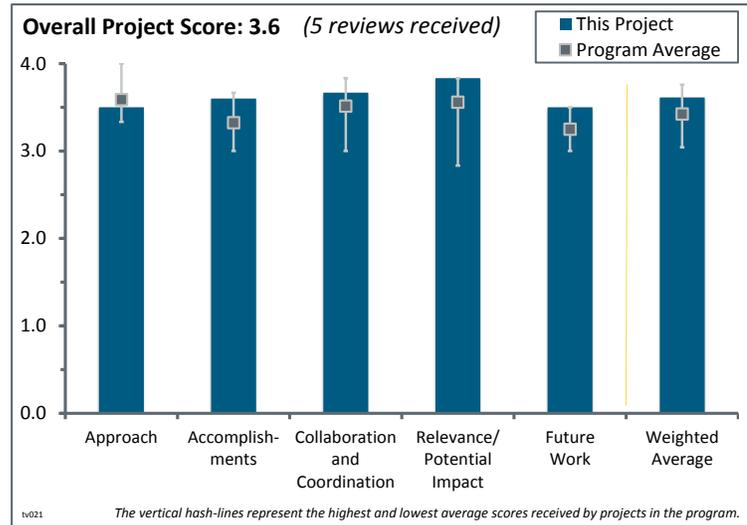
- Two reviewers noted that they had no recommendations for this project.

## Project # TV-021: Forklift and Backup Power Data Collection and Analysis

Jennifer Kurtz; National Renewable Energy Laboratory

### Brief Summary of Project:

The objectives of this project are to assess forklift and backup power technology status in real-world operations, establish performance baselines, report on fuel cell and hydrogen technology, and support market growth by evaluating performance relevant to the markets' value proposition. Technology will be reviewed through independent assessments, focusing on fuel cell systems and hydrogen infrastructure. Market growth will be supported through analyses of market value and reporting on technology status to fuel cell and hydrogen communities.



### Question 1: Approach to performing the work

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

- This project has a solid approach on analysis.
- The approach should have more focus on the key technology-restraining issues.
- The approach appears to be solid with technical data products, an analysis of operation and maintenance data, and close collaboration with system vendors.
- The National Renewable Energy Laboratory's (NREL's) business case analysis of the economic and operating performance of fuel cell forklifts has contributed to the sharp commercial ramp-up of fuel cell forklifts. NREL shares a key role in one of the "success stories" for commercial fuel cells.
- A draft report is due soon, and data are reported on a secure basis to NREL. The detailed product is shared with the data provider, and all information is published on NREL's website. The project also has a toolkit and leverages the data analysis work. So far, 1,302 fuel cell systems have been deployed, most in the form of backup power systems.

### Question 2: Accomplishments and progress toward overall project and U.S. Department of Energy (DOE) goals

This project was rated **3.6** for its accomplishments and progress.

- This project has had excellent success with many units, and safety and reliability have been demonstrated.
- An excellent set of data was presented for fork lift systems, but there was less information provided for backup systems. Slide 18 with failure modes for infrastructure was very informative.
- NREL has successfully brought economic analysis, such as cost of ownership comparisons that feature textured comparisons of fuel cell systems versus incumbent systems, into its reporting.
- Slide 13 comparing the costs of battery lift trucks versus fuel cell lift trucks should be a major selling point to encourage more warehouses and factories to convert to fuel cells.
- This project is significantly adding to the value proposition to the user for reliability and safety. The evaluation of the maintenance and reliability categories is helpful to demonstrate a reason for industry to determine the commercialization of these technologies.
- This is a noteworthy discussion of start-ups, reliability requirements, and the deltas and explains the cause of the deltas between requirements and actual performance. There is significant and valuable discussion on

the cost of ownership in comparison to battery forklifts. This project is an outstanding discussion of refueling and mean time between failure (MTBF).

- It is not immediately obvious what results have been obtained from the current project and what results were due to the previous American Recovery and Reinvestment Act (Recovery Act) project.

### Question 3: Collaboration and coordination with other institutions

This project was rated **3.7** for its collaboration and coordination.

- This project has a solid combination of team members and users.
- This project has outstanding data collection, analysis, and dissemination.
- The economic analysis could not have been as robust without NREL's ability to enlist the cooperation of its collaborators. This reflects an atmosphere of mutual respect, transparency, and trust among the collaborators.
- A wide variety of system providers are included that increase the validity of the data and conclusions. There appears to be some lack of data collection response from some vendors, but this is not the fault of the research team.
- The distinction between confidential and public results may mask some important insights that have been revealed only on a confidential basis.

### Question 4: Relevance/potential impact on advancing progress toward DOE research, development, and demonstration (RD&D) goals

This project was rated **3.8** for its relevance/potential impact.

- This project contributes to the goal of improving the reliability of fuel cells and hydrogen infrastructure, and will help define the value proposition for backup power. The compressor breakdowns are a red flag, and performance could be improved.
- The real-world data collection is essential to understanding barriers to greater commercialization, deployment issues, and technical limitations. Thus, high value and impact are delivered to fuel cell system suppliers and to DOE.
- It is unclear how the results of this study will be employed to help strengthen the expansion of fuel cell applications.

### Question 5: Proposed future work

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

- The quarterly reports and final reports are still to come. It is important to try to continue to improve compressor reliability.
- It is hoped that every demonstration program receives the same quality of analysis and reporting that NREL has provided for backup power fuel cells and fuel cell material handling equipment (MHE).
- This is a reasonable plan that outlines complete tasks, data sharing, and reporting key findings. It is not clear if there is a way or a plan to continue data collection with some installations to provide capabilities for trending data over several years.
- Every effort should be made to continue this project beyond June 2014. The continued collection of these data is very important to establish the long-term performance of fuel cells. Stopping now would effectively be throwing away an opportunity to establish a long-term record of lifetime. Some other entity would have to start over with a new fleet of systems to set up another long-term trial of fuel cell lifetime performance.
- The project is 60% complete and will end in fiscal year 2014.

### Project strengths:

- A significant amount of information about fuel cell systems has been obtained.
- This was a very complete presentation and a thorough project that identified systemic weaknesses.

- This project has good data collection, evaluation teams, and protocol. This project has good connections to end users, thanks to the implementation of the previous Recovery Act project.
- This is a good national approach to fuel cell analysis. There are early warnings of commercial problems, such as compressors. The project partners are happy to validate their equipment. The lessons learned from forklifts were very good.
- This project has an excellent roster of partners and a detailed data set for important emerging fuel cell system applications (MHE, backup power). Slide 13's stack-up of annualized costs is very informative and highlights key areas for improvement. This could be the basis for instructive sensitivity analysis as well.

**Project weaknesses:**

- This project has no weaknesses.
- Many important observations may be held on a confidential basis.
- The point about compressor failures as the problem was not identified/ discussed in the presentation.
- There are much more detailed drill-down data for forklifts than backup power.

**Recommendations for additions/deletions to project scope:**

- There are no recommendations for this project
- This project should continue the data collection.
- As noted in last year's feedback, a cost-of-ownership stack-up plot similar to slide 13 for forklifts would be a valuable addition for the backup power systems.
- It would be helpful to depict time-dependent performance trends, a risk-assessment of key issues and possible resolution paths for the identified issues. This work seems to be more of a snapshot, which is very informative, but depicting trends over several years would be even more salient. It is understood that funding is a limitation.

## 2013 — Safety, Codes and Standards

### Summary of Annual Merit Review of the Safety, Codes and Standards Program

#### Summary of Reviewer Comments on the Safety, Codes and Standards Program:

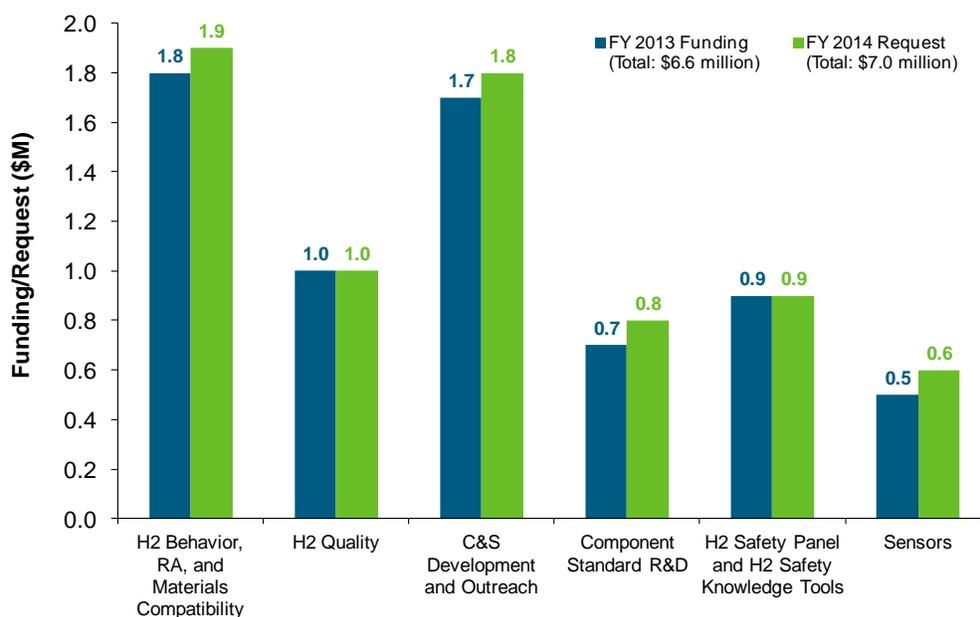
The Safety, Codes and Standards program supports research and development (R&D) that provides the critical information needed to define requirements and close gaps in safety, codes, and standards to enable the safe use and handling of hydrogen and fuel cell technologies. The program also conducts safety activities focused on promoting safety practices among U.S. Department of Energy (DOE) projects and the development of information resources and best practices. Reviewers recognized that the program continues to provide strong support in the following areas: hydrogen and fuel cell codes and standards including domestic and international harmonization, permitting and education, hydrogen sensor technology, hydrogen components and material compatibility, hydrogen behavior and fuel quality, hydrogen infrastructure risk assessment, hydrogen safety and related tools, and safety training for first responders and researchers. Reviewers made similar observations as they have in prior years, such as that projects in this program have effectively leveraged the resources and intellectual capital of academic institutions, standards development organizations (SDOs), code development organizations (CDOs), national laboratories, government agencies, industry, and other offices within DOE.

In addition, this year, reviewers commended the program for the strong international participation with the focus toward international harmonization for the safe deployment and early market commercialization of fuel cell and hydrogen technologies. Reviewers felt that the program was well focused and well managed, but noted that closer coordination with industrial partners and improved publication and outreach of technical work in safety implementation aspects of the program would enable better stakeholder and industry feedback on technical developments.

#### Summary of Safety, Codes and Standards Funding:

The fiscal year (FY) 2013 appropriation was \$6.6 million for the program. FY 2013 funding has allowed for continued support of codes-and-standards-related R&D and of the domestic and international collaboration and harmonization efforts for codes and standards that are needed to support the commercialization of hydrogen and fuel cell technologies. The FY 2014 request of \$7 million will continue these efforts.

#### Safety, Codes and Standards R&D Funding



### Majority of Reviewer Comments and Recommendations:

In FY 2013, nine Safety, Codes and Standards projects were reviewed, with a majority of the projects receiving positive feedback and strong scores. Reviewers' overall scores ranged from 2.8 to 3.6, with an average score of 3.3.

**Hydrogen Behavior, Risk Assessment, and Materials Compatibility:** Three hydrogen behavior, risk assessment, and materials compatibility projects were reviewed, with an average score of 3.2. Reviewers commended the strong analytical approach and methods found within these projects, strong research and experiments in validating data and models on hydrogen release behavior, and engagement with industry to maximize the impact on standards development. The reviewers suggested collaborating more closely with appropriate industry partner SDOs and CDOs, increasing publication and outreach to enable review and stakeholder feedback for future work, and considering applications for evaluating risk associated with equipment or processes.

**Hydrogen Quality:** One hydrogen quality project was reviewed, receiving a score of 3.4. Reviewers commended this project for its focus and alignment with near-term real-world needs and for being a key stepping stone toward the implementation of hydrogen fuel quality standards. Reviewers suggested reexamining the project scope to leverage other technical resources, investigating the cost-effectiveness of the analyzer technology, and collaborating with industrial partners to advance commercialization efforts.

**Codes and Standards Development and Outreach:** One codes and standards development and outreach project was reviewed, receiving a score of 3.3. The reviewers commended this project for its coordination with critical SDOs and CDOs, and for the importance of the work being done in California. However, the reviewers suggested that the project scope, approach, and plan should be improved to address a range of needs for codes and standards for hydrogen quality, metering, and certification of components and systems.

**Component Standard R&D:** One component testing project was reviewed, receiving a score of 2.8. The reviewers commended the project's strong coordination with SDOs and CDOs and national and international laboratories and the effective exchange of information between stakeholders. Reviewers suggested strengthening collaboration and coordination with industry and improving the definition of the project scope and milestones to better evaluate the project.

**Hydrogen Safety Panel and Hydrogen Safety Knowledge Tools:** One project in this area was reviewed, receiving a score of 3.6. Reviewers stressed the importance of this effort in providing information, guidance, and tools to improve industry awareness. Reviewers identified the need to involve third-party certifiers, improve coordination between the Safety Panel and safety planning in DOE-sponsored projects, and coordinate with SDOs and CDOs to build on the success of mobile platform safety knowledge tools.

**Sensors:** Two sensor projects were reviewed, receiving an average score of 3.3. Reviewers applauded the overall project management and strong collaboration and coordination with international and industrial partners. However, reviewers recommended improving communication regarding the role of sensors in meeting safety requirements and developing durability requirements and manufacturing, maintenance, and other cost estimates and targets for relevant applications. Reviewers also suggested investigating cross-sensitivity to methane and the use of wide-area detection and contact sensing technologies for early detection of leaks.

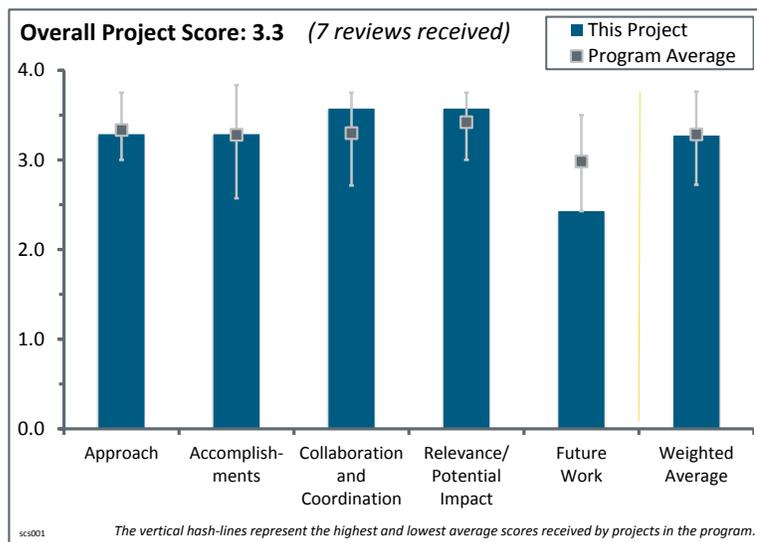
## Project # SCS-001: National Codes and Standards Deployment and Outreach

Carl Rivkin; National Renewable Energy Laboratory

### Brief Summary of Project:

The objectives of this project are to: (1) support code development for the safe use of hydrogen in commercial, residential, and transportation applications with a major emphasis on infrastructure for hydrogen fuel cell vehicle technologies; (2) advance hydrogen safety through collaboration and coordination with stakeholders; (3) facilitate the safe deployment of hydrogen technologies by working to incorporate safety data into codes and standards (C&S) projects and hydrogen technology deployment projects; (4) distribute hydrogen safety information through the most effective channels, including websites, technical reports, webinars, and in-person

presentations to reach key audiences such as project developers and code officials; (5) and conduct the research and development (R&D) needed to establish sound technical requirements for the safe use of alternative fuels with a major emphasis on hydrogen and fuel cell technologies.



### Question 1: Approach to performing the work

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

- The approach is well designed and has been coordinated with industry and standards organizations.
- The overall scope and approach of this work are very good. In the 2012 Hydrogen and Fuel Cells Program Annual Merit Review, this project was criticized for being too broad. However, the breadth is needed to adequately cover the critical regulations, codes, and standards (RCS) domain. The principal investigator (PI) clearly understands this space very well.
- The development of the templates provides a very useful resource. The National Renewable Energy Laboratory's (NREL's) work with California on hydrogen infrastructure is of high value as well; however, the approach (slide 4) needs to maintain its path as it expands—not shift entirely.
- Coordination work has been very effective in aligning resources and achieving harmonized C&S. Gap analysis is useful in prioritizing future work. Outreach is helpful, though hydrogen station permitting still seems to be a significant challenge.
- NREL has recognized that the major effort to develop C&S is close to completion—at least on the top level—and is wisely turning its emphasis to infrastructure issues as well as focusing more on outreach/communication.
- It is difficult to understand from the presentation what work researchers pursued, as well as why and when they pursued it. This makes it difficult to judge the approach. Presenting a project plan may be more useful next time.
- The focus appears to be limited to model building and fire codes, the International Organization for Standardization (ISO), and the United Nations' Global Technical Regulations (GTRs). These venues are important, but they are only part of the picture. Design codes, such as ASME B31.12, and product safety standards, such as the Canadian Standards Association (CSA) HGV4.1, also need support. The model codes indicate that hardware is to be “approved” or “listed;” however, the product safety standards need to be supported to make the model building and fire codes actionable. Additionally, much of the hardware being generated for hydrogen infrastructure is being developed by small companies. These companies

might not have the cash flow to fund the testing needed to become “approved” or “listed.” It is unclear if these issues are under consideration.

## Question 2: Accomplishments and progress toward overall project and U.S. Department of Energy (DOE) goals

This project was rated **3.3** for its accomplishments and progress.

- Important foundational work has been accomplished and key C&S are in place.
- The fact that much of the RCS for hydrogen and fuel cells have been developed is a significant accomplishment. NREL’s coordination effort is a significant part of that. NREL’s efforts aimed at furthering the acceptance of National Fire Protection Association (NFPA) 2 is very important, especially in getting it recognized by the International Fire Code (IFC). The NREL Hydrogen Safety Handbook will serve as a good complement to Pacific Northwest National Laboratory’s (PNNL’s) Hydrogen Best Practices website.
- The PI and NREL have done a very good job at keeping a focus on C&S and moving forward in a harmonized way. The harmonization between NFPA and the IFC codes was critical and very important. A lot of what the PI called “accomplishments” are really activities. This section still deserved a high score because those accomplishments that were listed were important and critical to the rollout of the infrastructure.
- The accomplishments regarding hydrogen safety and hydrogen fueling have been very good. There has especially been a lot of important information from NREL to assist in the J2601 standardization. However, efforts to accelerate analytical methods in the ASTM D.03 group have not been effective. The current activity in hydrogen quality is not focused on first finishing these sets of standards with round-robin tests, etc. Trying to find other ways of testing, such as in-line testing, are quite frankly misplaced and should be prioritized after that goal.
- Showing “Codes and Standards Basically Complete” in fiscal year 2013 is a gross misrepresentation of the state of C&S. The comment that industry will take over addressing all relevant C&S overestimates the manpower industry has to support this effort. Industry will have to prioritize the C&S to which it can dedicate manpower and therefore some will fall through the gaps. This is a critical point in time for support to meet commercialization needs. Work with Sandia National Laboratories (SNL), particularly on material compatibility and NFPA 2, was critical and a great accomplishment.
- The accomplishments noted by the PI are limited; more progress has been made in key areas. The PI is correct in reporting that NFPA 2 and the IFC/International Building Code work is progressing, and that ASME has amended Section VIII, Division III of the Boiler and Pressure Vessel Code for fracture mechanics (article KD-10) and added a new book section to the B31 Piping Code. Although, to this reviewer’s knowledge, nothing has been changed in articles 500–505 of NFPA 70: this should be verified. Other accomplishments include a domestic hydrogen fuel standard, SAE J2719, and an international standard that was harmonized with the domestic standard. The hydrogen fuel nozzle product standard, J2600, has been revised to define pressure classes so that the terminology of the automotive people and the stationary people agree; add the H70 hardware definition; and require the hardware to meet the national pressure technology requirements. This document, SAE J2600-2013, is published. ISO has also published a harmonized version of this document. It would be helpful to industry and DOE to expand the list of major accomplishments and include a status list on the progress of the remaining key documents.
- The statement that the C&S are essentially complete is misleading. It is true that much progress has been made, but there is still work to be done for more development and/or revisions, as well as for implementation. The assumption that industry will take over at this early date is not necessarily a good one. There was truth in the comment from an audience member who said that he “take[s] exception to the statement that industry needs to ‘do the heavy lifting.’ For the rest of industry (aside from the automotive original equipment manufacturers) this is very difficult, as there are not a lot of engaged parties—there is no short-term demand...” The work with California is extremely helpful and hiring a consultant (Bob Davidson) to work on the IFC proposals was also a great accomplishment. The Hydrogen Safety Handbook will also be good to see. If not done so already, it would be good to see positions supported by NREL (via DOE funding) re-engaged at this most critical time.

**Question 3: Collaboration and coordination with other institutions**

This project was rated **3.6** for its collaboration and coordination.

- The liaison work is very useful; it would be good to see more/continued efforts.
- DOE and NREL have very good connections both nationally with key standards development organizations (SDOs) (such as SAE, CSA) and code development organization (CDOs) (such as NFPA, the International Code Council [ICC]), and internationally with ISO and the GTR. The R&D collaboration with the Japan Automobile Research Institute (JARI) and others has been exceptional.
- By necessity (and successfully), this project collaborates well with the appropriate interested parties (such as NFPA, ICC, the Fuel Cell and Hydrogen Energy Association [FCHEA], other laboratories [SNL and PNNL], and particularly the California Fuel Cell Partnership).
- Working, collaborating, and coordinating with SDOs, authorities having jurisdiction (AHJs) in various areas, and others involved with furthering the development and implementation of hydrogen and fuel cells C&S is like herding cats. NREL is to be commended for its effort.
- The list of collaborations is sketchy. It is notable that the nationally recognized testing laboratories—which are working to develop the product safety standards—are not noted.

**Question 4: Relevance/potential impact on advancing progress toward DOE research, development, and demonstration (RD&D) goals**

This project was rated **3.6** for its relevance/potential impact.

- This project is very relevant to the needs of the DOE Safety, Codes and Standards program and to the rollout of the infrastructure. The role of coordinator is needed and executed well by this project.
- The relevance of appropriate RCS is obvious. Without it, market introduction of applicable technologies is limited.
- This work has been critical for supporting hydrogen infrastructure, where stakeholder resources are limited and significant learning is still required to achieve commercial readiness.
- This project is absolutely critical to the success of hydrogen and fuel cells—the expertise and coordination in C&S development is paramount to success, as outlined particularly in slides 11 and 12. There is no question that outreach and education on the progress is essential as well, but maintaining support in the development of C&S is still a high priority.
- Without RCS that are accurate, complete, acceptable, and understood, the implementation of hydrogen fuel cells will not happen on anything but the smallest scale. NREL's project is central to the development and implementation of RCS as well as to bringing the message to the hydrogen community, especially key AHJs. An emphasis on California is proper.
- The relevance is self evident. However, a more inclusive approach that is not limited to model building and fire codes would be helpful.
- Most project aspects align with the Hydrogen and Fuel Cells Program and DOE RD&D objectives. Much of the work in standardization is done; however, hydrogen quality cannot be measured universally due to the lack of finalized analytical standards.

**Question 5: Proposed future work**

This project was rated **2.4** for its proposed future work.

- The proposed future work is focused on the right areas.
- The project team should keep up the coordination in all areas.
- NREL plans to continue work in C&S coordination on a smaller scale, passing much of the work over to industry. NREL will focus on infrastructure C&S issues. NREL also appears to be stepping up its outreach activities, working with key AHJs. As hydrogen deployment ramps up in key areas (e.g., California) the outreach aspect will become more and more important. NREL's future work direction is proper.
- The proposed future work is discouraging. The task is only just started. Expanding the monitoring and support to be more inclusive by not being limited to the model building and fire codes would be helpful.

- To say C&S are complete is incorrect. Significant effort needs to go into addressing the U.S. Department of Transportation (DOT) requirements for shipping hydrogen tanks with hydrogen. Currently, this requires a special permit and is seen as a barrier for many market applications, such as mobile fueling. Additionally, industry has asked for years for a “hydrogen cleanliness spec” for hydrogen stations (e.g., what solvents can be used to clean a station after it has been built or maintained). This has never come to fruition and has apparently fallen off the table, if NREL states that all C&S are essentially complete. It is unclear where this is in NREL’s gap analysis.
- While there is truth in the notion that some of the heavy lifting has been accomplished by the CDO community to enable an infrastructure, there are still critical elements that are seriously needed (e.g., metering). So while the outreach efforts to support education in preparation for the infrastructure rollout are important, attention still needs to be given to the critical rate-limiting elements (such as metering, fuel quality, international harmonization, etc.). Now is not the time to pull back on the development of C&S for those critical elements, and now is not the time to lose track of the need to harmonize the U.S. efforts with international RCS activities.
- The conclusion slide and the responses to questions for proposed future work were very vague and weak. The plans have little relevance to eliminating barriers or advancing the Hydrogen and Fuel Cells Program. DOE should work with industry to make a list made of the top items left to assist in the commercialization of fuel cell vehicles and hydrogen infrastructure. Surely a concrete roadmap to get hydrogen metering to within 1.5% accuracy and analytical methods are some of the items that are needed as soon as possible, and the industry should be surveyed through the U.S. DRIVE Codes and Standards Tech Team and elsewhere to determine where support is needed.

#### Project strengths:

- The focus of the project is a strength.
- This project has helped to guide, inform, and coordinate a broad array of complex activities.
- The coordination with NFPA, IFC, and ASME is critical and very helpful to the industry.
- Strengths of this project include the researchers’ level of expertise and knowledge, progress/success to date, and coordination.
- Strengths of this project include its concise safety goals, communication, C&S coordination through FCHEA, and support of SAE Hydrogen Fueling (J2601).
- This project features coordination of a large number of C&S activities with various officials, SDOs, researchers, etc. Having the NREL Technology Validation database to draw from is another strength.

#### Project weaknesses:

- The project needs clear, significant deliverables and associated timelines.
- The focus of the project is also a weakness. The development of supporting design codes, product standards, and test methods needs support.
- There is a lack of planning to “finish the job” related to near term C&S development (Proposed Future Work).
- The outreach effort lacks metrics.
- It would be good to see three or four well-designed charts that visually tie all of the pieces of this work together. The project team should replace slide 6 (with the pyramid to the right) because this chart seems to depict the vehicle C&S as a roll-down of primary building and fire codes. The team should also connect to real-world goals: stations and vehicles and their interaction.

#### Recommendations for additions/deletions to project scope:

- C&S involving hydrogen quality needs to be addressed.
- Researchers should monitor field experience to confirm that the statement that “key C&S are in place” is really true.
- There should be work regarding the DOT requirements on composite tank shipment (on-road) with hydrogen.

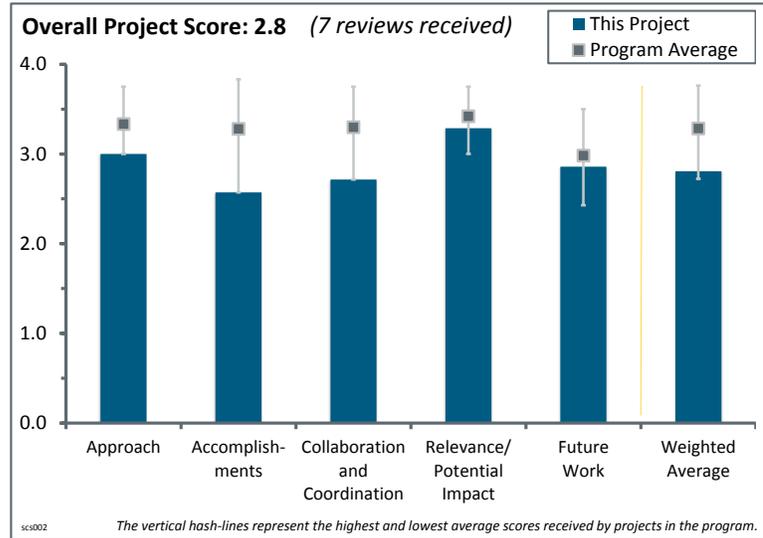
- The project team should expand the scope to include the supporting design codes, product standards, and test methods.
- The project team should continue to work with industry—the hose study is a good example—to facilitate progress in areas that may be of smaller relative scope (e.g., a hose versus a model fire code) but with just as much overall importance. Following are areas to expand upon (which are being addressed to some extent now): metering, the ability to sell hydrogen, and third-party certification of components and systems.
- The project team should create a “Near Term R&D Needs” document for C&S and canvas industry members at ASTM/CSA/SAE regarding needs, etc., to determine a roadmap. The team should be a part of “accelerating key” industry C&S. It should also delete all hydrogen sensor work; this is not valuable to the industry at all, per technical papers from the industry related to the status of hydrogen sensors. The team should also take the following actions:
  - Work with the ASTM D03 Gaseous Fuels Team to accelerate the hydrogen quality analytical methods that need to be finished as soon as possible. The other work being done for hydrogen quality is not as high of a priority as getting this standards round-robin testing completed and motivating the team and convener to finalize the technical work and publish the first set of standards. This is important.
  - CSA and SAE are not aligned regarding acceptance of materials compatibility; perhaps this needs to be accelerated. The stainless steels with high-nickel content needed for hydrogen storage systems are not available in North America—this is important. They must be shipped in from Europe or Japan or a custom order must be made at a steel mill. The standards could be a motivator, but they must be aligned.
  - Materials capability: This was stated a few times, but  $-50^{\circ}\text{C}$  must be used to determine embrittlement. It is unclear when SNL will have this capability.
  - CSA standards on dispenser components: The hose, breakaway, and connectors standards have not been tested before incorporation by the American National Standards Institute; this should be investigated with data.
  - SAE J2578/J2579: need data to validate before making recommendations to the standards. Topics such as stress rupture are inadequately covered in those documents.
  - Setback distances need to be aligned between the ISO and SAE worlds. This should be a coordinated data effort with the Japanese and European Union counterparts.
  - The hydrogen sensor work is obsolete because the industry has sensor solutions available in its production vehicles and stations. It is recommended to halt this project.
  - Hydrogen metering: Hydrogen metering is being evaluated through NREL, and there is already an additional funding opportunity announcement to investigate this. However, there needs to be a follow-on project that incorporates testing flow meters not only in the laboratory, but also in the field until a commercially acceptable flow meter is found to get within 2% accuracy.
  - Field testing (continuation of laboratory tests): Fueling standards should be further validated at a designated development station to show the positives and negatives (e.g., SAE J2601 versus the MC Method [total heat capacity method]). This station could also be a basis for metering and hydrogen quality testing.

## Project # SCS-002: Component Standards Research & Development

Robert Burgess; National Renewable Energy Laboratory

### Brief Summary of Project:

Safe deployment of hydrogen fuel cell technologies is dependent on components that are proven to perform safely and reliably as measured against new safety and performance standards. This project works with manufacturers, installers, and the National Renewable Energy Laboratory's (NREL's) Technology Validation program to prioritize gaps, then to close those gaps by conducting hydrogen component research and development (R&D) and performance validation. Root cause analysis and R&D testing are conducted to improve the safety and reliability of hydrogen system components.



### Question 1: Approach to performing the work

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

- The presentation featured a good, top-down hierarchical description. Making use of the NREL Technology Validation data is a good approach to advancing the safety database. The project's nature means that a significant portion of the work appears to be reactive—this is not necessarily a bad thing for this type of work.
- The project seems well coordinated with project SCS-001, with a good flow of information between NREL and standards development organizations (SDOs)/original equipment manufacturers (OEMs)/station providers.
- This project has the potential to bridge a gap in industry by providing capabilities for “in situ” testing of components in a high-pressure hydrogen environment. This is a critical need for industry. However, this work needs to be a collaborative effort with industry and recognized third-party testing laboratories. It was unclear in the presentation whether the information on “near misses” and incidents is being fed into the hydrogen incidents database and subsequently communicated to the appropriate SDOs. If not, this should be incorporated in order to provide important data to support the standards development. This presentation frequently referred to component-level issues being addressed in codes and standards. This needs to be corrected—component-level requirements and some system-level requirements are addressed in the safety standards. Codes are for installation and not to make component-level evaluations.
- Globally, the component R&D approach is good. It addresses several key barriers and will significantly contribute to close technology gaps that are essential to ensure safety. Although progressing well, further efforts could be done regarding the collection/integration of real-world data from OEMs and station providers. This is critical.
- The approach and input appear to be limited. The focus, based on this presentation, appears to be limited to work at SAE International (SAE) and the National Fire Protection Association (NFPA). Discussions with the generators of the design codes, product safety standards, and material test methods would be worthwhile. The project team should look at Tom Rockward's presentation as a way of handling multiple objectives.
- It would be good to see tighter partnering with other laboratories in this area—specifically the material science team at Sandia National Laboratories (SNL). The presenter did list the materials activities at SNL; however, on slide 6 under mechanical element testing, only a verbal comment was made with regard to SNL's efforts. This project and the materials science activities should be a close teaming effort; both

initiatives can benefit. It would also be good to see a focused approach to define which components are higher on the priority list for testing. For example, components needed for the commercial deployment of hydrogen should be placed higher on the list than those needed for production. There is an urgent need for dispensing and commercial equipment now in order to meet the infrastructure needs for a 2015 rollout.

## **Question 2: Accomplishments and progress toward overall project and U.S. Department of Energy (DOE) goals**

This project was rated **2.6** for its accomplishments and progress.

- The project seems to be on track. It is hard to fully evaluate the project at this stage, but this work and the capabilities developed should prove increasingly important over the next 5–10 years.
- Good progress has been made supporting codes and standards, especially SAE 2601. However, the rest of the accomplishments presented relate to “ad hoc” support activities that cannot be considered as tangible achievements (e.g., a webinar on refueling protocols). Efforts are needed to define a clear direction in terms of objectives and deliverables.
- It may be a result of the reduced budgets, but the funding for research to provide technical support for component-level standards has not been forthcoming. In situ PRD testing is needed and has been requested for several years (more than four years). With this project’s mandate to work closely with SDOs and develop data to provide technical justification for standards development, this needs improvement.
- The progress to date is gated by industry.
- It is concerning that some of the “accomplishments” presented were particularly weak. For example, NREL took credit for putting on a webinar that presented the status of SAE 2601; in reality, the presentation was given by two other representatives, neither of whom were NREL employees or part of NREL’s project. NREL’s role was one of support. This support role is also mentioned on other “accomplishments”—SAE J2601/NFPA joint call, and Non-Metallic Materials Workshop Participation. These listed accomplishments are not relevant to this component testing project. Next year, hopefully there are concrete accomplishments directly relevant to component testing, clearly differentiated from support, participation, and internal environmental safety and health requirements to enable an activity (periodic health assessments, etc.)
- Being able to support the SAE J2601 standard development by showing that, prior to refueling, hydrogen tank temperature (as a function of ambient temperature) is not as high as previously suggested by the standards committee is significant and may alleviate some refueling restrictions. But the presenter did not appear to know the tank temperature measurement locations. In addition, mention was made of the Emeryville incident (i.e., the hydrogen bus hydrogen leak/fire), but it is not exactly clear what this project’s involvement was in the investigation.
- This project suffers from a lack of technical achievements on components. There is no shortage of component-related issues; however, this project seems to have failed to identify, commence an analytical assessment of, or develop relevant project partnerships to achieve technically relevant results. It is unclear what the staff is doing beyond attending standards development committee meetings and generating quarterly, annual, and DOE Hydrogen and Fuel Cells Program Annual Merit Review reports. It is unclear what benefit the hydrogen community gains from this effort. The “Component Testing Report” was not available through the website even after an advanced search in the overall database. Furthermore, the presentation did not highlight the findings of the report. The summary states that “root cause safety/reliability issues” were identified by utilizing statistical data. The presentation only articulated one such statistical analysis—a vehicle fueling rate and temperature analysis. These results consist of already available data from the Technology Validation effort. It is unclear what value this effort provided besides communicating results to the technical committee (a useful but not technically significant achievement). The Emeryville incident investigation was a shared effort with many SCS laboratories that did not mention their participation as a major achievement (i.e., Pacific Northwest National Laboratory; Hydrogen Safety Panel members; and SNL, which conducted the majority of work in a contract for the California Air Resources Board). It is unclear why this project is articulating an achievement by mere involvement and what technical achievement beyond participation the project provided.

### Question 3: Collaboration and coordination with other institutions

This project was rated **2.7** for its collaboration and coordination.

- There is a large list of collaborators among standards developers, industry, and academia, both domestic and international. The project team appears to be well connected.
- The project shows very good collaborations with SDOs and international testing laboratories. However, more inputs from the industry will be required for testing activities at all component levels.
- The proposed future work areas are fantastic; however, there are an underwhelming number of project collaborators given the immense potential of the new capabilities (i.e., the Energy Systems Integration Facility [ESIF]) and previously spent efforts to develop project partners. The industry is a critical partner in this effort; this project seems entirely devoid of tangible and relevant industrial partners. This must be corrected in fiscal year (FY) 2014 for any benefit to result.
- This project/laboratory is “poised” to fill a gap in industry regarding the evaluation of components in a system-level, pure hydrogen environment. However, there are capabilities that exist through other nationally recognized testing laboratories (NRTLs) that need to be leveraged and coordinated with—especially given the fact that funds/budgets are tight. Capabilities of other NRTLs need to be investigated and coordination testing could be performed. Other laboratories have the capabilities to test some components. Given that the one purpose of spending DOE funds is to increase capability in the United States and build industry, pursuing collaboration with industry partners that currently provide third-party testing would serve this purpose. In addition, the third-party testing laboratories have staff that are trained and knowledgeable in testing products—to reproduce any of this at a national laboratory would put the laboratory in direct competition with industry/the private sector. Collaboration would provide the opportunity for the private sector to make manageable investments in what otherwise would be viewed as “high risk” activities. On slide 18, line 4.9 speaks of “certification and listing of components”—this is strictly the work of NRTLs, and NREL should not compete with the private sector. There is an “apparent” strong relationship between NREL, SAE, and NFPA. The presentation speaks of NREL working to provide “enforceable code language” for J2601. Similar activity needs to be initiated for other component-level national standards to drive “enforceable code language” for all systems and components where standards exist.
- The collaboration list does not appear to agree with the approach. The collaboration list implies a more expansive approach, which should be lauded.
- It would be good to see a much closer teaming collaboration between other activities supported by the DOE SCS program and outside SCS programs. There was mention of collaborative activities with others (e.g., the Emeryville incident and material mechanical component testing); creating a constructive teaming relationship with the appropriate parties rather than simply participating with other activities would strengthen this activity greatly. The project team should develop collaborative projects with others, such as by developing collaborative teaming activities. There is a perfect opportunity for NREL and SNL to team up on component testing and materials science and possibly other topics using the unique capabilities of NREL’s and SNL’s new fueling stations. Another example is the collaboration between NREL and the Joint Research Centre on sensor testing.

### Question 4: Relevance/potential impact on advancing progress toward DOE research, development, and demonstration (RD&D) goals

This project was rated **3.3** for its relevance/potential impact.

- This project fills gaps by providing shared capabilities that industry cannot yet maintain individually.
- This activity is very relevant to the needs of SCS and the general concerns of infrastructure rollout. This project should stay well informed with respect to the international community on component testing/qualification. The Japanese, for example, are very keen on the need to develop International Organization for Standardization (ISO) standards for station components.
- There is no doubt that component standard R&D is of high relevance for the rollout of hydrogen refueling stations. Components must comply with existing safety standards in the very short term and the new NREL

laboratory facility (the ESIF) will fully contribute to this goal. This project is therefore critical to the Program and DOE RD&D objectives.

- The emphasis on the component level to provide data to support compliance to existing standards is relevant to being able to use these components in deployed systems. Use of NREL’s ESIF to test components is worthy. Showing incident and near-miss data from the Technology Validation program was eye opening in that most (appears to be about 90%) of the near-miss data—more than 200 near misses—showed major or minor hydrogen releases (with no ignition).
- Slide 20 states that “NREL will continue to work with codes and standards technical committees to identify R&D gaps and to utilize the ESIF laboratory to conduct basic engineering R&D aimed at closing technology gaps.” A concern regarding the relevance and impact of this activity is that research dollars/space/time should be equitably allocated to the components that make up the systems. In addition, careful consideration needs to be taken to avoid competing with the private sector and to leverage knowledge and capabilities of third-party testing laboratories.
- The description of the approach does not represent the meat of the presentation. The meat is evaluating a generic fueling facility, determining the failure modes, and indicating where development work is required to reduce the safety risks associated with high-pressure gaseous systems. Outreach to the NRTLs is needed to assure them that NREL does not intend to compete with them, but rather provide support when requested by a NRTL.
- The unfortunate circumstance of this project is that it has incredible potential for impact to SCS efforts, but it has not delivered on that potential. There is a low degree of confidence that continued efforts, despite substantially improved capabilities (including the ESIF), will produce timely, trustworthy, or relevant results.

### Question 5: Proposed future work

This project was rated **2.9** for its proposed future work.

- The shift in emphasis toward safety and the reliability of components was a good idea.
- The project’s good list of future test priorities includes compressors, flow meters, hoses, a vehicle nozzle receptacle, and materials in service.
- Several gaps have been identified with regard to research and testing that is needed at the component level to support standards revisions/development. If NREL works to collaborate and provide the research support needed for SDOs with component-level standards, the progress and future work is in alignment. Collaboration with third-party testing laboratories is critical to establishing capabilities in the United States.
- The establishment of the ESIF laboratory is excellent news. Its technical capabilities are huge and will help overcome many barriers to the goals. Future test priorities have been planned, but further details could have been provided (e.g., connections with the industry). It was difficult to get a clear idea from the presentation about future accomplishments and the associated timeline.
- The proposed future work areas are fantastic; however, there are an underwhelming number of project collaborators given the immense potential of the new capabilities (i.e., ESIF) and previously spent efforts to develop project partners. The industry is a critical partner in this effort; this project seems entirely devoid of tangible and relevant industrial partners. This must be corrected in FY 2014 for any benefit to result.
- The future plans for this activity are good. It is not clear whether NREL has the capability in place to provide the necessary analysis and experimental data to provide input into the needs of flow meter accuracy. It will be very important to understand the mass flow rate as a function of time over the pressure and temperature domain as specified by a SAE J2601 compliant fill. It appears that the device being made for California is an end-point device; it is intended to measure the quantity delivered after the delivery has completed, not to quantify the mass flow rate during a fill. The ability to accurately measure the mass flow rate as a function of time at the required accuracy (dictated by HB44 and J2601) is critically needed to correctly qualify any mass flow rate meter. This is a particularly challenging effort. To qualify a meter, the testing device needs to be at least 10 times more accurate. For example, this means to qualify a meter at 1.5%, the qualifying device needs to be 0.15% accurate. Someone in the project needs to do this, and it does not appear that this is in NREL’s plans. The principal investigator should work on developing a well-thought-out, focused plan and developing testing priorities, among other items, to provide direction to this project.

- The future work is nebulous. The proposed work is limited to testing. The testing makes sense but does not appear to concur with the “approach.” A clarification on the work being done would be helpful.

#### Project strengths:

- The testing and implied collaboration with the NRTLs are strengths of this project.
- This project has the potential to provide in situ testing of components in high-pressure hydrogen environments. This will provide information on hydrogen compatibility and suitability for high-pressure hydrogen environments.
- This project’s strengths include the availability of ESIF, coordination with the Technology Validation data, and use of the wind-to-hydrogen project data.
- This project features effective information flow and fills gaps in resource-limited hydrogen industry capabilities, especially on the stationary side.
- This project’s strengths are in its capabilities and potential to deliver near-term, high-impact results. These strengths are substantial and unfortunately further underscore the project’s weaknesses and tepid results.
- Component testing is critically needed to advance the hydrogen infrastructure and to advance relevant regulations, codes, and standards. Basically, this project is well positioned to execute on this need. The new laboratory, when it is up and running, will clearly be a valuable asset to this community.
- Very good interactions with SDOs and national/international laboratories have been developed, which are clear strengths. The new laboratory facility, ESIF, is very promising and shows very high potential. This can provide a great leap forward in component R&D, thus overcoming most of the barriers. That is a very strong point.

#### Project weaknesses:

- The discussions on the project approach (goals) need some work.
- The presentation needed to elaborate more on the reasons for including the Emeryville incident.
- This project is still in its early phase and the results presented so far are still limited and lack consistency. A more consistent approach is needed to define clear, intermediate steps. Connections with the industry could/should be strengthened.
- There needs to be increased coordination/collaboration and support for the components and component-level standards that make up the system. Codes revisions need to be focused on installation issues, and the component safety requirements belong in the component-level safety standards. It is concerning that NREL is establishing “business” capabilities that will directly compete with private-sector, third-party certification laboratories. NREL needs to be in touch with these organizations to ensure they are not duplicating efforts/capabilities that already exist. Increased collaboration with existing laboratories is needed.
- The project’s weakness is its inability to use the unique position of frequent interaction with potential industrial partners through substantial codes and standards participation to develop any project partners. With the commissioning of the new laboratory capabilities, there are high expectations for this project to deliver substantial results. Unfortunately, it appears that opportunities to acquire project partners in advance of capabilities have been squandered and that the principal investigators will need to double efforts in FY 2014 to both acquire partners and produce results.
- Some of this project’s deficiencies could be because the project is relatively new and has a new laboratory. There is a strong need to team aggressively with others in the field to differentiate from simply participating. This will dramatically improve the quality/impact of the work, reduce overall cost, and help keep the work relevant and correct (cross-checking results).

#### Recommendations for additions/deletions to project scope:

- This project should deliver substantial results or face significant change considerations in FY 2014.
- The project team should improve teaming activities with other groups inside and outside the DOE SCS program.
- The project scope should be better defined, with clear milestones indicated.
- Leaks appear to be focused on the dispenser and compressor. In the stationary natural gas world, lines above 5 psi are required to be welded and instruments are seal welded or use non-tapered thread joints (i.e.,

pipe threads). It is unclear if the hardware tested meets the requirements in the B31.12 piping code. Compressor leakage is not surprising. Additionally, low mean time between failures would not be surprising for positive displacement pumping (compressors) hardware.

- It is important to stay one step ahead of industry. The project team may want to also add outreach at some point to transfer knowledge as industry grows and suppliers become ready to establish in-house capabilities.

## Project # SCS-004: Hydrogen Safety, Codes and Standards: Sensors

Eric Brosha; Los Alamos National Laboratory

### Brief Summary of Project:

The objective of this project is to develop hydrogen safety sensors for vehicle, stationary, and infrastructure applications and to demonstrate the technology through performance evaluation in simulated laboratory and field tests. Sensors are designed to be low-cost, durable, and reliable; they are subject to rigorous life testing to evaluate their performance in relation to codes and standards. Development of manufacturing methods and long-term testing in conjunction with industry partners will move the sensor technology toward commercialization.

### Question 1: Approach to performing the work

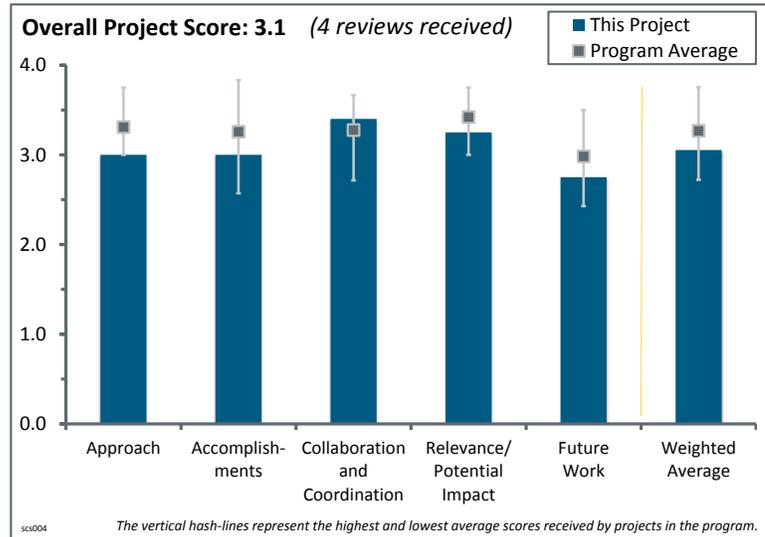
This project was rated **3.0** for its approach.

- The approach adopted in this project appears to be focused and coordinated. Shortcomings in sensor performance, highlighted by the National Renewable Energy Laboratory's (NREL's) testing (e.g., anaerobic operation), are addressed coherently and with positive results.
- This project approach has all of the hallmarks of a national laboratory/industrial collaboration—strong scientific results, good milestones, and an industrial “off-ramp” leading to a commercial product and step change to the current commercial ecosystem.
- Over the course of the project, durability, reliability, and sensitivity issues have been identified and systematically addressed to come closer to the sensors required to assess hydrogen leaks and concentrations in and around vehicles in accordance with safety criteria specified in codes and standards, such as SAE 2579 and the hydrogen fuel cell vehicle global technical regulation (GTR).
- As a higher level comment on sensor R&D, there have been multiple issues regarding moving toward an approach that can be adopted by industry for various reasons. The lack of sensor manufacturers at the table who can be available for discussion within the working group and are willing to come forward to address potential standards issues hampers the work needed to roll out a solution for industry. Sensor manufacturers need to be involved.
- Sensor development must be driven by the needs identified by the end users and system integrators. The workshop's influence on the development R&D program seems minimal, at best. As a whole, it is not clear how the approach will lead to a sensor that meets the targets specified. If not carefully managed, this project could be an open-ended sensor technology development process.

### Question 2: Accomplishments and progress toward overall project and U.S. Department of Energy (DOE) goals

This project was rated **3.0** for its accomplishments and progress.

- It appears that good progress has been made toward understanding the limitations and issues associated with these specific sensor technologies.
- The accomplishments listed under the Round 2 testing at NREL indicate significant progress has been made toward objectives and overcoming barriers. The principal investigator summed up the



accomplishments as “faster, better, and cheaper,” if technologies are moved from prototypes to commercial products.

- The results demonstrated are worthy of praise. In terms of value, it appears that DOE’s contribution of approximately \$5 million will produce a substantial benefit to the hydrogen and fuel cell industry and provide “backward compatibility” with the overall hydrogen and flammable gas safety market (a substantially larger commercial market in the near term). This “backward compatibility” is critical to the survival of sensor manufacturers ahead of vehicle deployments in 2015–2020. This project team has clearly identified that need and delivered a result that encompasses that critical aspect.
- Accomplishments toward the development of a sensing technology that shows promising selectivity to hydrogen, a robust working electrode, and resistance to changes in ambient temperature are encouraging. Accomplishments claimed in terms of “faster” and “cheaper” (unit cost) are difficult to evaluate based on the material presented. Nevertheless, the preparation for field trials and the focus on applying lower cost fabrication techniques suitable for mass production indicate the technology’s development in the right direction to achieve the objective to develop a low-cost, durable, and reliable hydrogen safety sensor for vehicle, stationary, and infrastructure applications.
- The sensor manufacturers need to be involved. In addition, standards need to be developed/identified that reflect the specific application for the sensor device.

### Question 3: Collaboration and coordination with other institutions

This project was rated **3.4** for its collaboration and coordination.

- This project demonstrates excellent coordination and utilization of the developed sensor testing capabilities at NREL. This provides a good model for future sensor development efforts funded by the DOE Fuel Cell Technologies (FCT) Office.
- This project features lots of collaboration between agencies, with complementary expertise with sensors, industry, and end users.
- The partnerships established with national laboratories and industrial entities appear to be appropriately and effectively coordinated. The involvement of industry lends confidence in the sensing technology’s ability to reach commercialization.
- The collaboration is good. Unfortunately, there seems to be a continued miscommunication between the project team and the NREL test laboratory. In addition, it is difficult to determine if the industrial partners are small start-ups or developed companies with established market share. It is important not only that a balance exists, but that the technology transfer has a very good chance of surviving in the market.
- The sensor manufacturers need to be involved. In addition, standards need to be developed/identified that reflect the specific application for the sensor device.

### Question 4: Relevance/potential impact on advancing progress toward DOE research, development, and demonstration (RD&D) goals

This project was rated **3.3** for its relevance/potential impact.

- This project is very likely to be transformative to the industry and provide a usable product for many applications.
- Devices that ensure the safe use of hydrogen are critical for the success of the transition toward a low-carbon, hydrogen-inclusive society. Clearly the development of a robust, cost-effective, accurate hydrogen sensor will increase safety and accelerate confidence in hydrogen technologies.
- As evidenced in existing and draft codes and standards and through the hydrogen incidents database, sensors for mobile and stationary applications are absolutely necessary to ensure safety. It has been clear that at the outset, sensor technology was not sufficient to meet the durability, response time, and sensitivity requirements of various applications. Safety is the first requirement of the deployment of new technologies. For hydrogen fuel cell vehicles, hydrogen sensors are absolutely necessary to manage fire and asphyxiation hazards.

- It is not clear that sensor development will have a big impact on the deployment of hydrogen and fuel cells systems (especially in the near term). It is not clear that this specific technology deserves so much focus by the DOE Hydrogen and Fuel Cells Program.

### Question 5: Proposed future work

This project was rated **2.8** for its proposed future work.

- All future work in sensor technology development funded by the FCT Office should be competitively selected. This project provides a good template for how the NREL facility can be leveraged by future sensor technology development activities.
- Continuing field testing, developing test protocols, and seeking commercial development partners will be useful in supporting affordable introductory products to the marketplace. It is unknown whether costs will be acceptable and whether all barriers to commercialization will be addressed.
- It is important in the final year that the future work includes a summary of the effort, not just a smooth transition to industry without a summary of the lessons learned and broader impacts that safety devices (more than just sensors) might have on the industry.
- The expectation for the coming year is that the field trials will validate the sensor's performance under laboratory conditions. Such field trials will demonstrate the sensor's performance under real-life operating conditions. Continued independent testing by NREL is encouraged; however, whether this should include "developing testing protocols" is questioned. The focus should now be toward fine tuning and commercialization.

### Project strengths:

- The collaborations with industrial partners are commended. The progression from laboratory testing to field testing is very encouraging and will test the sensor's real-life performance and provide a true test of this technology. The results from these field tests are eagerly awaited.
- The project team has a strong scientific competency in sensors. The project demonstrates good coordination with critical partners (e.g., NREL test facility).
- This project features great project management, good project partners, and a clear vision from start to finish with high confidence that the project will come in on time and on budget with a high likelihood of commercial success.

### Project weaknesses:

- As a whole, it is not clear how the approach will lead to a sensor that meets the targets specified. If not carefully managed, this project could be an open-ended sensor technology development process.
- The influence of some species on the sensor baseline is of concern. This is particularly the case with CH<sub>4</sub>, a species that may feature in future hydrogen applications such as refueling stations, where the influence on the baseline is extensive.
- It is unclear whether the industrial partners are robust enough to market and allow the substantial DOE investment to survive the next few years until light-duty vehicle deployment and the broader fuel cell market take hold. The principal investigator should articulate this in the final presentation in fiscal year 2014.

### Recommendations for additions/deletions to project scope:

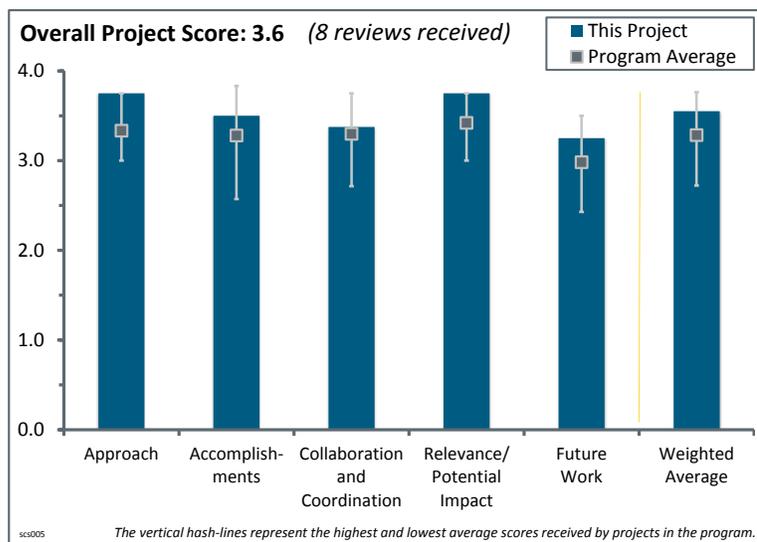
- All future work in sensor technology development funded by EERE should be competitively selected.
- Specific applications for these sensors are unclear, and it is also not clear whether there are specific cost and durability requirements for each application.
- The project team should further investigate cross-sensitivity to CH<sub>4</sub> to understand the unusual response to CH<sub>4</sub> observed in the presence and absence of hydrogen. Information on sensor manufacturing costs and indicative costs for maintenance/calibration would also be useful.

## Project # SCS-005: R&D for Safety, Codes and Standards: Materials and Components Compatibility

Aaron Harris; Sandia National Laboratories

### Brief Summary of Project:

The Safety, Codes and Standards program coordinates critical stakeholders and research to remove technology deployment barriers. The overall objectives of this project are to enable technology deployment by providing science-based resources for standards and hydrogen component development and to participate directly in formulating standards. The goals for fiscal year 2013 include developing and maintaining a material properties database, identifying material properties data gaps, developing more efficient and reliable materials test methods in standards, designing and qualifying the safety of standards for components and materials testing, and executing materials testing to address targeted data gaps in standards and critical technology development.



### Question 1: Approach to performing the work

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

- The approach taken to address the barriers identified was presented very clearly, as was the relevance and importance to standardization. The importance of providing robust data for the development of effective standards cannot be overestimated. The project has provided such data and has proposed improved test methods.
- The work presents a logical structure, a logical approach, and logical involvement of relevant stakeholders. It contributes to filling necessary knowledge gaps.
- The approach is consistent with current industry practice.
- The project is addressing targeted data gaps, transferring data and conclusions to standards development activities, and providing effective international engagement to increase harmonization and reduce potential for competing requirements.
- Sandia National Laboratories (SNL) is using a valid approach to provide material/component data that will allow codes and standards to be modified or augmented. SNL is addressing several key compatibility issues including hydrogen effects on steel used in pressure vessels and hydrogen effects on welds. SNL is also working with standards teams. The approach appears to be a good one.
- The current approach is sound and accurate; however, it could be improved. It contributes to overcoming only some of the barriers. Researchers must develop the capability to test to  $-50^{\circ}\text{C}$  or else the results are questionable.

### Question 2: Accomplishments and progress toward overall project and U.S. Department of Energy (DOE) goals

This project was rated **3.5** for its accomplishments and progress.

- This activity clearly supports DOE Hydrogen and Fuel Cells Program goals.
- Good work has been done on materials that are of interest to industry. Learnings have been used as the basis for standards development.

- This project has featured very good accomplishments to date. SNL should be complimented on its leadership in accelerating and assisting in completing the hydrogen compatibility standards.
- Completion of the test matrix of two different steels is an important accomplishment. The fact that this has been done in collaboration with industry (steel suppliers) compounds its relevance to the industry. The investigation on the effects of welding practice on tensile ductility yielded interesting behavior. A deeper understanding of the reasons for these effects may be relevant.
- The work is still ongoing. The project team has made excellent progress in developing test methodologies to accelerate data generation without compromising data accuracy. This is important to fill data gaps where long-term testing would otherwise be required. It allows data gaps to be filled more quickly.
- The project addresses a number of challenges that have been identified. The progress in mechanical testing does not seem substantial compared to the previous year.
- SNL has found that crack growth for a lower strength steel is not affected as much by hydrogen pressure as a higher strength steel. However, it is not clear from the presentation whether the testing proves that steel strength is the reason. It appears that more types of steel should be tested. It is recognized that testing is necessarily slow. SNL has also shown that welds, due to their microstructures, are more likely to become embrittled by hydrogen than non-welded materials.

### Question 3: Collaboration and coordination with other institutions

This project was rated **3.4** for its collaboration and coordination.

- There is great collaboration with the European original equipment manufacturers (OEMs) (i.e., Opel, BMW) and standards development organizations (SDOs) (i.e., Canadian Standards Association [CSA] and SAE International [SAE]).
- SNL is working with SDOs, industry, and international researchers; these are all necessary and proper for furthering the completeness and accuracy of standards. SNL is also working with universities, specifically using student design teams. Training the next generation is always good.
- The project focuses not just on research and development, but also on active participation of project personnel in SDOs—this is highly commended and facilitates the direct injection of the results of this scientific research into standards. More explicit information on the nature and degree of the collaborations with the named industry partners would be useful to critically evaluate the effectiveness of these collaborations.
- It is excellent that project members are participating directly with appropriate standards development committees. One slide provided for reviewers only (Critical Assumptions and Issues) notes the following: “We must maintain and expand relationships with industry partners and SDOs not only so that we have a supply of materials but also access to their input into materials testing parameters.” Active participation in Fuel Cell and Hydrogen Energy Association (FCHEA) working groups may be a suitable way to achieve this. SNL is already a member of FCHEA and has access to the working groups.
- Collaboration covers the correct range of stakeholders, both for guiding the issues to be addressed and for dissemination to safety, codes and standards (SCS) committees. Because hydrogen embrittlement and compatibility issues between hydrogen and materials in general have been widely investigated in the past by a large number of research programs across the world, it may be useful to identify in the presentation the efforts that have been made in exploring the relevance of this body of knowledge for the Safety, Codes and Standards program to avoid duplication with earlier work.
- The National Institute of Standards and Technology (NIST) (Colorado) is doing similar work. It would be preferable for SNL to collaborate with NIST and other researchers to avoid duplication and possibly share equipment and tooling to reduce cost and expedite data generation by minimizing non-recurring engineering costs (set up time, fixtures, etc.). ASME might be a good venue for this coordination. It is public and would hopefully be the beneficiary of the research (via inclusion in the pressure technology codes).

**Question 4: Relevance/potential impact on advancing progress toward DOE research, development, and demonstration (RD&D) goals**

This project was rated **3.8** for its relevance/potential impact.

- This activity is clearly relevant for a hydrogen infrastructure.
- The direct input of robust, independent scientific research into standards is essential. This project contributes positively to standards development and the material properties knowledge base.
- Filling gaps in the knowledge of materials behavior in a hydrogen environment and feeding the information into standards and code development organizations is a necessary precondition for technology deployment.
- A solid understanding of materials behavior in intended hydrogen operating environments is crucial as industry shifts from small-scale demonstration toward commercial volumes with optimized designs.
- The methodologies allow data development of critical gaps in knowledge. The results of the work on welds are relevant and unique. The results help answer many questions from the technical community on pressure vessel and hydrogen system construction.
- SNL was a key reason why the appendix SAE J2579 was so successful.
- There is obvious relevance; there is a need for data that will allow standards to be set. The presentation implies this but does not state it. However, the emphasis on targeted data was stressed many times and focuses the project in relevant areas.

**Question 5: Proposed future work**

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

- The proposed future work seems to build suitably on the work performed to date. Complementary work in direct collaboration with industry would give added value.
- SNL is looking to continue the mechanical properties work to further the understanding of crack initiation and growth in materials and welds. Most of the future work seems to focus on this important area.
- Project principals are documenting work done so far; it will be good to read about the details of the work.
- Researchers must show a plan when -50°C capability will be possible.
- The majority of the proposed work makes sense. It must be pointed out that pipelines operate in a small temperature band, but storage, pressurization equipment, and appliances see a much higher range (i.e., -40°C to 85°C for vehicles, and up to 500°C for hydrogen generators). The effects of temperature should be examined.
- To enhance the transferability of laboratory results to real-life applications, the project should consider screening the effect of residual stresses in the fatigue test program. The relevance of testing weldments (1) under pre-charged conditions rather than directly in a hydrogen environment and (2) in short-term tensile tests only should be explained and justified. An explanation should be given on the need for and relevance of testing in hydrogen under variable temperatures.

**Project strengths:**

- This project is doing fundamental work on materials in hydrogen applications unique to transportation or early hydrogen and fuel cell markets.
- This project features effective interaction with SCS bodies.
- Strengths of this project include its communication with industry, analytical methods, and integrity of data.
- A solid scientific approach is adopted in this project. The direct relevance and input to standards development is clear.
- The collaboration with ASME and the pipeline needs are strengths of this project.
- This project is making it possible to fill data gaps more quickly than previously possible. Other strengths include how it is focused on the highest impact data and its direct involvement in standards activities to transfer data.
- This project features a good collaborative team with the International Institute for Carbon-Neutral Energy Research (I<sup>2</sup>CNER). Another strength is how it is getting international “buy in.” Obtaining sufficient

information on specific hydrogen effects on metals and alloys as functions of temperature, pressure, and concentration is very important.

**Project weaknesses:**

- This project features limited testing capability to date.
- Stronger direct support to industry would strengthen this project (i.e., relevance to industry needs).
- The project team must show the capability to test at -50°C to have credibility for embrittlement testing.
- The data on two steels is not enough to draw conclusions about steel strengths versus crack growth.
- Weaknesses include the lack of collaboration with other government-funded related research and limited data at alternative temperatures.
- This project is not as comprehensive as it could be with sufficient resources and time. While it is not possible to test every material under every condition, the presentation spurred a desire to see more. More direct and focused discussions with the fuel cell and hydrogen industry may aid in identifying parameters of greatest interest and in obtaining suitable materials.
- To clearly demonstrate the lack of potential duplication with related research elsewhere in the world, clear identification should be given of how the project's work plan is different. This includes gaps identified, specificities and/or complementarities addressed, etc.

**Recommendations for additions/deletions to project scope:**

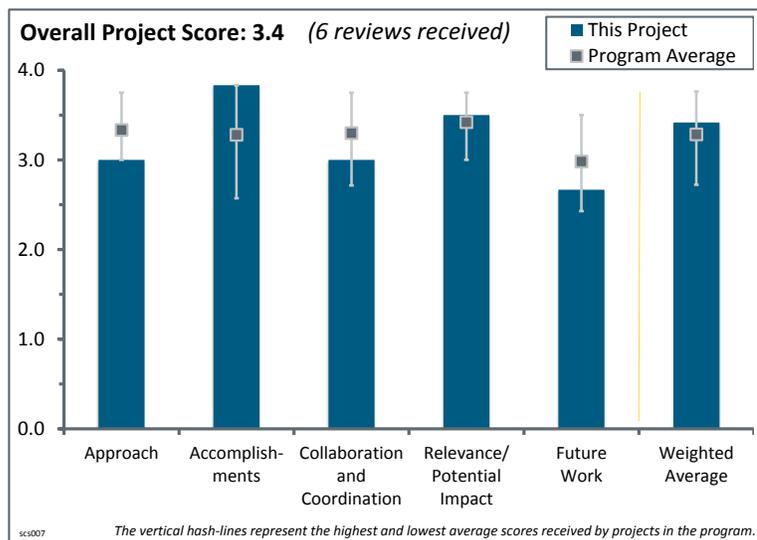
- This project should address the weaknesses identified by reviewers.
- Further investigation of the influence of welding practice on material properties may yield useful information.
- In addition to addressing weaknesses, the project team should assist in the harmonization between SAE and CSA, especially with regard to the accepted stainless and aluminum materials list proposed by the OEMs.
- The project team should pursue more publication of research and preliminary results and conclusions to enable review and feedback for future work. This may also facilitate additional research by others to both validate and expand upon this project. It would be nice to see some data over a larger temperature range.

## Project # SCS-007: Hydrogen Fuel Quality

Tommy Rockward; Los Alamos National Laboratory

### Brief Summary of Project:

Qualifying the hydrogen fuel grade for polymer electrolyte membrane fuel cell (PEMFC) systems is a priority to ensure fuel cell viability. Minimal amounts of impurities are detrimental to the performance and durability of PEMFCs, and an in-line hydrogen analyzer to continuously monitor impurities is needed. The objectives of this project are to develop an international standard for hydrogen fuel quality by determining levels of impurities that become detrimental to fuel cell performance and to demonstrate proof-of-concept of an electrochemical analyzer designed to detect impurities.



### Question 1: Approach to performing the work

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

- This project has three approaches (goals). The presentation is divided into three sections. This is a wise approach.
- The work on the in-line analyzer is much needed. It will be good to see its implementation at a station.
- Great work has been done, but at some point a cost trade-off model should be added to the project to look at the balance between stack cost reduction (reduced platinum loading) and fuel costs (increased purification effort). In addition to studying the effects of the maximum allowable impurity levels, the project team should also look at “expected” impurity levels.
- This is very important, good work. The only concern is with the in-line fuel quality analyzer. It is not clear that attention is being given to the final cost of the technology. If this is going to be widely implemented in dispensers, then the technology needs to be cost effective. The principal investigator (PI) needs to address this issue, and if the technology cannot meet a reasonable cost target, then this needs to be addressed. A techno-economic analysis really should be made to ensure that this will yield a cost-effective solution. Priority should be given to this part of the project. The measurement of fuel quality as delivered is necessary for a successful rollout of the infrastructure, which is targeted for 2015–2016—less than two years from now.
- The approach for publication of ASTM methods is unclear. There is no project plan for the interlaboratory study (ILS) (precision and bias statements) process for each standard test method. This needs to be addressed. Although these standards have been published, very few, if any, laboratories know how to use these methods. Without laboratory capability to test hydrogen contaminants at the levels required by ISO 14687-2 and SAE J2719, the fuel quality standards, and now regulations, are moot. It is unclear what the project plan is for moving ASTM standards through ILS and getting more laboratories set up to test hydrogen to these levels.
- The approach suffers from distracting priorities. The work should either focus on developing an in-line analyzer or work in membrane electrode assembly (MEA) impurity testing. At this point, MEA work should fall under the Fuel Cells program, not the Safety, Codes and Standards (SCS) program. In-line analyzer development and test method round-robin efforts are closely aligned and would greatly benefit the industry. If this project were to refine the approach and use the sensor testing effort at Los Alamos National Laboratory (LANL) as an example, a significant accomplishment could result. This would require

refocusing the project to identify potential commercial partners for this analyzer and dedicating efforts toward that end. This is the best option for this project.

### **Question 2: Accomplishments and progress toward overall project and U.S. Department of Energy (DOE) goals**

This project was rated **3.8** for its accomplishments and progress.

- LANL is without a doubt one of the most highly regarded hydrogen quality experts. The testing being conducted and methodologies being developed are innovative.
- The progress and accomplishments to date meet DOE goals.
- Participation with ASTM and completion of ISO 14687-2 are very good and important accomplishments. The attention to fuel quality effects on stacks is a natural next step; this is also an important teaming opportunity with others in this area (e.g., the Joint Research Centre [JRC]).
- Full standards for hydrogen fuel quality are now in place.
- It is clear that the technical competency of this group is world-class. Progress toward the goals should be refined to focus the efforts, perhaps by bifurcating this work into a Fuel Cells project examining the MEA impact of impurities and an SCS project aimed toward an in-line analyzer.
- There is a need to better communicate these successes to those in the fuel cells world (but outside of the “hydrogen quality” world) as a message to policymakers that progress is happening.

### **Question 3: Collaboration and coordination with other institutions**

This project was rated **3.0** for its collaboration and coordination.

- The emerging relationship with the Japan Automobile Research Institute (JARI) is very encouraging. It would be good to see this activity also team with other international entities that are working on (or will be working on) fuel quality issues on stacks. The efforts with the standards organizations are excellent.
- Regarding the comment from last year’s DOE Hydrogen and Fuel Cells Program Annual Merit Review on collaboration, this is a good start. Perhaps there is an opportunity to collaborate with others (e.g., Germany). The project team should maintain contact with industry stakeholders as a “check” on synergy between the “real world” and research.
- The collaboration with various institutions is adequate. The lack of feedback to the SAE J2719 team is a notable oversight.
- Contributions and collaborations from project partners identified on the opening slide were not clearly detailed in the subsequent presentation, except for a scoping meeting with JARI and, of course, the work with ASTM. This project would substantially benefit from deeper collaboration with industry, particularly if the suggestions to focus on developing an in-line analyzer are followed.
- There was no apparent collaboration with laboratories conducting hydrogen quality sampling in the real world, such as Atlanta Analytical and Smart Chemistry. It is unclear if the project team has identified the needs of these laboratories and how the project can provide support. The project team could use its expertise to help other laboratories, such as California’s Division of Measurement Standards (DMS), which will be required by law to regulate the quality of hydrogen. It is unclear if the project team has worked with California DMS. Also, on slide 24, JARI highlighted the need to look into particulates. It is unclear if the project team is doing any work on that, or if there is a plan for particulate work.

### **Question 4: Relevance/potential impact on advancing progress toward DOE research, development, and demonstration (RD&D) goals**

This project was rated **3.5** for its relevance/potential impact.

- LANL’s innovation and expertise in hydrogen quality is and has been very influential for determining constituent levels in fuel.

- The effects of fuel impurities on PEMFCs and the requirements to minimize certain impurities in hydrogen set the requirements between the station and the vehicle. This is the key link between fuel provider and fuel consumer.
- This work is critical for implementing hydrogen infrastructure and fuel cell vehicles (cars, buses, etc.) and needs to keep a rapid pace. If additional personnel are needed, it seems appropriate to allocate the funding.
- Fuel quality standards for delivered fuel are a necessary element for the commercial sale of hydrogen and for the performance of the stack. This work is spot on, and it is recognized globally for its contribution to the standards community.
- Researchers need to look at cost trade-offs. The requirements seem somewhat one-sided from the stack perspective versus the fuel provider perspective.
- The opportunity for impact from this project is substantial if it can refrain from becoming distracted by efforts in characterization of MEAs (which appears to be a legacy activity now caught in an SCS project—a bad omen from a project management standpoint). The utility of a commercial product in-line gas analyzer in the next 3–5 years is a substantial need within the industry and perhaps represents a “step change” innovation for the commercial sale of hydrogen (a potential barrier to vehicle deployment).

### Question 5: Proposed future work

This project was rated **2.7** for its proposed future work.

- Researchers should add a cost trade-off model.
- The project team should try to keep some focus on near-term needs, along with innovative advancements.
- There is no clear project plan for the ASTM standards.
- The focus on NH<sub>3</sub> and CO as a function of catalyst loading is important. The focus on H<sub>2</sub>S as a function of catalyst loading is not. Experience shows that sulfur is either present in large quantities or not present. Thus, additional data on the effects of sulfur concentration versus time and catalyst loading may not be as profitable as data on the effects of the other impurities, which are generated in the fuel processing. Recovery techniques that can be done on the vehicle would be very useful.
- It would be good to see an economic analysis and/or a discussion on the cost effectiveness of the in-line analyzer. The commercial development of such an analyzer is critically important to the commercial sale of hydrogen. The clock is ticking—indeed, one can argue that this development is already late. With that said, it is strongly recommended that the analyzer development effort aggressively seek an industrial partner suited to the commercialization of this technology, positioning it for deployment during the early rollout of a hydrogen infrastructure. In addition, it would be good to see outreach to others proposing work on fuel quality effects on stacks, such as JRC.
- This project suffers from competing technical interests—MEA characterization for speculative loading targets and gas quality analysis and analyzer development. The project should have identified this growing distraction and suggested steps to address it. If this issue is not addressed, this project will likely under-deliver on both technical areas, thus missing the potential impact of a more focused project. In short, the technical aspirations of the project are spread too broadly for the available resources for the project and the overall scope of the funding available to the Fuel Cell Technologies Office.

### Project strengths:

- This project is the basis for successful implementation of hydrogen fuel quality standards.
- This project’s strength is the project team’s expertise.
- Focus and dedication are the strengths of this project.
- The ASTM D03.14 work (publications) and in-line analyzer work show great alignment with near-term/real-world needs.
- This project’s strengths are the project team’s technical aptitude and capability to produce transformative commercial product prototypes in gas analysis at LANL, as demonstrated by the SCS-004 project presentation.
- This PI has been working on fuel quality effects on membranes for several years. The contribution to this very important problem is very good and well recognized. This project is making a significant impact in the

field and is satisfying a very important need. The participation in relevant standards bodies and leadership provided in these bodies (i.e., ASTM) is excellent.

#### **Project weaknesses:**

- The reluctance to put sulfur to bed is a weakness of this project.
- Perhaps this project needs more support in terms of person hours/personnel.
- It is concerning that attention to the cost practicality of the in-line analyzer has not been explored; at least, it did not come out in this review. An industrial partner to accelerate the commercialization of the in-line analyzer needs to be found.
- It would be good to see cost analysis—stack materials costs versus fuel purification costs and respective impacts on total vehicle cost of ownership. It would also be good to see data on actual contaminant levels in fuel streams from state-of-the-art hydrogen supply chains and dispensing equipment.
- This project suffers from competing technical interests—MEA characterization for speculative loading targets and gas quality analysis and analyzer development. The project should have identified this growing distraction and suggested steps to address it. If this issue is not addressed, this project will likely under-deliver on both technical areas, thus missing the potential impact of a more focused project. In short, the technical aspirations of the project are spread too broadly for the available resources for the project and the overall scope of the funding available to the FCT Office.

#### **Recommendations for additions/deletions to project scope:**

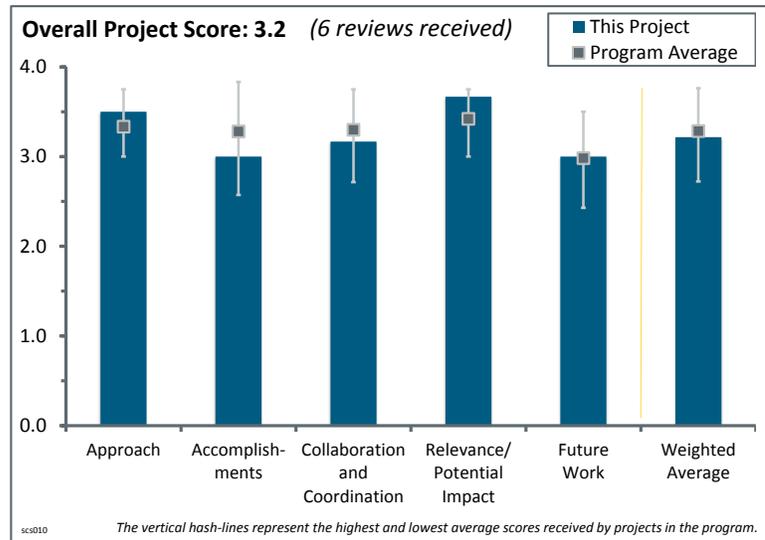
- The project team should put ASTM standards through ILS to train laboratories and share its expertise.
- The project team should investigate the cost effectiveness of the in-line analyzer. The work needs to be on track to develop a low-cost, effective device. An industrial partner to accelerate the commercialization of the in-line analyzer needs to be found.
- The project team should focus on the tolerance of cells at various catalyst loadings to process impurities (not housekeeping impurities such as sulfur) and recovery techniques for all impurities that can be incorporated into the vehicle design. A previous DOE-supported contract was a quality control process improvement project (ION Power) that might include periodically supplying improved MEAs to the researchers.
- The project team should delete the project scope for MEA characterization at low platinum loading levels. This is the right technical group to perform this work but the wrong FCT program to fund this effort. This should be done under the Fuel Cells program, which would allow this work to better align with all of that program's efforts in low platinum targets. The researcher should add the development of a commercial in-line gas analyzer to the project scope to help target both the round-robin test method validation and the in-line gas analyzer efforts toward a "Specific, Measurable, Achievable, Relevant, and Timely" (SMART) project goal.

## Project # SCS-010: R&D for Safety Codes and Standards: SCS Project Overview – Hydrogen Behavior

Aaron Harris; Sandia National Laboratories

### Brief Summary of Project:

The objectives of this project are to conduct experiments to understand dominant release, ignition, and combustion phenomena for unintended hydrogen releases and to provide data for the development and revision of regulations, codes, and standards (RCS), as well as best practices. The research will support consequence analysis in the “risk informed” approach, model release dynamics from relevant leak scenarios, determine ignition and flame-up probabilities, and quantify thermal radiation and overpressure hazards. The research will address the lack of safety data and technical information relevant to the development of codes and standards (C&S) for hydrogen delivery.



### Question 1: Approach to performing the work

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

- This project features a good approach.
- This science-based approach is quite relevant for the development and revision of hydrogen safety C&S. There is no doubt that the conducted experiments (e.g., noncircular openings) and the project’s inputs into the integrated quantitative risk assessment (QRA) toolkit (via the consequence module) address critical barriers.
- The research being done on characterizing gas dispersion is important to supporting the development of C&S requirements. The “science” has been missing for quite some time in this area and different propagation and mitigation methods need to be modeled and validated in order to understand what could happen once the systems are installed. This work will also support first responders and repair and maintenance technicians in understanding how they approach leaks.
- The approach is comprehensive, scientific, and clearly targeted to inform RCS that govern hydrogen leakage, dispersion, and ignition under comprehensive use conditions. Continuing support for the integrated QRA algorithm will continue to increase confidence in accurate predictions of the consequences (and causes) of hydrogen release.
- The project fits into a well-defined overall concept (namely an integrated QRA algorithm) that aims to address and quantify the effects of unintended hydrogen releases in general. The oral presentation mentioned that the special consideration of separation distances is but one of the applications of the approach; however, the information contained in the slide presentation seems to unduly emphasize this particular application.
- Hydrogen behavior, particularly with hydrogen releases, has been identified by industry, both nationally and internationally, as an important aspect to ensure safety in design and installation. This project leveraged data and used it to improve data sets and the accuracy of QRA. It will be clearer how this work addresses critical barriers when it is complete and can be implemented by stakeholders.

## Question 2: Accomplishments and progress toward overall project and U.S. Department of Energy (DOE) goals

This project was rated **3.0** for its accomplishments and progress.

- Good progress has been shown.
- This project is still in the discovery phase of understanding and characterizing different leak modes and their effects and ignition distances. Further research to develop a base understanding of how hydrogen behaves is important. Good progress has been made to date.
- This project meets the Safety, Codes and Standards (SCS) program goal of performing high-priority research and development (R&D) that benefits C&S data needs. Data goals seem to be progressing well. A concern for this project is that in order to support consistent RCS, much more outreach is required in the form of publications and presentations to stakeholders, both nationally and internationally. This is needed to inform stakeholders about the work and to solicit feedback that helps identify any potential inconsistencies with outside research and shape future work.
- The broad scope of hydrogen behavior as it relates to the different industry partners—including component, cylinder, and automotive manufacturers; fuel suppliers; stations; local authorities having jurisdiction (AHJs); standards development organizations (SDOs); and end users—breaks this project down into several areas. The project is a long one, spanning 13 years. Every year there are additional technical accomplishments in various areas, with various collaborators, that are pulled together through harmonization efforts. Accomplishments are on target for data-driven C&S in all of these areas (with regard to large hydrogen releases).
- The integration of the consequence analysis module into the QRA algorithm represents excellent progress. Good progress has been made with regard to data collection and the development of the different modules (overpressure module and radiative heat transfer model). However, it is difficult from the presentation to really assess the level of progress on these modules and the associated gaps. Also, no slides were presented that highlighted the current progress made in terms of impacts to RCS and harmonization. Good results have been obtained from ignition probability experiments, but they were not addressed during the presentation. These accomplishments should have been incorporated in the main presentation rather than in technical back-up slides. The future integration of the results stemming from the noncircular opening experiments into the QRA toolkit could have been discussed in more detail. Fast-fill experiments and modeling activities were conducted in fiscal year (FY) 2012. It is unclear if this research work stopped in FY 2013.
- The work definitely addresses DOE Fuel Cell Technologies Office and SCS program goals. However, it is unclear from the presentation whether and to what extent the items for future work that were identified in the 2012 DOE Hydrogen and Fuel Cells Program Annual Merit Review have been addressed, and what progress has been achieved with respect to those items. This comment applies both to the R&D and the input that the project has provided to SDOs.

## Question 3: Collaboration and coordination with other institutions

This project was rated **3.2** for its collaboration and coordination.

- The collaboration with other national and international institutions is outstanding.
- The project has very good collaboration with international private and public partners that have great experience in hydrogen behavior experiments and modeling. However, the slide on collaborations only provides a list of names; additional information could have been provided about the type of collaboration and how this benefits the project.
- The project features good industry support; it needs to include SDOs and the Fuel Cell and Hydrogen Energy Association in the mix to understand how this can support the research done by manufacturers. SDOs can act as the buffer between the specific needs of the integrators in driving research that will meet their needs. Organizations such as the Compressed Gas Association (CGA) and CSA Group should specifically be included in these discussions because they are the SDOs that represent the industry's voice. There is apprehension with the station integrators in regard to operating outside of the published code

requirements. There is general agreement that the code requirements are very conservative due to the risk of litigation in the event of a catastrophic failure.

- The collaboration with the relevant groups is good; however, it is unclear what level of involvement the partners listed on the Overview slide actually have. It is not clear if there are defined roles for these partners or whether they are simply groups that have been identified as stakeholders with whom formal or informal channels of communication have been established. It is not clear how the collaboration with the International Energy Agency (IEA) Hydrogen Implementing Agreement (HIA) Task 31 impacts RCS. A sentence or two on this would be useful. One or more papers published on the subject would help connect a few dots. It is important to distinguish between IEA Task 31 and IEA-HIA Task 31. More discussion on how the collaboration efforts further the aims of the project may be beneficial.
- Though much U.S. collaboration has been shown, the collaboration with the newly formed International Organization for Standardization (ISO) TC 197 hydrogen technologies working group needs to take place. There is a major rift between the setback distances in Japan, the United States, and Europe. QRA is not widely accepted, and before the project concludes it must not only investigate the National Fire Protection Association approach, but also the approach used in other European countries and in Japan.

#### **Question 4: Relevance/potential impact on advancing progress toward DOE research, development, and demonstration (RD&D) goals**

This project was rated **3.7** for its relevance/potential impact.

- The project addresses a critical step in an overall approach for acceptance of hydrogen fuel cell technologies.
- This project meets the DOE objective of performing high-priority R&D. It also helps to develop science-based requirements for RCS.
- The research and collaboration here are very relevant to the goal of safe deployment of hydrogen vehicles and infrastructure. More research is needed to address the safety of cryogenic hydrogen.
- This project addresses technical gaps that are critical to DOE's objectives through experiments/modeling (and validation) of hydrogen release behavior that is crucial for the development and revision of C&S. Support to the QRA process development (project SCS-010) through the integration of reduced order models (consequence analysis) is of high relevance.
- Siting and supporting the AHJs is critical to the successful launch. This research will hopefully go directly into the codes to provide greater confidence for safe placement of on-site fuel storage. Further research on different plume dispersions as well as liquid fuel releases needs to be done to complement the work that has been done on compressed fuel. Separation distances have been and continue to be a big barrier to installing hydrogen stations in public access areas. Right now the separation distances are so large that the typical refueling station property is not suitable to provide the necessary room for storage and other forecourt equipment. Reducing setback distances will be important if hydrogen is to be placed in existing locations.

#### **Question 5: Proposed future work**

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

- The proposed future work aims to improve past technical accomplishments and the QRA toolkit, which offers support for international research collaboration and RCS harmonization.
- It is critical to expand the research to include other types of fuel releases and modes to further the knowledge base for station designers and ensure safe placement of fuel storage devices and piping. The plan is still quite open because the project is still in the learning phase. Once the base research is done, a more deliberate plan on how the research can be pragmatically applied to the codes and other outreach papers will be important. Also, it will be critical to develop more quantitative risk values that can feed into the QRA model.
- The proposed future work is consistent and will provide valuable inputs to the consequence analysis for QRA. However, given the complex nature of the project, the research gaps to be filled should be prioritized. Significant progress is necessary with regard to the radiative heat transfer and ignition probability models in support of the QRA toolkit. This was not stressed enough during the presentation.

- This was an OK proposal, but this QRA approach must be judged by more of the industry (perhaps also by members of the fueling community, such as oil companies and more hydrogen providers) than what is listed in this presentation.
- The project focuses on quantifying consequences of unintended releases on humans (in particular, health). It is definitely correct to emphasize this first. However, in the future, the effects on neighboring infrastructure, equipment, and installations should also be investigated.
- The effect of gas temperature is planned to validate QRA models, including the overpressure reduced order model. An investigation into sustained flame and efforts to produce accurate prediction of conditions that lead to jet light up will also be conducted. This project is presently planned to be completed in September 2015. It is not certain that the goals will all be realized by that time. Additional time for feedback loops and additional follow-on that may be identified may be warranted. Feeding the results into RCS activities that have multi-year development cycles will be a critical activity to meet the goal of impacting C&S.

#### **Project strengths:**

- This project is analytical and features good planning for model validation.
- This project's strengths include its scientific competence and thoroughness, both experimental and numerical.
- This project features in-depth research and experiments to validate data and models and to begin to fill in data gaps.
- The research collaboration, support for C&S development, and international harmonization efforts are all excellent.
- This project feeds directly into the output of the QRA model—this is a good attempt to provide quantitative risk values. The project team needs to run more scenarios.
- The project team has great experience in conducting experimental and modeling research activities on hydrogen release behavior throughout all stages. The researchers have also developed very good collaborations all over the world, which is a clear strength. The outcomes of their research are of great importance for both the industry and SDOs through the revision/creation of standards.

#### **Project weaknesses:**

- Researchers still face challenges regarding equating this work into the codes, which is a driver for this work. This research cannot be used as a basis for code development—it is a good understanding of the physics. The models will need to be tested and vetted.
- Not enough information about the work is easily accessible to the public. It would be good to see more frequent publication with focused topics to help a general audience understand the importance of the work and the impact of the research. It is unclear how some of the collaborations are working.
- The project team should conduct more work on cryogenic release.
- The project is relatively complex and ambitious. The researchers should make efforts to simplify/clarify the objectives and provide a comprehensive overview of the progress made so far and of future plans. For instance, no information was provided about the research activities on fast-filling that were presented last year.

#### **Recommendations for additions/deletions to project scope:**

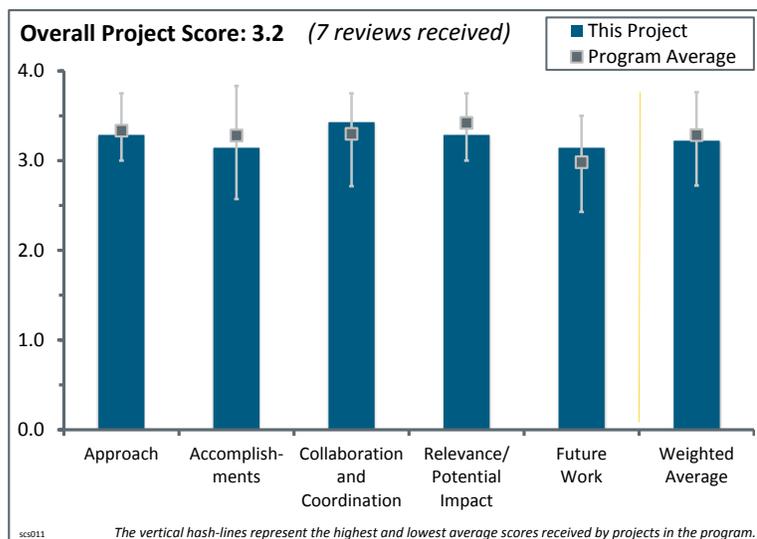
- Because of the conservative nature of the gas suppliers, gaining their direct support for this project will be difficult. Their direct input will be needed in order to make this successful. The project team needs to consider including underground storage in the fuel storage matrix.
- This project needs more frequent and widespread publication and outreach, as well as more time for following RCS activities through multi-year development cycles.
- There is a lack of international coordination, especially with ISO TC 197.

## Project # SCS-011: R&D for Safety Codes and Standards: SCS Project Overview – Risk

Aaron Harris; Sandia National Laboratories

### Brief Summary of Project:

The objectives of this project are to develop and demonstrate methodologies to support the use of quantitative risk assessment (QRA) as a tool for development and revision of regulations, codes, and standards (RCS), as well as safety best practices. The project will address the lack of safety data and technical information relevant to the development of codes and standards (C&S). A QRA toolkit will be developed through identification of risk drivers and their associated consequences. Engaging with stakeholders will build awareness of QRA and related activities to reduce risk.



### Question 1: Approach to performing the work

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

- The approach adopted in this project is robust and focused. The project has made major progress in communicating the usefulness of QRA to the hydrogen community.
- The project team used a pragmatic approach to pursuing the goals that were in alignment with U.S. Department of Energy (DOE) objectives. The approach was aligned with industry needs and kept industry involved throughout the process.
- The use of QRA as a tool is critical to assuring safety without relying on overly restrictive requirements. This project includes significant engagement with the relevant industry and regulatory stakeholders. The project also developed algorithms to facilitate tools for enabling access to the data. It is good that the data algorithms are being developed by the same organization that developed the QRA model. This increases confidence that any resulting tools will represent the data accurately. Development of the algorithms also appears to have facilitated refinement of the risk model.
- The approach has been integrated with other efforts, specifically the hydrogen behavior program, to apply risk assessment techniques for use in the development of C&S and best safety practices. Engaging stakeholders to use the QRA to inform RCS aids harmonization and increases confidence in safety metrics.
- The approach is very good. Although somewhat complex, this integrated QRA process combines all processes into a single code. The consequence module will be regularly improved thanks to research and development efforts from the hydrogen behavior task (project SCS-010), which is a very good point.
- As outlined, the overall approach—as well as its breakdown into a number of consecutive steps—is targeted at establishing a validated QRA toolkit. The availability of such a toolkit constitutes an important element for customer and public acceptance of hydrogen technologies. The work presents a logical structure, approach, and involvement of relevant stakeholders. It contributes to filling necessary knowledge gaps. Once the tool is available, measures should be put in place to ensure that the strength of the tool cannot be “abused” by non-specialists using it in an incorrect way.

## Question 2: Accomplishments and progress toward overall project and U.S. Department of Energy (DOE) goals

This project was rated **3.1** for its accomplishments and progress.

- The project team quantified an approach to risk that outlines risk assessment in the environment that is within this application. The QRA model was actually represented.
- Progress is noteworthy in terms of reaching DOE goals for increasing access to and the availability of safety-related information and data, as is the project's contribution to the development of C&S. Use of the fatal accident rate (FAR) metric conveniently allows risk comparison with other industries. The project is successfully creating a toolkit to provide robust and reasonably accurate results to the user.
- This year, the researchers have developed a QRA toolkit to provide results for specific scenarios that should be addressed in RCS. They have applied the QRA toolkit to the indoor fueling scenario, have improved the previous QRA process by including the FAR metric for comparisons to other industries, and are developing a hazard to harm module.
- It is acknowledged that this work is not the end product; however, the work is required to develop the tools that put the data within easy reach of users. This work is unique and will enable the data developed over the past few years to be used in QRA toolkits. Future work for acquiring user feedback and improving the toolkit is an important step in getting the data in an easy-to-use form into the hands of users. This will facilitate installations.
- The project has demonstrated good accomplishments. In addition to the creation of the integrated QRA algorithm, significant progress has been made through the estimation of the FAR for comparisons to similar industries, and the integration/developments of modules. However, the predicted FAR value is obviously subject to many uncertainties that could have been mentioned during the presentation. Although partly covered in SCS-010, it would have been interesting to see the progress made on the development of ignition probability models, which are critical for such analysis. Also, one slide could have been presented highlighting the main differences between QRA v.0 and QRA v.1 (and the upcoming versions).
- The project strongly contributes to the Safety, Codes and Standards (SCS) program goals. However, for the reviewers to be able to express a judgment on the achieved progress as well as on the efforts deployed in achieving it, the presentation contained insufficient detailed information on progress regarding the topics identified for further work in the 2012 DOE Hydrogen and Fuel Cells Program Annual Merit Review. It is suggested to include a traffic-light table on the identified topics of future work in the presentation. It is not clear how and to what extent frequency data provided by industry partners have been considered and used. Although the importance of having access to reliable “denominator numbers” was stressed in the oral discussion, no information has been provided on whether the provision of such data has been successful (i.e., whether it has proved fit-for-purpose) and sufficient.

## Question 3: Collaboration and coordination with other institutions

This project was rated **3.4** for its collaboration and coordination.

- This project features collaboration with national and international stakeholders, standards development organizations, and government regulators.
- This project shows very good collaborations and is connected to many industry and research partners. Support and feedback from the industry will be essential for the development of the QRA toolkit.
- The outreach activities of the project and the input of feedback from stakeholders appear to be an effective way to further develop and improve the QRA toolkit. Activities such as the International Energy Agency workshop provide tangible means to evaluate whether the research coordinates with industry and other stakeholders needs.
- The principal investigator continues to seek out collaborators to further develop his model. He should collaborate with the natural gas vehicle (NGV) industry and compressed natural gas (CNG) utilities because they have real application data for this type of environment—this can be the basis for qualifying similar models for hydrogen where the data set is limited.
- This step—collaboration and coordination with other institutions—will become more important with the next stage. The QRA toolkits will be limited by the data sets available to the users. The principal

investigator suggested that this is a limitation that the researchers would like to continue to address. This is good, and it will be nice to see healthy discussions of relevant stakeholders to minimize limitations and increase take-up of the tools.

- Collaboration covers the correct range of stakeholders, both for guiding the issues to be addressed and for disseminating information to SCS committees. It is strongly recommended to have the tool “vetted” by other experts who are not involved in the current project.

#### **Question 4: Relevance/potential impact on advancing progress toward DOE research, development, and demonstration (RD&D) goals**

This project was rated **3.3** for its relevance/potential impact.

- This project provides feedback for revision to codes task groups on specific hazardous scenarios.
- The project addresses a critical step in an overall approach for the acceptance of hydrogen fuel cell technologies.
- There is a need to develop a quantifiable risk-based approach. This is a novel way of presenting the data to outline the true risk associated with the applications.
- This is important work in a highly specialized area. It is a multi-year effort and needs to continue in order to realize its ability to support progress toward SCS program goals.
- The development of this integrated QRA tool is quite relevant to support the development/revision of hydrogen safety C&S. Although it is in its early stage, the QRA toolkit is introducing science into the risk assessment process and will constantly benefit from research efforts of the hydrogen behavior project SCS-010 (consequence models). This project fully supports DOE RD&D objectives.
- The relevance of this work to the development of specific standards is alluded to in slide 12, but it is not explicitly described in the presentation in terms of the degree of Sandia National Laboratories’ contribution and the work performed.

#### **Question 5: Proposed future work**

This project was rated **3.1** for its proposed future work.

- The proposed way forward is logical and builds on previous achievements.
- This is important work in a highly specialized area. Future work to engage stakeholders, as defined by the principal investigator, is necessary to prove the ability of this project to support progress toward the Program’s goals. Future work needs to engage industry to help guide the direction for improvement.
- Continued improvement of the toolkit is important, but it would be interesting to investigate how the scope of the toolkit could be broadened.
- The proposed future work addresses critical barriers and is planned in a logical manner. Alongside incremental improvements of the different modules, key points refer to the integration of a sensitivity analysis and the access to data. However, it would have been interesting to see a prioritized list of research efforts for the different modules. Also, improving ignition probability models was already a point to be addressed for fiscal year (FY) 2013 (as outlined in the 2012 presentation). It is unclear what the progress has been in FY 2013.
- Future work focuses on integrating the overpressure model, improving ignition probability models, facilitating industry adoption of the QRA database/toolkit, and gaining user feedback. When that starts to occur, expect the value of the QRA to be easier to quantify.
- There are inherent challenges to the direction of the project because the assumptions that are critical to the QRA project need to be mitigated and adapted. There is a significant challenge due to the immaturity of the application. Trying to understand when the algorithm is truly reflective of the actual risk will be a challenge, given the sparse and unrefined data set. It is recommended that researchers try QRA on other fuels, such as propane and CNG, because a more mature application may provide more data to develop and validate the assumption set. Experimental and empirical data will need to be developed to truly test some of the more critical assumptions. The project team may want to consider some kind of affinity or sensitivity analysis to understand what factors have the greatest impact on the models.

**Project strengths:**

- The ability to compare risk with other industries (through the FAR metric) is a major improvement.
- The project is based on best practice approaches at refiners and nuclear reactors. These applications are well defined and risks can be mitigated early on with controlled access of trained operators and staff. The challenge is that the Hydrogen Refueling Station application is open to untrained laymen, and therefore a QRA for this application needs to be very carefully vetted if it were to be adapted into practice by industry.
- This project is highly specialized. It is critical for enabling siting of hydrogen projects—particularly refueling stations in real-world spaces.
- The project has very good technical capabilities and benefits from science-based inputs from SCS-010, which is clearly a strength. The researchers also have very good collaborations, which is another strength.
- This project's strengths include its scientific competence and thoroughness and its relevant and timely involvement of stakeholders. There is a possibility of parameter screening for assessing the impact on resulting risk numbers and using the results to feed back into an improved design.
- Two reviewers did not respond to this question.

**Project weaknesses:**

- Most of the critical assumptions are based on limited data: this therefore challenges the validity of the result. The approach is good, but quantification of the “numerator” and “denominator” of the risk still needs improvement.
- This is in the early but critical stage of the work—the project team needs to engage stakeholders in the next phase.
- It is unclear what other scenarios will be modeled in future versions besides indoor refueling.
- There are no apparent weaknesses at present. In the future, a potential weakness may be the inappropriate use of the QRA toolkit by non-experts.
- There are questions about how misuse of the toolkit will be prevented, whether there could be liability issues, and whether access to the toolkit will be controlled or will users have to be “trained” in order to ensure that the tool is used and the output interpreted correctly.
- The relative complexity of this QRA toolkit could be considered a weakness, especially if the tool is to be manipulated by end users. It is a very ambitious project that is still in its early development phase. Although it is on the right track, there is a long way ahead before it can provide tangible results that can be used for revising/creating standards. Collaborations with industry partners are essential in this respect.

**Recommendations for additions/deletions to project scope:**

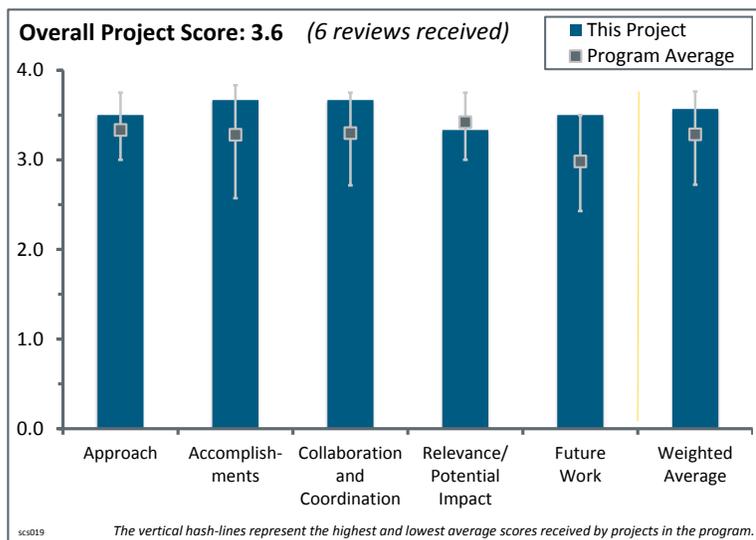
- This project should be continued, with stakeholder input to be used to shape future work.
- It would be interesting if the toolkit could be applied, not only for FAR but also for the risk to equipment or processes.
- Component standards for critical components related to the risk (e.g., leaks) need to be considered as a method to better quantify and drive the behaviors of industry. Insurance companies would directly benefit from this approach.
- This effort should be compared with HySafe in the European Union.
- There are no specific recommendations, but given the time frame (i.e., 2015), the project should try to better plan future research work in order to be more efficient.

## Project # SCS-019: Hydrogen Safety Panel and Hydrogen Safety Knowledge Tools

Nick Barilo; Pacific Northwest National Laboratory

### Brief Summary of Project:

The objective of this project is to provide expertise and recommendations for identifying and integrating safety planning and best practices into funded projects to ensure that all projects address and incorporate hydrogen and related safety practices. Collecting information and sharing lessons learned from hydrogen incidents and near-misses will help prevent similar safety events from occurring in the future. A vast and growing knowledge base of hydrogen experience will be captured and made publicly available to the hydrogen community and stakeholders.



### Question 1: Approach to performing the work

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

- The approach is clear.
- The three-pronged approach is rational.
- Industry practices are critical and need to be maintained, managed, and broadcast to the public.
- This work on the Hydrogen Safety Panel (the Panel) is very important, and the approach is spot on. Indeed, the principal investigator embraced the suggestions of the reviewers in previous reviews. The field app is a direct result of previous reviews—this is excellent.
- The Panel is continuing to thrive under the management of Nick Barilo. Pacific Northwest National Laboratory (PNNL) demonstrated an exemplary leadership transition process. The Panel’s focus on participation early in the projects (e.g., kick-off meeting participation) is valuable. The Panel is clearly adding value to safety planning and finding ways to help projects be successful.
- This project has done a good job at identifying issues; working toward solutions with industry; and, when necessary, getting the information into the hands of the standards development organizations (SDOs) that need the information to revise the standards. With the future focus of understanding “third party certifications,” it seems appropriate that the Panel should include representatives from this industry/area. Third-party certifiers are well versed in laboratory testing and field evaluations. This could provide additional insight for addressing situations with “existing equipment/installations” as well as moving forward. Allowing the system to work—“standards-> codes-> third-party certification”—supports the work of authorities having jurisdiction (AHJs) and will serve to expedite the process.

### Question 2: Accomplishments and progress toward overall project and U.S. Department of Energy (DOE) goals

This project was rated **3.7** for its accomplishments and progress.

- The progress to date is suitable and appropriate.
- It appears that this project has been quite successful in gaining AHJ approval and implementing best practices. Safety should continue to be the number one priority. It was good to see the metrics for site visits on slide 8.

- The Panel is an excellent resource for the Safety, Codes and Standards program. The review of hydrogen projects is critically important and the work load is not insignificant. The statistics on reviews, actions, etc., speak for themselves. Particularly impressive was the “self improvement” exercise by the Panel entitled “...What have we learned about our review process.”
- The project has made significant progress each year and is providing tools to industry for the deployment that is happening in the “precommercialization” phases. The next step of evaluating how third-party certification impacts the role/job of the AHJ is a much-needed step for commercialization. Other industries have demonstrated that the system works—“standards-> codes-> third-party certification”—this supports the AHJs, expedites the process, and increases consumer safety in a large-scale manner.
- The effort in Hawaii provides a good example of how the Panel has added value to the DOE Hydrogen and Fuel Cells Program by staying at the forefront of technology research, development, and demonstration (RD&D). It is also able to perceive gaps in safety understanding that are then fed back into the research and development (R&D) program. The mobile application for the safety knowledge tools is forward thinking and innovative. A plan should be drafted to ensure sustained upkeep and maintenance of this software tool. There should be a partnership with an entity that is well positioned to push the product forward in the years to come.
- The project team needs to accelerate the work from the Panel that is related to defining the certification requirements for industry. This will be critical for AHJ support. The app for project planners and AHJs is a very useful tool to support the best practices and the review of locations and construction.

### Question 3: Collaboration and coordination with other institutions

This project was rated **3.7** for its collaboration and coordination.

- The Panel, as shown on slide 4, appears to be a solid mix of laboratories and industry, which is critical.
- This project has demonstrated superb coordination with stakeholders that is enhanced by demonstrated integrity and technical excellence.
- PNNL is tied very closely to the leading organizations who are working to move hydrogen to a commercial solution.
- The collaboration and coordination are appropriate. At this point, outreach to the various state and municipal fire and building authorities may be appropriate.
- The increased awareness and dissemination of information to the SDOs to address issues is excellent. Given the increased focus of the Panel and this activity to understand certification and the role it plays for society and AHJs, representation from third-party certifiers in the fuel cell and hydrogen area needs to be incorporated in the Panel’s discussions. Without that portion of industry representation, the Panel may be duplicating or performing a role that existing third-party certifiers are already equipped to handle.
- It is a bit hard to accept the list of “collaborators” provided on slide 20 of the presentation (e.g., a Panel meeting at the Hawaii Natural Energy Institute hardly counts as a collaboration, and the National Fire Protection Association [NFPA] Conference and Expo is a conference, not a collaboration). However, the breadth of the Panel in-and-of-itself provides an outstanding span of collaboration.

### Question 4: Relevance/potential impact on advancing progress toward DOE research, development, and demonstration (RD&D) goals

This project was rated **3.3** for its relevance/potential impact.

- This activity has the potential to facilitate the introduction of hydrogen infrastructure.
- This activity is critically important and relevant to the safe performance of the Hydrogen and Fuel Cells Program. It is clear that the level of attention to safety and the impact this project has had on the overall safety culture is excellent. The outreach (publications, white papers, etc.) is excellent.
- This project is critical and enhances safety through knowledge development and information sharing. The Fuel Cell Technologies (FCT) Office needs to be more proactive in leveraging the Panel to encourage improved and consistent safety planning in its entire portfolio of programs.
- This has been one of the best ways to capture, catalog, and reference field incidents and reports of field failures. The direct support of SDOs and codes development organizations is critical to ensure that these

lessons learned can be captured in the regulations, codes, and standards. The proactive approach is also very important to ensure that future station construction is reflective of the best practices.

- There is some skepticism about usage of the mobile app.
- Education and outreach are critical to successful deployment of hydrogen and fuel cells. Assistance with the initial deployments/permitting of stations, etc., is a key component of this outreach. Incorporating the third-party certifiers in the process will help the Panel understand the capabilities of nationally recognized testing laboratories (NRTLs) and will also assist in educating the AHJs (if they are not aware). As industry moves forward, this activity will need to be picked up by the NRTLs—now is a good time to get all involved parties at the table to build awareness from all sides.

### Question 5: Proposed future work

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

- The proposed future work is good. The development of the mobile app is right on and moving it to Android devices is a necessary (and recognized) move. The only concern is that there needs to be attention given to establishing a mechanism to maintain the mobile app. This seems to be missing in the current and proposed scope of work.
- It appears that the safety plan review has been quite successful. Industry support of any input to NFPA 2 is critical.
- The proposed work is appropriate. A caution on the app is in order. The project team should define the audience and then address the app to the audience. If the intended user is an AHJ, the project team should write the information in the app for a fire marshal, not a PhD or a researcher. This is easier said than done.
- In general, the project is a good tool set for the industry stakeholders to make them aware of and to support the application of best practices in the field. PNNL has a pragmatic approach and understands its role as a communication content provider. The new and innovative methods to expand visibility of the database are important. Other innovative platforms are expected with anticipation.
- The FCT Office should be more proactive in encouraging Panel participation in all funded projects to help provide consistency in safety planning and engineering.
- With the increased focus of the Panel and this activity to understand certification and the role it plays for society and AHJs, representation from third-party certifiers in the fuel cell and hydrogen area needs to be incorporated into the Panel's discussions. Without that portion of industry representation, the Panel may be duplicating or performing a role that existing third-party certifiers are already equipped to handle. In addition, as industry moves forward, this activity will need to be picked up by the NRTLs—now is a good time to get all involved parties at the table to build awareness from all sides.

### Project strengths:

- This project's strengths are its focus and dedication.
- This project provides guidance and tools to increase awareness for industry as new technology is introduced. It is providing feedback to SDOs to support revisions to standards to address known safety risks.
- This Panel is performing very well and providing a critical service to this community. The construction of the mobile app demonstrates the willingness to grow beyond traditional roles—this is excellent.
- The Panel is providing a critical forum for sharing safety information, enhancing safety planning, and identifying safety R&D gaps. The information tools are a consistent resource for industry, laboratories, and universities because they provide valuable information.
- The Panel and its collaborators are strengths of this project. Keeping these Panel members is critical to the success of this initiative. This project should continue to be funded at its fiscal year 2012 levels so that the innovative ways of getting this out to industry are expanded.

### Project weaknesses:

- There is not enough funding.
- The project team needs to involve third-party certifiers (NRTLs) in the process.

- Weaknesses include the limited safety reviews and the need to determine the audience for the app.
- The FCT Office needs to be more proactive in leveraging the Panel for encouraging adequate safety planning in projects with DOE Office of Energy Efficiency and Renewable Energy investment. There is evidence that the link between the Panel and the projects has been not been as consistent as needed. The FCT Office needs to incentivize interaction with the Panel. A strategy needs to be developed for the continued development and maintenance of the safety knowledge tools. These are critical and it would be bad to see them get stale.

**Recommendations for additions/deletions to project scope:**

- The Panel should continue to seek out ways in which the enormous talent of its members can continue to be exploited on behalf of the hydrogen community. Keep it up!
- The project team needs to involve third-party certifiers (NRTLs) in the process and continue providing feedback to SDOs.
- The project team should increase the safety reviews and start outreach to the AHJs.
- The concept of providing safety knowledge tools on mobile platforms to increase value is innovative and critically important. It is a great idea to build on this initial effort to develop a comprehensive strategy around mobile platform application development—this has the potential for the highest impact in the field.

## Project # SCS-021: NREL Hydrogen Sensor Testing Laboratory

Bill Buttner; National Renewable Energy Laboratory

### Brief Summary of Project:

Sensors are a critical hydrogen safety element and will facilitate the safe implementation of hydrogen infrastructure. The objective of this project is to provide critical safeguards including an alarm at unsafe conditions, ventilation activation, and automatic shutdown to hydrogen delivery systems. Safety systems need to detect and mitigate circumstances such as a lack of hydrogen detection, a lack of combustible gas monitoring or training, or alarms that do not specify the danger detected.

### Question 1: Approach to performing the work

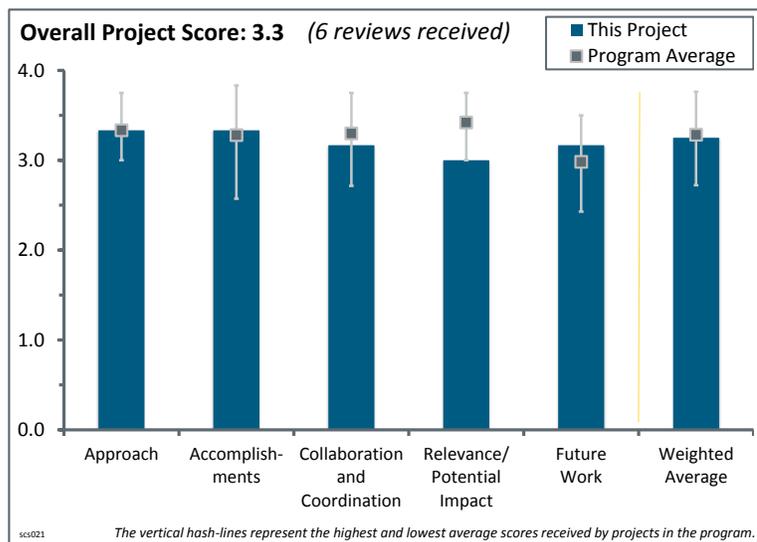
This project was rated **3.3** for its approach.

- This is a good project and the overall approach is very good.
- The project presentation mainly focuses only on a single fiscal year effort, and it is recognized that funding is determined annually. It seems, however, that the success of the project depends on multiyear support. It would be helpful to see the approach and planning in the context of the overall long-term goals as well as the annual goals for the work, and progress for both. This was addressed late in the presentation, under future work. Early discussion of the importance of the longer term goals would be beneficial.
- All of the barriers identified are important, especially barriers F, G, and H (from the *Fuel Cell Technologies Office Multi-Year Research, Development and Demonstration Plan*), which this project is targeting. The project team should keep focused on the ultimate goal of ensuring that end users get the sensing technology they need; for example, facility sensors (as highlighted in slide 5) versus vehicle sensors.
- The approach is sound. However, direct detection of leaks may not be appropriate in many applications. Currently, sensors are costly, require maintenance, and are often unsuitable for a number of applications. The results are often spurious alarms or no detection—both are issues. Sensors might become an issue and not a solution.
- The independent assessment and qualification method for the development of sensors is valuable. The workshop provides a forum for influencing the work that is performed. It is not clear if (a) the most critical end users are adequately involved and (b) the feedback from industry participants is actually influencing the project.
- The National Renewable Energy Laboratory's (NREL's) dual approach of providing independent sensor testing to developers, end users, and codes and standards developers together with gap identification is very good. One caveat, however, is that testing must be entirely independent of development. The project team should not be involved with sensor research and development (R&D).

### Question 2: Accomplishments and progress toward overall project and U.S. Department of Energy (DOE) goals

This project was rated **3.3** for its accomplishments and progress.

- All in all, the project has a very good path forward. The project team has achieved nice accomplishments to date and is realistic about the barriers and issues that still need work.



- This project features an excellent mix of accomplishments. The collaboration with the Joint Research Centre (JRC) seems especially valuable and produced some very interesting outcomes, including the lack of accuracy of sensors tested in the round-robin testing and the inappropriateness of oxygen displacement sensors for hydrogen measurements. Also significant was the gap analysis result that sensor maintenance is a large cost and that sensors need to be calibrated often (the researchers suggest no less often than semi-annually). In the past, some sensor manufacturers would claim that their sensors could be calibrated every couple of years.
- The ability to assess sensors with a vehicle crash test is nice. Whether there is a need to include a sensor on a vehicle is still open to debate.
- Supporting the Global Technical Regulation (GTR) was a critical accomplishment; however, there was no mention of the previous work by Sandia National Laboratories on hydrogen concentration in vehicles (a GTR-driven study). This is cause for concern; perhaps these researchers are operating a bit in the dark. The finding that one-third of the sensors tested did not even perform as well as the manufacturers' specification is incredible. This finding alone is critical.
- It is not clear that the work in support of the GTR resulted in quantifiable recommendations for the proposed requirements. NREL's sensors team needs to develop strategies for quantifying performance of deployed sensors. The Fuel Cells and Hydrogen Joint Undertaking (FCH-JU)-funded JRC collaboration resulted in consistent results in both laboratories showing value in the round-robin testing.
- It was not clear from the presentation how R&D on sensors directly contributes to DOE goals. There is a reference to the *Fuel Cell Technologies Office Multi-Year Research, Development, and Demonstration Plan*. The presentation could be more effective by going back to specific goals and demonstrating how the project contributes to achieving the goals. It was worthwhile for the presenter to clearly articulate the important role of this project in helping industry develop sensors that can meet existing and future standards. As sensors do not yet meet the existing standards, this project provides a cost-effective way to evaluate and improve developing sensor technologies.

### Question 3: Collaboration and coordination with other institutions

This project was rated **3.2** for its collaboration and coordination.

- This project features excellent collaboration with JRC.
- The collaboration with JRC is excellent.
- This project demonstrated outstanding coordination through the round-robin testing. The coordination with the FCH-JU-funded project provides a good template that the FCT Office (can leverage for other international efforts. Better domestic coordination could be achieved through leveraging the needs identified for sensors from Technology Validation or other FCT Office investments.
- The collaboration with JRC is commendable. The presentation included an excellent, clear description of this collaboration, showing clear benefits. The presentation could be improved by providing more details on the collaboration and coordination efforts with the other named partners and collaborations.
- The collaboration appears to be limited to other national and European Union laboratories. Outreach to major manufacturers (MSA, RKI Instruments, Detronics, etc.) is not mentioned.
- NREL talks about its collaboration with JRC and the U.S. Department of Transportation quite extensively, but it does not list them on its collaboration slide. It does list Element One and the Colorado School of Mines, among others, but includes no explanation about these collaborations.

### Question 4: Relevance/potential impact on advancing progress toward DOE research, development, and demonstration (RD&D) goals

This project was rated **3.0** for its relevance/potential impact.

- This project is very relevant for applications at hydrogen fueling infrastructure and repair facilities.
- There was a very good discussion of the relevance of sensor work. The discussion of NREL's approach implies that its work is relevant to the overall sensor need.
- The overall relevance of this work to the Safety, Codes and Standards program and the community is very good. Sensors are required by code, so the quantification of sensor performance and reliability and working

with the codes development organization/standards development organization community is also very important. The execution of a round-robin test was also very nice.

- The option for a robust sensor(s) is attractive and relevant. It is not clear whether a sensor is the best technical solution.
- This project does not address a critical need facing the deployment of hydrogen fuel cell systems. It is not clear what critical issues will be overcome if this project is 100% successful.
- It would be good to see the presentation more specifically discuss the existing standards relating to sensors—particularly those used for qualifying sensors to existing regulations, codes, and standards—particularly ISO 26142: 2010 Hydrogen Detection Apparatus - Stationary and UL 2075 - Gas and Vapor Detectors and Sensors, as well as progress in the development of sensors to meet existing standards. More discussion is needed on how the project helps to harmonize requirements for sensors. Sensors do not yet meet the existing standards, so this project provides a cost-effective way to evaluate and improve developing sensor technologies.

### Question 5: Proposed future work

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

- The proposed future work is rational and appropriate.
- The proposed future work is excellent. The future work discussion mentions plans to investigate wide-area monitoring. Wide-area monitoring will overcome the shortcomings of point-wise measurements.
- NREL presented a reasonable schedule for the next several years in the hydrogen sensor area. It is proposing to include wide-area sensing as part of the plan. It appears that much of NREL's future work will be based on it moving into the new Energy Systems Integration Facility (ESIF).
- This project needs to focus on independent testing and test methods development. It was stated that future work will be 50% new sensor development. Any new sensor technology development needs to be competitively selected and should be led by industry. EERE should not directly fund sensor development through a non-competitive process.
- It was very good to see the multi-year project plan in the presentation. Future guidance on sensor placement is a concern. While industry and other stakeholders are interested in guidance on hydrogen sensor placement, it is critical to avoid any misperceptions that sensors are the only way to achieve the desired levels of safety. Researchers delivering messages relating to sensor placement are advised to use caution to be clear that the guidance applies when sensors are chosen as a method for achieving the desired safety parameters. Performance-based standards for systems and equipment are careful to specify a required level of safety, but they do not specify the method to achieve it. Therefore, sensors can be considered one of many options for achieving the safety levels desired.
- It seems that the ESIF will be instrumental in future work, especially in assisting with field testing. It may be difficult (depending on the application) to do comparisons in the "field," so setting up real-world scenarios at the ESIF might prove very useful.

### Project strengths:

- This project's focus and dedication are its strengths.
- This project is very good, relevant, and well executed, and it features good teaming with international partners.
- This project provides an excellent example of effective collaborations with projects funded by the FCH-JU.
- This project provides an avenue for sensor developers to improve sensors and measure progress toward goals (DOE goals and those stated in published standards).
- This project is working to understand needs from industry.
- The collaboration with JRC is yielding some very good results. The ESIF will increase the team's capabilities. Gap analysis revealed the need for increased scrutiny on calibration.

### Project weaknesses:

- The concept that sensors are required is an area of weakness. However, that is a policy question.

- This project is at risk of appearing to develop and test sensors for the sake of developing and testing sensors rather than to address a critical need facing the deployment of hydrogen and fuel cell technologies.
- More information is needed on collaborations outside of JRC (as this collaboration was adequately described). More context is desired at the beginning of presentations, publications, and workshops to help put the role of sensors into context with other methods available to meet requirements to ensure safety.
- The collaboration with Element One and the Colorado School of Mines is unclear.

**Recommendations for additions/deletions to project scope:**

- The project team should ensure that there is continued focus on sensor calibration protocol.
- The project team should add a caveat “for applications requiring a sensor.”
- This project needs to stay clear of sensor development. The FCTO needs to rely on a competitive process for any sensor development activities.
- The project should include messaging to avoid confusion about the role of sensors to achieve safety levels defined in codes and standards.
- The project should investigate (or reinvestigate) the use of wide-area detection. Also, contact sensing technologies (color change, etc.) should be investigated. The potential for such technologies in many applications could prove to be very valuable (more so than point measurement systems) in early detection of leaks from common sources such as valves, joints, welds, pipe fatigue cracks, etc.

## 2013 — Market Transformation Summary of Annual Merit Review of the Market Transformation Program

### Summary of Reviewer Comments on the Market Transformation Program:

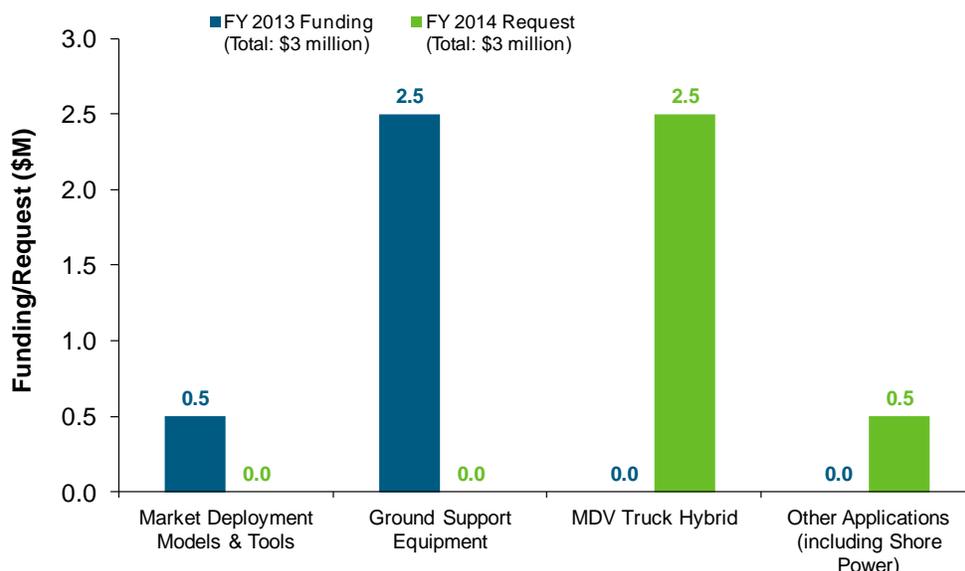
The purpose of the Market Transformation program is to spur market growth for domestically produced hydrogen and fuel cell systems. By supporting increased sales in key early markets, this program helps to identify and overcome non-technical barriers to commercial deployment and to reduce the life cycle costs of fuel cell power by helping to achieve economies of scale. The current focus of the Market Transformation program is to build on past successes in lift truck and emergency backup power applications (part of the U.S. Department of Energy’s [DOE’s] American Recovery and Reinvestment Act of 2009 [Recovery Act] efforts) by exploring the market viability of other potential and emerging applications. Six projects were reviewed this year, and these projects are highly leveraged, with more than half of the funds provided by DOE’s partners. This substantial commitment of external resources shows the high level of interest in exploring applications and markets where the hydrogen and fuel cell industry can expand and the technologies can play a valuable role.

Generally, reviewer comments on the program were positive, noting that activities were considered to be important to enabling the commercialization of hydrogen and fuel cells. Reviewers considered the program to be well managed and noted the extensive collaboration present in the projects and the substantial leveraging of federal funds by cost-sharing. However, a number of reviewers felt that the program lacks an overall cohesive market transformation strategy and that the current projects do not seem to be part of an integrated plan.

### Market Transformation Funding:

With the market successes that have been achieved by fuel cells in lift trucks and backup power applications as a result of fiscal year (FY) 2009 and Recovery Act funding, the focus of FY 2013 funds was on a new application: airport ground support and specialty vehicles. As shown in the chart below, other applications (including shore power) will be a new focus that will achieve leverage by partnering with other federal agencies and stakeholders to deploy fuel cell systems in their operations. Another focus will be battery/fuel cell medium-duty hybrid trucks (MDV) that will demonstrate a value proposition for parcel delivery fleets. Although not reflected in the FY 2013 budget, DOE invested \$42 million under the Recovery Act to enable the deployment of more than 1,000 fuel cells for early market applications such as forklifts and backup power. The Market Transformation program budget for FY 2013 was \$3 million.

**Market Transformation R&D Funding**



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### Majority of Reviewer Comments and Recommendations:

The Market Transformation program's projects were rated average to high, and overall ratings ranged from 2.8 to 3.6, with an average score of 3.2. The projects were judged to be relevant to the DOE Hydrogen and Fuel Cells Program's activities, with good or adequate technical approaches used. Reviewers recommended that future data collected and analyzed from all deployment activities be used to develop business case reports that can be used to support further market expansion.

**Stationary Applications (Micro Combined Heat and Power):** One project was reviewed, with an overall score of 3.6. Reviewers commented that this project was clearly relevant and could help build significant market share for hydrogen and fuel cells in the near term. They also observed that this project was well designed for collecting and analyzing data. However, reviewers expressed concern that too much effort is being spent on modeling and more attention is needed on understanding the results of the fuel cells in the real world.

**Airport Ground Support Vehicles:** One project was reviewed, with an overall score of 3.2. Comments were supportive of the project's approach in that it was modeled after successful lift truck or material handling equipment (MHE) deployment projects. More than one reviewer was concerned that the schedule was very aggressive but also noted that concrete go/no-go decision milestones will minimize risks. One commenter stated that the market size may be too small and that other applications should be brought in. It was stated that, if this project is successful, the associated hydrogen infrastructure is expected to be the model for other airports to begin similar projects, which is needed to help commercialize fuel cell road vehicles. Expansive team and stakeholder involvement was positively noted. Also noted was that the project aligns well with the Market Transformation program objectives.

**Direct Methanol Fuel Cell Material Handling Equipment:** This project, which was focused on deploying and testing fuel-cell-powered MHE and compiling operational data for validation, received an overall score of 3.2. Reviewers noted the value of exploring technologies that offer effective alternatives to hydrogen fuel cells, particularly the usefulness in developing a business case and making technology improvements. Reviewers also commented on the significant operating data and experience being obtained from the 75 units deployed (as of June 2011). While some issues have been identified, illustrative data from "good" and "failed" stacks were reported and issues have been corrected. One reviewer recommended maintaining more information on costs, life, and customer experiences, and reporting more information on the details of the fuel cells.

**Landfill Gas-to-Hydrogen:** This project achieved an overall score of 2.8 for its efforts to validate the business case and technical feasibility of using landfill gas (LFG) for hydrogen production and sharing lessons learned that may be applicable for other candidate waste streams. Reviewers recognized that the project is well focused on market transformation for fuel cell technology instead of proving the science of LFG-to-hydrogen. The project team was also commended by reviewers for showing foresight and flexibility to adapt to changes beyond the control of the project team.

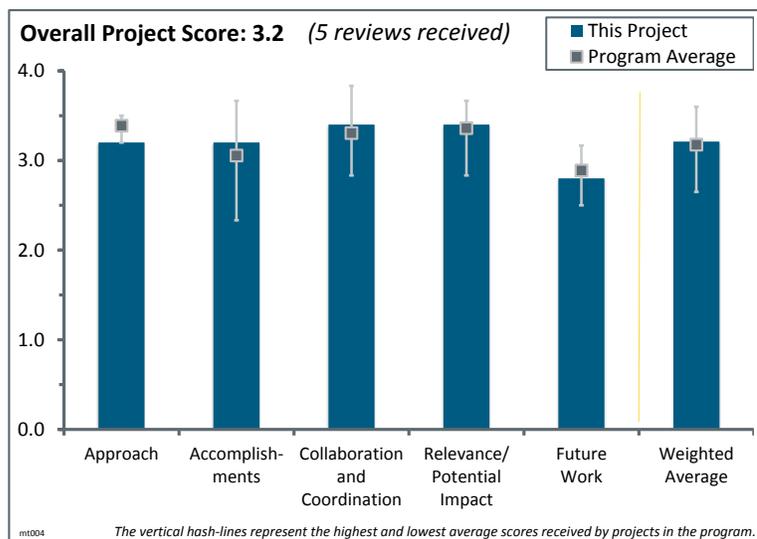
**Hydrogen Energy Systems as a Grid Management Tool:** This project received an overall score of 3.2 for its efforts in modeling, testing, and validating potential applications for hydrogen energy systems to address grid stability issues. One reviewer commented that this project has significant potential to demonstrate a solution for larger-scale applications. Reviewers also praised the Hawai'i Natural Energy Institute for leading a well-coordinated team effort alongside its partners and recognized the high degree of collaboration among federal, state, and private entities.

## Project # MT-004: Direct Methanol Fuel Cell Material Handling Equipment Deployment

Todd Ramsden; National Renewable Energy Laboratory

### Brief Summary of Project:

The National Renewable Energy Laboratory (NREL), in collaboration with Oorja Protonics, built and maintained direct methanol fuel cell (DMFC) Class III material handling equipment (MHE) systems for commercial food distribution warehouses. Oorja Protonics deployed and operated DMFC-powered MHE and methanol infrastructure and compiled operational and maintenance data. Performance of the infrastructure was validated by NREL under real-world conditions. An independent technology assessment evaluated the reliability and durability of the fuel cell systems, performance of the infrastructure, and overall value proposition. This project also provided support to the market for fuel cells in material handling applications by providing relevant results for key stakeholders.



### Question 1: Approach to performing the work

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

- The approach is sound. This is a pilot demonstration with limited imposed restraints. These real-world data should be useful.
- This is a well-designed experiment, but the failure of the initial 75 units had a significant impact on the project. There should, perhaps, have been some initial testing of a few units to shake out any issues before the decision to produce and purchase 75 was made.
- Fuel cell-powered MHE is being evaluated in this project. The battery is recharged by an onboard DMFC. NREL is collecting the data on its operations.
- The project approach was sound given the constraints that existed. It would have been preferable to have multiple DMFC vendors, but that may have been constrained by the market or resources. The use of the NREL Hydrogen Secure Data Center (HSDC) is well understood and prevents duplication of already existing analysis capabilities; it also potentially leverages data across platforms, uses, and technologies. This allows for some comparative analysis (for example, hydrogen-powered MHE versus DMFC-powered MHE versus battery-powered MHE). It is not clear what the non-technical barriers were and how they were addressed. This hopefully will be contained in the final report.
- The approach is focused on data collection and not on implementation barriers in the real world. There is very little discussion of the value proposition and the advantages over incumbent technologies. It is unclear if there will be enough data and lessons learned in the end to develop a recommendation on next steps. Additionally, the project focuses on one manufacturer, whereas multiple DMFC products would possibly present additional challenges not considered or presented. Overall, improvements to the effort and approach might be possible by focusing on the value proposition in addition to data collection.

## Question 2: Accomplishments and progress toward overall project and U.S. Department of Energy (DOE) goals

This project was rated **3.2** for its accomplishments and progress.

- The accomplishments are interesting. The references to safety issues are important.
- Valuable information has been collected showing the hours operated, the power generated, and degradation data. The fuel cell system did not perform that well with a high degradation rate. The data collected are valuable, although more data on performance and cost should be sought. The data suggest that more stack development work is needed.
- Despite the failure of 75 units and the lack of sufficient data to do value analyses, the project showed the possible utility of a methanol fuel cell as an onboard battery charger with easy refueling.
- It is hard to adequately evaluate given current data status. This was only rated as fair because it seems to have missed several project goals for performance (units not operational, operating hours not achieved, MW/hr generated, fuel cell degradation, etc.).
- One key barrier will be the cost compared to incumbent technologies, which is the key to analyzing the value proposition. Insufficient data have been cited in providing this analysis. Technical barriers are addressed, but without cost and value data, this project is lacking overall value in terms of moving forward with a business case for commercialization of this technology.

## Question 3: Collaboration and coordination with other institutions

This project was rated **3.4** for its collaboration and coordination.

- This project has good collaboration between the sites, the MHE provider, and NREL.
- While it would have been valuable to integrate multiple DMFC manufacturers into this project, the team did an outstanding job leveraging their partners. Getting multiple sites and 131 units deployed is impressive.
- This project should verify good cooperation between Oorja and the “grocery” sites. This project needs better cooperation and data exchange between Oorja and NREL.
- The collaboration should have included one other reference, the local authority having jurisdiction (AHJ). The AHJs speak with each other. If the AHJ is included in the project, it makes the next project easier to site because the AHJ of the new project can chat with the AHJ of the previous project. This word of mouth ends up being an endorsement and eases the next AHJ’s reluctance to allow a project.
- This project is limited with only one manufacturer. That may be a feature of the current development base, or resource constrained, but it makes data sharing more difficult. The collaboration with users was good, and multiple users and sites helped this. For market transformation, the reviewer is hopeful that the actual forklift manufacturers start pushing out these types of options for consideration or become primes in the demonstrations.

## Question 4: Relevance/potential impact on advancing progress toward DOE research, development, and demonstration (RD&D) goals

This project was rated **3.4** for its relevance/potential impact.

- The relevance/impact is as should be expected.
- The use of methanol in a real-life application is excellent; it eliminates all the perceived issues with hydrogen.
- One of the goals of the Fuel Cell Technologies Office’s Market Transformation program is to conduct deployment projects “to enable life cycle cost and performance of fuel cell power lift trucks.” This project enabled the deployment and subsequent collection of data on 131 follow-on commercial deployments. Data collected should inform the life cycle cost and performance of fuel cell-powered lift trucks.
- Using a liquid fuel, instead of hydrogen, can significantly reduce the refueling infrastructure cost. Methanol has a low well-to-wheels efficiency. There is also a concern about methanol spills getting into the groundwater. Charging the batteries with a fuel cell is beneficial in that it increases the productivity of the

equipment. It is expected that the study will help with analysis of the suitability of this configuration with both a battery and a fuel cell contributing to the capital cost. An analysis of life cycle cost to compare against other configurations is also needed.

### Question 5: Proposed future work

This project was rated **2.8** for its proposed future work.

- The proposed analysis of the data should be completed.
- The proposed plan, given sufficient funding, is absolutely the right approach.
- A post-project debrief should be considered in which lessons learned are discussed and then amended to this report. The lessons learned may facilitate similar projects.
- The project is about to end, and the team identified issues stemming from a lack of data; no clear resolution was discussed to address this.
- Future steps all seem focused on just closing out a report and study on this project. The current lack of data (four months after project completion) makes this risky to some degree and suspect. There was no discussion about how the results/learnings/findings might roll into future improvement and development efforts, and Oorja was not present to discuss and elaborate.

### Project strengths:

- This project is a great real-world application of fuel cells with a commercial fuel.
- Project strengths include focus and attention to detail in generating, collecting, and reducing the field data.
- Project strengths include project management and data collection, as well as collaboration between host sites and manufacturers.
- Data are being generated on DMFC system performance and durability. It allows exploration of another type of fuel cell in the MHE application. This is very valuable.
- This is a straightforward plan and demonstration to look at DMFC in an operational environment. It is very much built on the template from other MHE deployments. This provides some comparability among technologies.

### Project weaknesses:

- This project needs better understanding of reasons for performance degradation and better access to performance data.
- Currently, the lack of data and inability to hit several of the performance objectives make it very hard to establish the value proposition at this stage.
- The Market Transformation project ultimately must prove commercial viability of the technology. This project does not fully demonstrate whether this will be competitive in the marketplace. The value proposition is key, and not much attention was paid to that analysis.
- This project needs additional data and information. For example, it is unclear what requirements and costs were associated with meeting the environmental safety and health standards, especially for methanol, which is toxic, absorbable through the skin, and water soluble. It is unclear what methods are in place to prevent operators' breathing in methanol vapor, or what the stack efficiencies were at the beginning and end of its life.
- As part of the safety input, while this is prototype hardware and would not have product listings, the hardware should have been designed to the applicable standards, such as UL 2267 "Fuel Cell Power Systems for Installation in Industrial Electric Trucks." The same holds true for the dispenser. It would also have been nice to note that CH<sub>3</sub>OH is a heavier-than-air fuel that has the fire properties listed in NFPA 496. In future demonstration projects, this project should include the local AHJ in the activity early and include the AHJ as a collaborator. It will help with getting adoption of additional projects by the local AHJ.

**Recommendations for additions/deletions to project scope:**

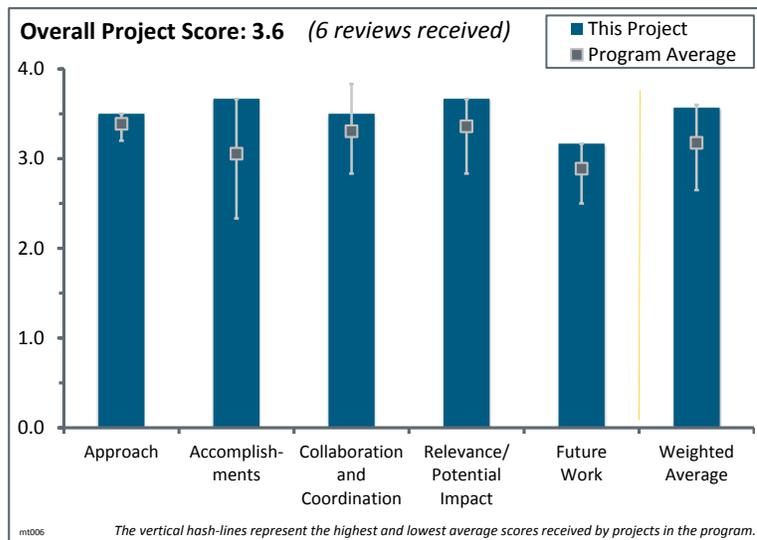
- This project should provide a business case for deployment by the industry, independent of DOE.
- The life cycle cost analysis is essential and preferably should be compared with other configurations, fuels, fuel cell types, etc.
- This project should place better attention on the quality of the methanol. Safety work is not necessary until the cell performance degradation issue is solved.
- A post-project debrief should be considered in which lessons learned are discussed and then amended to this report. The lessons learned may facilitate similar projects.
- The final study/report should highlight the areas and specific improvements/corrections that must be made for this technology in this type of operating environment.

## Project # MT-006: Fuel Cell Combined Heat and Power Commercial Demonstration

Kriston Brooks; Pacific Northwest National Laboratory

### Brief Summary of Project:

The objectives of this project are to demonstrate combined heat and power (CHP) fuel cell systems, objectively assess their performance, and analyze their market viability in commercial buildings. Fuel cells for CHP should demonstrate environmentally friendly technology, movement toward cost competitiveness with conventional technologies, reduced risk of electric grid disruptions and enhanced energy reliability, stability in the face of uncertain electricity prices, usefulness for applications such as base-load backup power or as a foundation for other renewable alternatives, reduction in the need for new transmission and distribution infrastructure, and enhancement of power grid security.



### Question 1: Approach to performing the work

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

- This project has done a great job identifying and directly addressing specific barriers and achievable goals. Feasibility has been proven through deployments and successful operations, and the project is well rounded by being rooted in deployment of commercial technology and focused on education.
- The project was started in fiscal year 2011 and is scheduled to conclude in 2015. The project approach was laid out very well, and progress is continuing as planned. It is a very good evaluation and demonstration, with units currently in the field producing electricity and results.
- Polybenzimidazole (PBI) fuel cell-based CHP units have been set up for demonstration and data collection at four commercial facilities. Data from these systems will be collected and analyzed to gauge performance, while familiarizing the public with this new method of small distributed heat and power. A total of 15 CHP units are planned in this project. The planned five-year evaluation is more valuable for determining durability and conducting a life-cycle analysis.
- The approach is well described and seems to encompass the most important elements for consideration. However, the project length (five years) seems longer than necessary. It is described as an attribute (better than other three-to-six-month studies); however, it would seem that after a couple of years (two seasonal cycles), most of the necessary data and details would be available, unless a lot happens in performance in years 3–5 that is not necessarily demonstrated by the results. With the rapidly developing markets and technologies, this is a considerable time to be under study.

### Question 2: Accomplishments and progress toward overall project and U.S. Department of Energy (DOE) goals

This project was rated **3.7** for its accomplishments and progress.

- Overall, the project has made progress toward achieving the DOE goal of demonstrating micro-CHP. The fact that the rated 5-kW capacity of the unit has not been achieved (and reset to 4 kW) impedes

demonstration of total system value. It appears a mitigation/revision plan is in place with original equipment manufacturers (OEMs) to rectify the decreased performance.

- All systems have been installed in previous years. Some modifications and updates to the balance of plant are in progress. The operation's working at lower-than-originally-rated capacity has improved performance and availability. This project has very good documentation of performance and analysis of costs.
- This is an excellent validation project. The CHP market will probably focus on the usage of the heat, and the generated electricity will be a secondary factor. If electricity is in surplus, it will be sold back to the grid. If a deficit is encountered, the grid would supplement. CHP for off-grid applications will be difficult to balance efficiently because the usage profiles vary.
- This is a commendable list of accomplishments, results, and actions taken as it relates to the project and improvement. This project is hitting some impressive numbers.
- This project is hitting all of the major milestones and addressing barriers as they occur. During the field trial, fuel cell degradation was identified. The manufacturer spotted the problem and is in the process of implementing corrective actions. This project has led to a product redesign by the manufacturer, which will improve the industry as a whole and supports the DOE's goals to improve U.S. industry. Past year milestones were met, and the data being collected are being compiled to supplement the previous year's work.
- Identifying that the units were not performing as expected, and working with the manufacturer to improve their product, demonstrates the high quality of this project and project team. This is very valuable to the manufacturer and could possibly prevent potentially very damaging impacts if it were to happen with a future real-world customer. While not presented in the peer review meeting, the business case developed along with this product will be very valuable to proving this technology in the real world.

### Question 3: Collaboration and coordination with other institutions

This project was rated **3.5** for its collaboration and coordination.

- It appears the collaboration among participants was very good. Some different types of users help to form the potential market basis a little better.
- The project seems to have a great working relationship with the fuel cell manufacturer, and both seem to be striving to make this project a success. The host sites are also supportive of the project and seem to be active participants in this demonstration.
- The diverse set of end-use customers provides valuable data applicable across several markets. Collaboration with the end-use customers has and will continue to be key in developing the business case.
- The collaboration should have included one other reference, the local AHJ. The AHJs speak with one another. If the AHJ is included in the project, it makes the next project easier to site because the AHJ on the new project can chat with the AHJ of the previous project. This word of mouth ends up being an endorsement and eases the next AHJ's reluctance to allow a project.

### Question 4: Relevance/potential impact on advancing progress toward DOE research, development, and demonstration (RD&D) goals

This project was rated **3.7** for its relevance/potential impact.

- This project directly addresses DOE's goal of reducing life-cycle costs and improving the performance of light commercial/residential power systems.
- The relevance is appropriate. CHP has the potential to greatly reduce energy costs by more effectively utilizing the waste-from-heat from current applications.
- This project is certainly relevant to DOE's targets and goals. But it is not clear what the market of small commercial buildings is. One slide talks about hotels, hospitals, and food operations, but many of these are sized well beyond the micro-CHP levels. Perhaps some discussion and quantification of this market would be helpful in the analysis and impact consideration.
- This project is offering commercial facilities the opportunity to experience the benefits of the fuel cell-based distributed micro-CHP. It is crucial that these systems deliver on their promise of high efficiency and availability. The data gathered will be very valuable in identifying the areas that need further development.

The set point change has increased the capital cost. It is unclear what the resulting gain in electrical and combined efficiencies has been.

- This project is providing a needed field demonstration and evaluation of commercially available fuel cell technology. The viability and feasibility are being tested. This demonstration is advancing the industry; already results from this project have allowed the fuel cell provider to perform a major redesign of the product to improve performance and minimize the fuel cell degradation that was observed during the demonstration. This project supports the DOE's goal to improve the U.S. economy/industry under the Market Transformation program.

### Question 5: Proposed future work

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

- A post-project debrief should be considered in which lessons learned are discussed and then amended to this report. The lessons learned may facilitate similar projects.
- It is important to identify opportunities for improvement, especially efficiency. It is unclear what will fuel the truck auxiliary power unit (APU). Increasing the test period to at least a 1000 hours is suggested.
- Future work includes completing the business case and continuing the field demonstration to provide robust, long-term field results. A related research project involves the evaluation of the APU fuel cell demonstration. If progress continues in a similar fashion, this follow-on work should provide good results also.
- The project is well managed and on target. Future work includes expanding to additional markets and the completion of a very comprehensive business case. The improved systems triggered by the discovery of less-than-expected output should be incorporated, if possible, into the demonstration and data collected, especially if the costs are increased.
- It seems that all the future work for the next two years is composed of additional data collection and report writing. There is no discussion of how the present and future work will move the needle on the micro-CHP market. For example, it is unclear what and how action is being taken so that another request for proposals released in a year will result in more than one bidder. The relevance of the truck APU to the micro-CHP project is not obvious.

### Project strengths:

- The project management and planning is a strength of this project.
- This project is very successful in capturing performance and cost-related data.
- This project is an excellent opportunity for data collection.
- The focus and attention to detail in generating, collecting, and reducing the field data is a strength.
- This is a well-laid-out and -executed research project that is hitting the milestones and producing good useable results.

### Project weaknesses:

- Only one manufacturer is included; however, there are limited manufacturers in this range of CHP systems.
- This project lacks information on areas needing technical improvement (research and development).
- In future demonstration projects, this project should include the local AHJ in the activity early and include the AHJ as a collaborator. It will help with getting adoption by the local AHJ on additional projects.
- Although the approach was solid and the user partners are from different "markets," it appears all installations were in relatively moderate climates. Perhaps the study and demonstration would benefit from at least one "cold"-weather installation.

### Recommendations for additions/deletions to project scope:

- Some additional details in the report/analysis would be useful.
- This project should continue as laid out in the statement of work. As more U.S. fuel cell manufacturers provide commercially available products, additional demonstrations may be required.

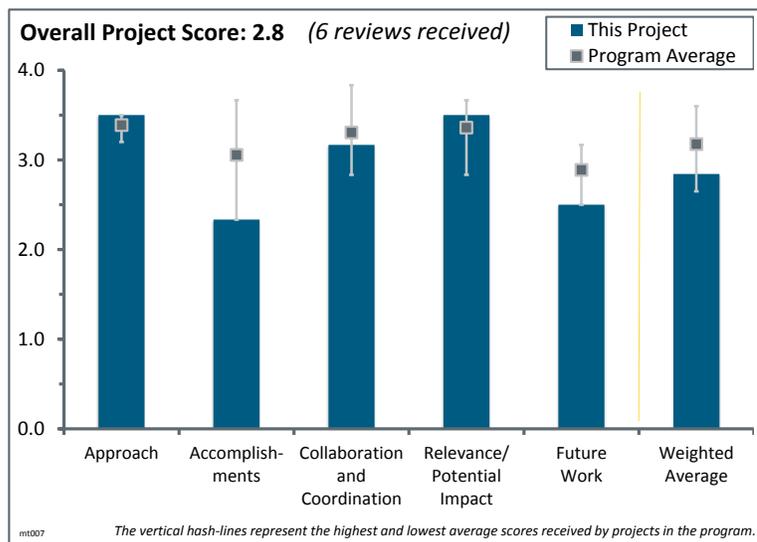
- This project should track the cost of ownership and then project it for the life cycle. The project should also compare the greenhouse gas emissions over the life cycle and compare them to a state-of-the-art central power plant for equivalent natural gas consumption.

## Project # MT-007: Landfill Gas-to-Hydrogen

Shannon Baxter-Clemmons; South Carolina Hydrogen and Fuel Cell Alliance

### Brief Summary of Project:

The objectives of this project are to validate the business case and technical feasibility of using landfill gas (LFG) as a distributed generation option for hydrogen production and to transfer lessons learned that may be applicable for other candidate waste streams. This project surveys commercially available equipment to draw conclusions regarding the economic viability of the LFG-to-hydrogen approach for potential end users; demonstrates the technical viability of current systems to produce sufficiently pure hydrogen for use in automotive or other applications; and confirms that there is no adverse impact on fuel cell systems that operate on LFG-sourced hydrogen.



### Question 1: Approach to performing the work

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

- The project quickly focused on major barriers, such as the LFG cleanup and the economics of producing hydrogen using LFG versus cryo-hydrogen.
- This is a good demonstration project where the host (BMW) looks at using landfill gas to reduce their consumption of fossil fuels. Their willingness to host material-handling equipment (MHE) powered by fuel cells and fueled by hydrogen from LFG is a tremendous opportunity for a good demonstration project.
- The initial plan was well laid out, but issues arose in fiscal year 2012 that were detrimental to the schedule, and the project has not yet recovered. The schedule and outcome of the project will suffer. A major barrier to the appropriate purity of the hydrogen has not been overcome. If the course correction is made, this could still be a very good and successful project.

### Question 2: Accomplishments and progress toward overall project and U.S. Department of Energy (DOE) goals

This project was rated **2.3** for its accomplishments and progress.

- This project has made outstanding progress in cleaning up LFG with the major impediment—the showstopper—identified.
- The project seems to be facing a serious hurdle in separating the nitrogen and oxygen from the LFG. The high nitrogen and oxygen content is unusual, indicating a serious issue in the separations unit.
- This project is significantly behind schedule. The main point of the project is to look at the viability of using LFG to make hydrogen onsite. The project should be more creative in solving the gas clean-up problem, and maybe should have some foresight to avoid it.
- The project is approximately 70 percent complete, but full demonstration of the equipment has not been accomplished. As this is the main goal of the project, there is some concern that the schedule will not be met. In research, not every project meets all of the goals set out in the statement of work, but the project missed an opportunity to reach back to DOE and DOE’s partners to get help. The feasibility study portion of this project is accomplished and well received. With the issue of the purity of the hydrogen, the schedule is not likely to be accomplished without an extension.

- When drawing the gas from the landfill, air is often entrained. This results in high nitrogen and oxygen levels in the feed stock. The nitrogen becomes an issue due to being a diluent and forming trace amounts of  $\text{NH}_3$  in the reformat.

### Question 3: Collaboration and coordination with other institutions

This project was rated **3.2** for its collaboration and coordination.

- There is fantastic coordination among all participants, particularly in terms of doing work at a real manufacturing facility.
- The host seems to have been accommodating, considering the delays. The Gas Technology Institute (GTI) and its gas separation vendor may need to work closely together to resolve the problem.
- The project has worked very well with its project partners, including BMW, GTI, Ameresco, and the South Carolina Hydrogen and Fuel Cell Alliance
- The excellent collaboration with BMW remains a stellar aspect of this project. An unsung benefit is the rather large amount of in-kind support BMW is providing. Although not actually credited in the project's overall financials, this de facto co-funding is a key to the project's potential success.
- Based on the issues noted above, the collaboration needs to be increased.

### Question 4: Relevance/potential impact on advancing progress toward DOE research, development, and demonstration (RD&D) goals

This project was rated **3.5** for its relevance/potential impact.

- The relevance is clear. This has the potential to be a model demonstration project.
- LFG is a potentially fantastic source of hydrogen for forklift fuel cell trucks.
- The project offers good opportunities on several levels. Cleanup of the trace impurities is often a challenge. It is unclear if this project has resolved this issue.
- This project supports the goals of DOE very well and could showcase a way to utilize a fuel source that could provide cost-competitive hydrogen. Multiple entities in the industry have been contacting the principal investigator of this project to track the progress and inquire about implementation at additional sites. It seems that there is good interest in the industry to see this application or similar applications succeed.
- This project has direct relevance to the Market Transformation program mission. The project takes advantage of local resources to build a demonstration site that pioneers a "doubly-green" technology. Even if the reformer never produces usable hydrogen, the project still has some relevance.

### Question 5: Proposed future work

This project was rated **2.5** for its proposed future work.

- The removal of nitrogen was identified as an issue, but there is no clear path to do it.
- The project needs to focus on solving the hydrogen purity issue and complete the six-month demonstration.
- Others are able to create good-quality gas (i.e., stuff suitable for use in SMR) from landfill emissions. The South Carolina Research Authority (SCRA) should have already contacted some of these groups and had a good handle on the next steps.

### Project strengths:

- This is an excellent opportunity to use a renewable fuel in an MHE application.
- This is a well-laid-out concept with industry applicability. The project has not yet been completed, and industry is asking for the results. The feasibility study has been completed and shows good potential for future applications of a certain size to be cost-competitive.

**Project weaknesses:**

- The lack of expertise in landfill gas and pressure swing absorptions is this project's weaknesses.
- There are no clear paths to remove nitrogen. This project should do preliminary economics to see if it is economic, assuming nitrogen can be removed at a minimal cost. This should be a go/no-go decision.
- This project incurred a major hurdle with the hydrogen purity issue. This delayed the timeline. The project is asking the right questions to solve the problem now, but a couple of attempts that lead to dead ends delayed progress. This project can still be successful. An extension will need to be put in place for the project to complete all of the goals laid out. They will probably not be able to meet the current timeline.
- This reviewer has misgivings about the effectiveness with which SCRA has handled things with the supplier of the gas cleanup system, but as that outfit is not really a "collaborator," this did not affect the collaboration and coordination score.

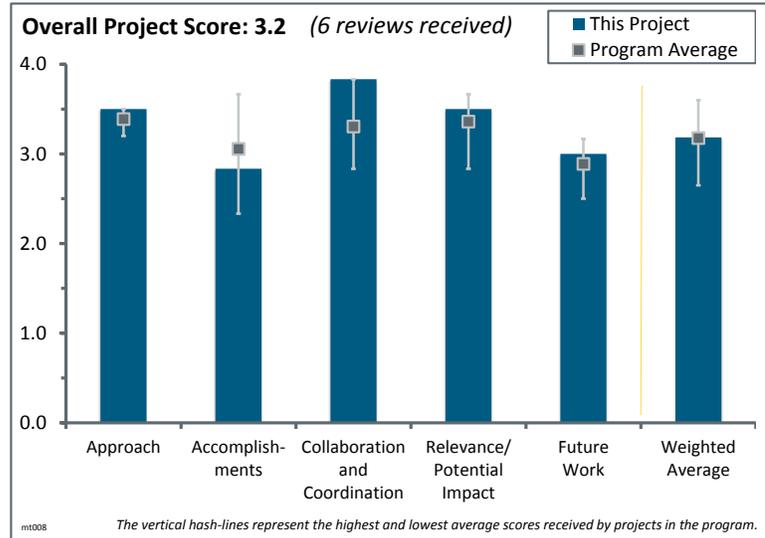
**Recommendations for additions/deletions to project scope:**

- An extension will need to be put in place for the project to complete all of the goals laid out in the project.
- This project should consider third-party evaluation/an alternate vendor for gas separations.
- This project should not continue experiments on nitrogen removal until the economic case is completed, assuming minimal cost for nitrogen removal.
- In future demonstration projects, this project should include the local AHJ in the activity early, and include the AHJ as a collaborator. It will help with getting adoption by the local AHJ on additional projects. A post-project debrief should be considered in which lessons learned are discussed and then amended in this report. The lessons learned may facilitate similar projects.
- The project should spend a few thousand dollars to locate and hire, as a consultant, a world expert on cleaning up LFG. Even if there is not enough money now to follow the suggestions, this could provide valuable insight into what it will take to make this a viable approach to providing feedstock for SMR systems in industrial environments.

**Project # MT-008: Hydrogen Energy Systems as a Grid Management Tool**  
 Mitch Ewan; Hawai'i Natural Energy Institute

**Brief Summary of Project:**

The objective of this project is to evaluate hydrogen energy systems for grid management through (1) demonstration of the use of electrolyzers to mitigate the impacts of intermittent renewable energy by regulating grid frequency; (2) characterization of the performance/durability of commercially available electrolyzers under dynamic load conditions; (3) supply of hydrogen to shuttle buses operated by the County of Hawaii Mass Transit Agency and Hawaii Volcanoes National Park; (4) performance and cost analysis to identify benefits of an integrated system, including grid ancillary services and off-grid revenue streams; and (5) evaluation of the effect on reducing overall hydrogen costs offset by value-added revenue streams.



**Question 1: Approach to performing the work**

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

- The project addresses all barriers from technical and operational barriers to getting signed agreements in place.
- This project uses a currently available hardware to encourage a utility company (a very conservative industry) to try something novel.
- The project approach is ambitious and well planned. However, it is not clear how the project will address the first objective of demonstrating electrolyzers as a grid management tool. It seems that all the work is through modeling and not through the actual installation and connection to the grid.
- Running an electrolyzer does provide a viable approach to converting geothermal energy to a form that can be (a) transported and (b) instantly converted to electrical energy. Comparing this storage medium with batteries is a good idea. However, it is not obvious how the comparison will be made or how rigorous it will be. Taking advantage of the resource (a hydrogen production facility) that results in the mainstream of the project by using its output hydrogen to run buses produces further “green” leverage that should make this project attractive to the local populace.
- This project has some serious problems getting all permissions and agreements with the owner of the location of the electrolyzer, and also with public acceptance due to the use of geothermal energy. However, the project has resolved the issues and managed to have everything ready now. They have also found a nice solution for the use of the hydrogen produced, which could lead to public acceptance because of its visibility. However, the project now has many fronts open including the hydrogen production with geothermal energy, the demonstration of grid balancing, the use of the hydrogen stations, and the use of the buses in very hard conditions. There is a risk of dispersing the efforts and that problems in one part of the project jeopardize the rest.

### **Question 2: Accomplishments and progress toward overall project and U.S. Department of Energy (DOE) goals**

This project was rated **2.8** for its accomplishments and progress.

- The accomplishments and progress are excellent.
- This is an ambitious project that is often confronted with challenges. The main one here is obviously keeping on the timeline. There is not much progress in the actual demonstration of the electrolyzer in grid management.
- The project has made good progress by modeling the impact of a fuel cell on stabilizing the grid to securing agreements and funding from a number of sources. The stability of the electrolyser under real fluctuating loads still needs to be determined.
- The progress is slow. It has taken too long to get all permissions and to put all the equipment in place.
- Progress this year has been slow but seems to have picked up in the past few months.. The resulting need for a no-cost extension is very real; one hopes that the period requested is long enough to account for any more unforeseen delays. On the positive side, it seems that all but the regulatory-delayed activities have progressed as rapidly as possible, and the community acceptance issue now seems to be getting resolved.

### **Question 3: Collaboration and coordination with other institutions**

This project was rated **3.8** for its collaboration and coordination.

- The collaboration and coordination are excellent.
- There is good collaboration between partners and also with other programs.
- This project has many, many partners and funding sources. The overall cooperation is impressive.
- This is probably one of the best lists of partners/collaborators on a project and includes levels of government and industry that are stakeholders. This adds to the complexity and coordination needs of the project, which has already had a slight impact on the schedule.
- This is one of the best-leveraged projects seen. Although significant non-DOE funds still come from the federal government, it is really impressive to see such a long list of contributors, all of whom seem genuinely interested in advancing the objectives of this project.

### **Question 4: Relevance/potential impact on advancing progress toward DOE research, development, and demonstration (RD&D) goals**

This project was rated **3.5** for its relevance/potential impact.

- The relevance of this project should be self-evident. This project allows for the full utilization of the generating equipment (which is variable) and yet still results in a stable and predictable grid. This is a cool project.
- This project will have great impact on the ability of the grid to use fluctuating and steady-state renewable energy sources.
- The use of electrolyzer and hydrogen offer significant opportunities in the grid management and energy storage arena. It is not clear if the project will be able to fully deliver answers to some of the questions posed, but the relevancy and importance are certainly there.
- If the project succeeds, the use of hydrogen production for balancing the grid could become an option for the utility companies. This would greatly aid the use of renewable energy for Hawaii. The use of buses will help gather more data and allow the project to learn about their performance.
- The participation of the U.S. Department of Defense (DOD) in the project points to a national security-level interest in the project.

**Question 5: Proposed future work**

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

- This project was rated as good because the stability of the electrolyzer to fluctuating loads should be shown in the lab before going to a field test.
- This sounds like a commercial project.
- Most of the activity focused on completing the project is devoted to finishing out the work.

**Project strengths:**

- The concept and cooperation are strengths of this project.
- The collaboration and project objective in support of grid management are laudable.
- The high level of outside (state/DOD and other) participation is the main strength of the project.
- The ability to get all the partners to work together and get additional funding sources is a strength of this project.
- This project could have a lot of “visual” impact by the use of the buses. It covers all aspects, from renewable hydrogen production to its use for transport.

**Project weaknesses:**

- The project focus is very dispersed, and since it covers so many things, there are many risks.

**Recommendations for additions/deletions to project scope:**

- This project should develop an option to expand and deliver some grid management capability.
- This project should increase the number of buses and connect the electrolyzers to a wind farm.
- This project should identify other potential uses for hydrogen and get real, off-site data on the impact of cycling loads on electrolyzer life.
- A post-project debrief should be considered in which lessons learned are discussed and then amended to this report. The lessons learned may facilitate similar projects.
- The project team should add an explicit task to develop an analytical format for comparing the benefits of the hydrogen approach with the battery approach. Although this comparison is mentioned as a key goal of the project, there seems to be a lack of attention to the way in which it will be done. The findings of the project will be much more useful to other sites if a formal cost–benefit analysis, or something close to it, comes out of it.

## Project # MT-011: Ground Support Equipment Demonstration

Jim Petrecky; Plug Power

### Brief Summary of Project:

This project creates a hydrogen-fuel-cell-based solution as a cost-competitive and more energy-efficient power source for baggage tow tractors (airport vehicles) compared to the incumbent internal-combustion-engine-powered vehicles. The fuel cell solution reduces consumption of gasoline and diesel fuels, achieves lower carbon emissions, and demonstrates a value proposition that shows decreased energy expenditures when compared to diesel-powered airport vehicles.

### Question 1: Approach to performing the work

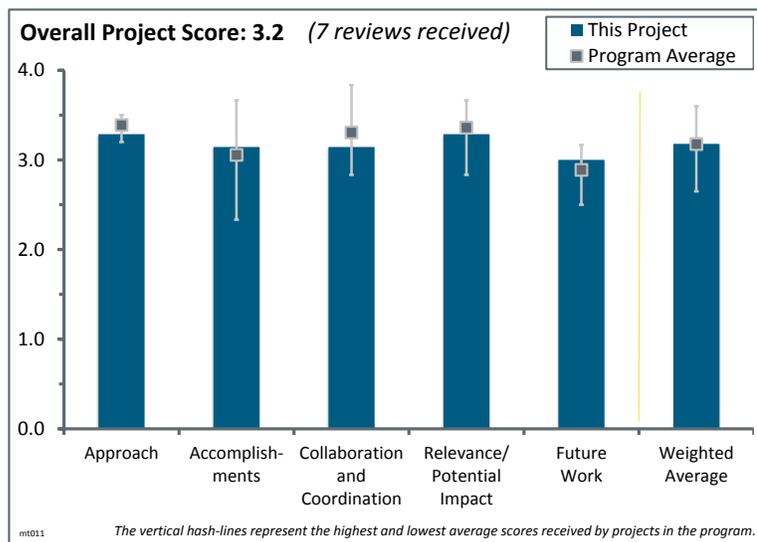
This project was rated **3.3** for its approach.

- The project is just starting, but it is very well focused and organized.
- This project and demonstration have a strong and solid approach. This has been a proven approach over several similar material handling equipment (MHE) demonstrations. The one component that is significantly new is the outside exposure.
- This is a well-planned project that appears to meet all of the requirements for a successful market transition effort. Working with the largest customer and the leading original equipment manufacturer (OEM) in the market is a good way to approach the final product engineering and early deployment. The phased project plan, with a concrete go/no-go decision point, minimizes risk.
- The project will replace diesel engine baggage tow tractors with fuel cell- and battery-powered units. Hydrogen will fuel the fuel cells.
- The project kicked off in January 2013, and the component requirements have been identified. The biggest issue will be the timeline provided. In the first year, Plug Power states that both alpha and 15 beta units will be produced. This seems to be a very aggressive schedule and timeline.
- There is no clear path from demonstration to commercialization and several unknowns, which do not seem to be addressed. For example, it is unclear how these systems will operate outside, how the air quality at the airport sites will affect the units, and how the modified unit will perform. With a market of only 26,000 units per year nationwide, it is unclear how this technology will be expanded to other applications. This is a difficult deployment; however, these considerations should be part of the approach. Also, the choice of designing for one manufacturer limits the commercialization of this unit. While there seem to be some uniform standards across the industry, this is a unique tractor in that the seating is in the rear. It is not clear how this will be integrated into other units if the prototype is designed specifically for the Charlotte unit.

### Question 2: Accomplishments and progress toward overall project and U.S. Department of Energy (DOE) goals

This project was rated **3.1** for its accomplishments and progress.

- The work performed in only two months is already very promising.
- The accomplishments and progress are as to be expected.
- The project kicked off less than two months ago. The requirements have been defined, and partner coordination is in progress.



- The project was kicked off in January, and good progress has been made getting all players together and involved. Development of the new unit for deployment could delay this project and should be watched carefully.
- The rating is principally based on where the project is at this point, which is just getting under way. No significant progress has been made on objectives or barriers that can be accurately judged. Hopefully, this will move up during the next DOE Hydrogen and Fuel Cells Program Annual Merit Review.
- The project has only the groundwork laid, including the identification of requirements and some initial planning. Work on the alpha units needs to begin to meet the first year's deadlines. This project's kick-off meeting was held at the end of March, even though award was made in January.
- This project is only two months old. It appears to have started on time and to be proceeding according to schedule. It is important to note that DOE allows performers to "get ahead on the curve" on new projects by doing the first 60 days of work at their own risk before getting on contract. Had Plug Power done this, the progress would be ranked as outstanding.

### Question 3: Collaboration and coordination with other institutions

This project was rated **3.1** for its collaboration and coordination.

- The Plug Power-led team is working with a hydrogen producer, airport authorities, the tractor manufacturer, and the end user.
- This is a good list of partners and is the best type of operating environment to demonstrate the value proposition.
- The coordination between the partners seems good for now. The close coordination between the baggage tow tractor (BTT) provider, the fuel cell system provider, the hydrogen station provider, and the end user is critical.
- Getting buy-in from the airport partners and Federal Express (FedEx) in this short timeframe is impressive. Careful management of these collaborations should be a priority. They will be key in the deployment stage of the project.
- Plug Power has assembled a good team of partners that seem to have bought into the project. The support from two host locations and FedEx will help this project succeed. Nuvera has also become a partner to supply the hydrogen fuel, which is a good partnering, as they bring experience doing these types of demonstrations.
- Although the performers appear to have established good working relationships with Charlotte and FedEx, contacts with other end-market customers and OEM suppliers seem to be limited.

### Question 4: Relevance/potential impact on advancing progress toward DOE research, development, and demonstration (RD&D) goals

This project was rated **3.3** for its relevance/potential impact.

- The reported relevance is valid, and the task is commendable.
- Although it is relevant and has some potential impact, it is unclear how big a market this truly is. After FedEx, UPS, and a few major airports, it is unclear if this market dries up.
- This project opens a new market for fuel cells. It has good potential not only for the U.S. market but also for exportation to other markets.
- The project will replace diesel engines with clean fuel cell power, meeting Tier 4 emission standards. The fuel cell/battery systems are expected to reduce downtime since current diesel engine units need to regenerate the filters. A successful demonstration may attract other smaller airports to adopt these electric drive BTTs.
- The relevance of this project is aligned with the goals of the program; however, with the limited market size, the overall impact of this project, if successful, will be less significant in proving this technology against conventional technologies.
- This project could create a new product for the fuel cell industry, which would align well with the Market Transformation program goals. The overall impact may be smaller than hoped, as there need to be fairly specific situations for the fleet to be cost-effective. There may not be widespread applications that are

feasible, but there may be enough of a market to make it profitable for the fuel cell industry when bundled with other hydrogen/fuel cell applications.

- This project is well aligned with the Market Transformation program objectives. The projections of a two-year payback on investment for shippers at each major airport that adopts hydrogen-fueled Eagle MTT Electric Tow Tractors seems a little optimistic, but if true, it will certainly enable the life-cycle cost and performance so that it is on par with conventional technologies. (This is a Market Transformation objective in the 2012 *Fuel Cell Technologies Office Multi-Year Research, Development, and Demonstration Plan*.) Even if the payoff takes three years, commercial adoption of hydrogen for vehicles in a demanding application like this one will get the attention of users in other transportation markets.

### Question 5: Proposed future work

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

- The lessons learned were good, and hopefully that includes how to work with the authorities having jurisdiction (AHJs).
- The project has laid out a multi-year plan with go/no-go options. If it can meet all the milestones, this could be a successful project. An issue may occur with the very tight timeline in the first year to develop an alpha and 15 beta units. The future year's work seem reasonable and well laid out.
- The team is aware of potential setbacks and has built in go/no-go decision points that are appropriate. No decision point is outlined for proving the value proposition of this unit; this is key to aligning it with program goals and objectives.

### Project strengths:

- Collaboration is the strength of this effort.
- The concept, collaboration, and the proposed future work are strengths.
- Collaboration and real-world potential are strengths of this project.
- This is an interesting project that builds on past forklift experience.
- This is a good project plan, and the very clear path to market makes this an attractive project.
- The demonstration of clean electric drive technology and the promise of capital cost recovery in 2.5 years due to fuel savings are strengths of this project.
- This project involves good partners and is well coordinated. It is well structured and, if successful, will open a new market for fuel cells.

### Project weaknesses:

- The single unit and limited market team must outline how this technology can be applied to other markets.
- The hydrogen cost of \$12/kg is high but understandable. Hopefully Nuvera and the team will explore options to reduce this cost.
- The market may require significant ground support equipment (GSE) population, which will limit the potential market.
- The market this project is targeting is very demanding and will give only one opportunity. The project has the potential to open a new market, but also risks closing it. The comparison with diesel vehicles is unfair since the comparison should be with battery vehicles. If the comparison is done against diesel, it is not clear if the environmental impact of hydrogen production has been included in it.
- The timeline of the first year is very progressive and may be too much for the project to accomplish. This may cause all the deliverables for the project to slip. The project must supply sufficient manpower dedicated to the project for it to be successful and meet the goals set up in the schedule.
- The number of sites at which this precise approach can be used is limited. Clearly the large-scale-shipper-material-transfer-truck market is not enough to sustain a business. What is unclear is whether this market will ever be net-positive for the Plug Power team/supply chain without DOE support.

**Recommendations for additions/deletions to project scope:**

- This project should evaluate the use of steel tanks since the extra weight could reduce the need for the ballast and potentially reduce the cost of the system.
- This project should track the cost of ownership and greenhouse gas emissions and compare to the diesel-powered units they replaced. Projection of the costs and emissions should be done for the product life cycle. The independent assessment of project metrics will have higher credibility.
- The project should look at modifying the first-year deliverables. The project will probably not be able to create both alpha and beta units by the end of calendar year 2013. They will have trouble with permitting and need to address this early on in the project. The government point of contact should confirm and track progress on the permitting issues and track progress and milestones closely.
- The project should have serious discussions with other MTT truck makers as soon as possible. It might be good to add a specific task to the project that calls for the team to look at ways to rapidly add other fuel cell electric vehicle customers at the airports where reformers will be installed.
- This project should include other manufacturers in the design phase to plan for commercialization across the industry. Not including others could lead to tough competition during any commercialization stage.

## Project # MT-012: Fuel Cells as Range Extenders for Battery Electric Vehicles

Aymeric Rousseau; Argonne National Laboratory

### Brief Summary of Project:

The objective of this project is to evaluate the potential of using a fuel cell system to double the range of current battery electric vehicles. Aspects addressed in this research include the cost effectiveness of fuel cell systems versus battery systems for storage and for delivering power and determination of the optimal power usage in fuel cells to provide the lowest levelized cost of driving. The results are impacted by hydrogen cost, vehicle life, driving distance, and battery cost.

### Question 1: Approach to performing the work

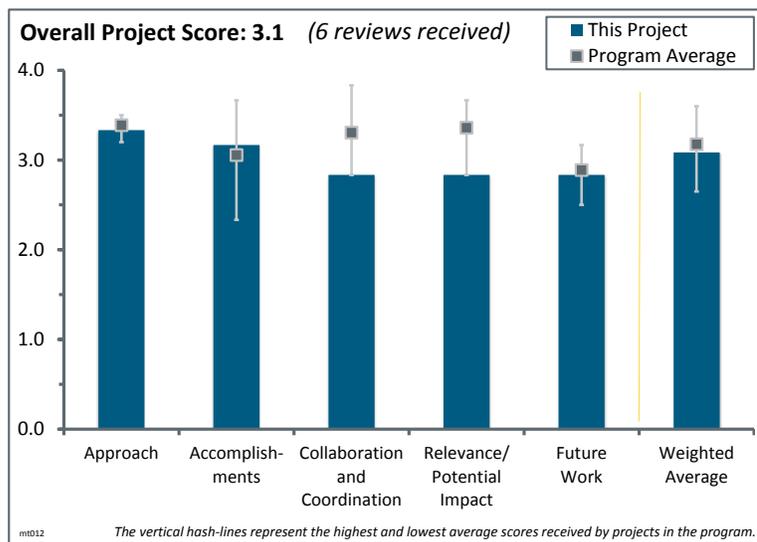
This project was rated **3.3** for its approach.

- This is a well-designed project from an analytical viewpoint.
- The modeling approach appears robust and sound. The current report does not compare the use of a gas engine as range extender for comparison purposes. That should be incorporated into the next look. Additionally, the analysis also considers the current state of battery technology, and it is constantly improving.
- The project has performed as expected. However, the results are predictable, and the way they are presented with the different charts is not clear (there is no resolution in the charts to really see any difference between options for the heavier vehicle).
- As this project is based purely on simulations, it is a low-cost way of evaluating fuel cells as battery range extenders. Definitive conclusions were produced, and this information will be valuable in proving the value proposition for fuel cells as battery range extenders.

### Question 2: Accomplishments and progress toward overall project and U.S. Department of Energy (DOE) goals

This project was rated **3.2** for its accomplishments and progress.

- This project was completed on time and produced clear and defensible results.
- This project definitely showed the potential benefits of using a fuel cell as an electric vehicle cost reducer.
- The progress and accomplishments are as expected.
- The project has delivered the expected results.
- This study produced a relatively robust set of results, with specific findings that seem to validate the business case for the fuel cell electric vehicle (FCEV) approach to extending zero-emission vehicle range. If manufacturers and potential customers believe in these results, the study could be used to help promulgate this particular market as an early entry point for fuel cell systems.



### Question 3: Collaboration and coordination with other institutions

This project was rated **2.8** for its collaboration and coordination.

- There has been some collaboration with other laboratories to obtain the necessary data and to harmonize results.
- The work of this project was accomplished almost entirely with in-house resources. Very little collaboration was necessary. The fact that the project objectives were accomplished on time and within budget means that relations with the subcontractor (Autonomie) were well handled.
- There is really no opportunity for coordination.
- This project lacks collaboration with real-world vehicle manufacturers.
- The level of collaboration from original equipment manufacturers (OEMs) is unclear.

### Question 4: Relevance/potential impact on advancing progress toward DOE research, development, and demonstration (RD&D) goals

This project was rated **2.8** for its relevance/potential impact.

- This project has great relevance for FCEVs.
- This project met the need for a timely study of the FCEV hybrid approach to doubling the range of zero-hydrocarbon vehicles. The results seem to indicate that, in places where hydrogen is available, this approach would be more cost-effective than simply doubling the battery size, particularly for heavier vehicles.
- While this project was successful, it is based on a simulation and unfortunately has only so much value in achieving the goals of the program, which are to prove fuel cell technologies in real-world situations.
- It is hard to judge given the results and the current level of collaboration. The study suggests some opportunities, but it is unclear how that gets taken to the market.
- Hybridizing a battery electric vehicle with a fuel cell has very little potential. The study only tells us something that is already known: batteries are limited as a storage medium for electricity; hydrogen is a much better option. Hydrogen and fuel cells are more expensive when providing main power.

### Question 5: Proposed future work

This project was rated **2.8** for its proposed future work.

- Evaluating the approach for 2015 and 2020 using fuel cell cost targets is a great idea.
- The suggestion to look at different drive cycles and vehicle classes is probably worthwhile.
- Of the potential follow-on projects cited, validation of the study results using actual hardware embodiments of some of the vehicles studied would be the most interesting. Unfortunately, it also would be by far the most expensive. Looking at other vehicle classes (another proposed follow-on task) might be interesting, too.
- It is uncertain whether continuing this effort will provide value-added. The optimization of a system based on only a couple of variables can lead to questionable conclusions.
- The relevance of the results of the project, even if very interesting from a scientific/technical point of view, will not contribute to fuel cell and hydrogen deployment, nor to battery vehicles.

### Project strengths:

- The results are clear and defensible.
- This was a well-rounded, well-executed project.
- The technical expertise in modeling is strong.
- The models seem sound, and the organization of the project is good.
- This project showed the impact of changing some variables on conclusions.

**Project weaknesses:**

- This project has no real-world demonstration and does not include vehicle manufacturers.
- The lack of real-world input and the limiting of the design parameters are weaknesses.
- It was not clear what the impact of CC on range was. Also, the project does not have good information on the impact of variable fuel cell costs.

**Recommendations for additions/deletions to project scope:**

- This project needs to show the impact of varying fuel cell costs on cents per mile.
- This project should include vehicle manufacturers in the analysis or at least to review findings.
- This project has ended and has achieved its goals. Adding a third dimension to the trade-off matrix (hydrogen fuel cost) to address the sensitivity of this scheme to the availability of hydrogen would probably be the best use of any additional money allocated to extend this project.
- The need for this effort should be reassessed.

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## 2013 — Systems Analysis

### Summary of Annual Merit Review of the Systems Analysis Program

#### Summary of Reviewer Comments on the Systems Analysis Program:

The reviewers considered the Systems Analysis program to be an essential component of the U.S. Department of Energy (DOE) Hydrogen and Fuel Cells Program's (the Program's) mission. The projects were considered to be appropriately diverse and focused on addressing technical barriers and meeting targets. In general, the reviewers noted that the Systems Analysis program is well managed and demonstrated the ability to address immediate analytical needs and overall objectives and plans, especially to implement the new initiative, H<sub>2</sub>USA.

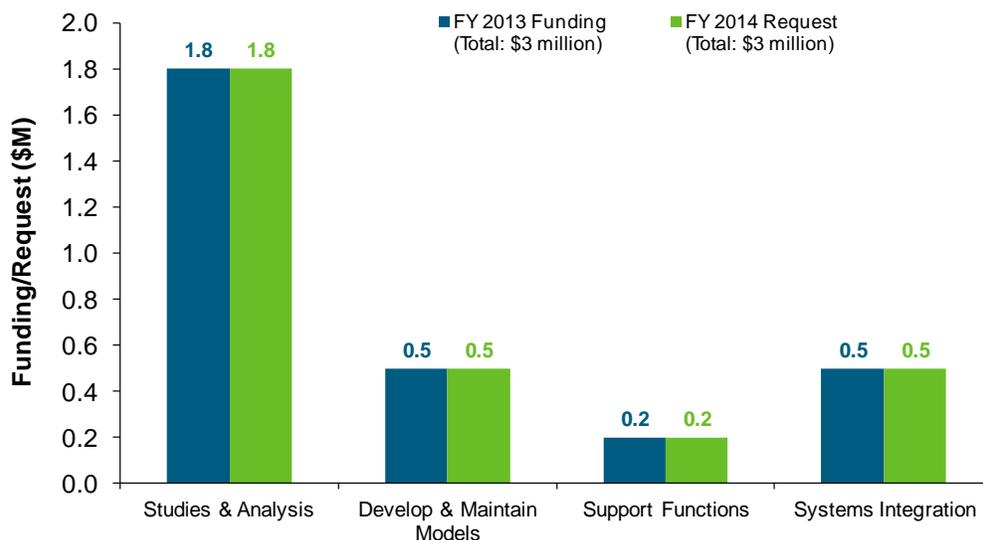
Some reviewers commented that the program is effective in providing analytical support and key insights for the Program's research and development (R&D) efforts and that it is helpful in appropriately directing R&D efforts to address key barriers. Reviewers also commented that the analysis and model portfolio was making good progress toward understanding the issues, challenges, and opportunities related to achieving the Program's technical targets. Some reviewers commented that the use of flowcharts to articulate the interactions between the types of analysis and applications was effective in describing the program's analysis process.

Key recommendations for this program included the following: (1) more emphasis on near-term market barriers is warranted, given the status of fuel cell vehicles and the challenges with infrastructure deployment; (2) analysis is needed to assess the policy options to incentivize stakeholders and finance mechanisms for infrastructure and fuel cells; (3) analysis is critical to the Program; and (4) the level of funding for this program continues to be a concern.

#### Systems Analysis Funding:

The fiscal year (FY) 2013 appropriation for the Systems Analysis program was \$3 million. Funding for the program continues to focus on conducting analysis using the models developed by the program. In particular, analysis projects are concentrated on infrastructure development for early market fuel cell introduction, the use of hydrogen and fuel cells for energy storage, biogas resources, life-cycle analysis of water use for hydrogen production, employment impacts of developing infrastructure to supply hydrogen for fuel cells, and the petroleum and greenhouse gas emission reduction benefits of various pathways. The FY 2014 request level of \$3 million, subject to congressional appropriation, provides greater emphasis on analysis of hydrogen for energy storage and transmission, early market adoption of fuel cells, continued life-cycle analysis of water use, levelized cost of hydrogen from future hydrogen production pathways, cost of onboard hydrogen storage options and associated greenhouse gas emissions and petroleum use, and other impacts such as job creation.

### Analysis R&D Funding



#### Majority of Reviewer Comments and Recommendations:

The maximum, minimum, and average scores for the Systems Analysis projects were 3.5, 2.9, and 3.2, respectively.

**Infrastructure:** The analysis projects reviewed in this topic area received a favorable average score of 3.2 for assessing the costs of hydrogen infrastructure development and understanding the hydrogen infrastructure costs compared to other alternative vehicle infrastructure. Reviewers acknowledged the insights gained from a wide array of stakeholders and analysis of the economics of hydrogen refueling stations in a dynamic context. The suggested next steps included the following: linking station siting and overall station needs to vehicle choice modeling and expected fuel cell electric vehicle (FCEV) purchases, continuing to calibrate the findings with key stakeholders and other studies, and expanding the analysis projects to a more comprehensive and integrated study of vehicle/infrastructure rollout.

**Model Development and Systems Integration:** Two projects involving model development were reviewed (one for assessing the employment and economic impacts of deploying fuel cells and hydrogen infrastructure and one for life-cycle analysis of water use for hydrogen production) and each received a score of 3.2. These projects received favorable reviews and were regarded as well aligned with the current program goals and objectives.

Reviewers commented that the JOBS model provides valuable economic and job creation information for project funding justification. Reviewers recommended that the project continue to expand the model to include assessment of the employment impacts of infrastructure construction.

Reviewers acknowledged that expanding the Greenhouse Gases, Regulated Emissions, and Energy Use in Transportation (GREET) model platform to include water use life-cycle assessment addresses critical and relevant Program issues associated with hydrogen production. Reviewers pointed out that the model would have to be expanded to include all fuels so a proper comparison can be completed. The project will benefit from collaboration with industry stakeholders.

**Programmatic Benefits Analysis:** The reviewers commented that the analysis projects to assess the program's benefits (in terms of reducing greenhouse gas emissions and petroleum use) for multiple hydrogen pathways and the inclusion of various onboard storage options for hydrogen pathways are relevant to the Program's objectives and provide valuable projections of the impact of FCEVs and hydrogen in the U.S. transportation mix. Systematic

evaluation of the pathways and with future onboard storage options for cost and greenhouse gas emissions is critical to the overall systems analysis effort and guiding research goal settings and prioritization.

**Resource Analysis:** This project received a favorable review for assessing biogas resources available for *renewable* hydrogen production. Reviewers specifically appreciated the insights the analysis provided about using waste in a way that not only provides clean fuel for FCEVs, but also eliminates costs and environmental problems associated with solid waste and associated biogas. Future work will include additional waste feedstocks, economic analysis, and costs.

**Studies and Analysis:** Six analysis projects were reviewed, with an average score of 3.2. The projects covered a range of topics including energy storage, fuel cell integration with biofuels facilities, and the global status of FCEV technology. In general, the reviewers felt that the projects supported Program goals, but they also agreed that the results of the analysis projects need to be (1) disseminated to a wider audience outside the fuel cell community, (2) used to modify goals and assumptions used for various analysis and modeling exercises, and (3) used to examine other applications.

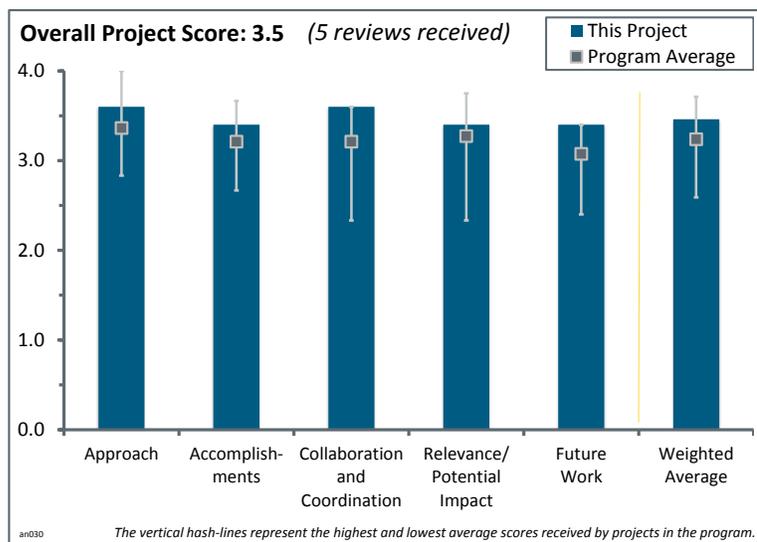
The analysis project to assess the worldwide status of hydrogen FCEV technology and prospects for commercialization was commended for its thorough approach and collaboration with automobile original equipment manufacturers (OEMs) to acquire critical data for modeling input. The project provides critical insight on fuel cell technology progress; trends; and the plans of major OEMs that should be incorporated in research, development, and demonstration planning and future direction.

## Project # AN-030: Worldwide Status of Hydrogen Fuel Cell Vehicle Technology and Prospects for Commercialization

David Greene; Oak Ridge National Laboratory

### Brief Summary of Project:

The goal of this project was to establish the status of fuel cell electric vehicle (FCEV) technology and commercialization plans in Japan, Korea, the European Union, and the United States. Benchmark progress has been seen by original equipment manufacturers (OEMs) in the performance of FCEV technology, manufacturing costs, and the timing of commercialization. Government and industry plans for deployment of FCEVs were documented, and the data collected were used to recalibrate the market transition models. FCEV performance will be ready for commercial introduction by OEMs in 2013, 2015, 2017, and 2020, depending on the availability of refueling stations.



### Question 1: Approach to performing the work

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

- This is a very thorough approach to obtaining data and insight for study and analysis with targeted partners.
- This project includes a comprehensive approach, utilizing available data and analyses supplemented with direct input from OEMs.
- This project is contacting relevant stakeholders in different countries and seeking detailed insights from them. This is a valuable approach, and such interactions should be continued on a regular basis so as to keep abreast of relevant developments and to receive insights that could shape future research decisions.
- The approach was comprehensive. The data was presented in a useful and informative way and directly addressed the barriers of FCEV component cost and performance. This project also highlighted areas where improvement is needed, such as in the interplay between platinum loading and durability.
- This project has access to multiple sources of information and data that are required for this analysis, although there seems to be a disconnect between the status of the technology, the focus of the research program, and the information coming from the U.S. DRIVE Tech Teams. Additional discussions are needed to ensure that information collected from stakeholders is indeed representative.

### Question 2: Accomplishments and progress toward overall project and U.S. Department of Energy (DOE) goals

This project was rated **3.4** for its accomplishments and progress.

- This project provides a comprehensive assessment of FCEV status and commercialization prospects.
- This is a great collection of data. It is hard to predict if cost and rollout of stations and vehicles will match the estimates.
- Based on the information obtained from OEMs, the analysis points to particular issues that can be used to focus research efforts in other programs. This is an important outcome of any analysis project. The information should be vetted with the appropriate subprogram leads and checked against the technical teams.

- The project made significant progress in understanding projected future costs for components of FCEVs and vehicle costs, which is a major factor in future market adoption. The project also helped address the barrier of inconsistent data by gathering and analyzing cost data from diverse OEM sources. The work made significant progress toward its goal of better understanding future costs, a key driver for market adoption of FCEVs. This project also helped clear up inconsistent data on FCEV costs and performance.

### Question 3: Collaboration and coordination with other institutions

This project was rated **3.6** for its collaboration and coordination.

- There is great collaboration with countries and OEMs, especially with South Korea.
- The project includes excellent collaborations with government agencies, vehicle OEMs, and non-government organizations.
- The project drew on industry data and coordinated with diverse international programs on hydrogen and fuel cells in Japan, Germany, South Korea, and the United States. This project succeeded in getting projections on costs, which are difficult to obtain. It is not clear if the report was fully up to date on regional infrastructure plans, but this is not surprising given how fast they change. The overall conclusions were still very useful.
- This project has access to knowledgeable collaborators who provide needed data that can be used to improve the believability of the results. Additional discussions with the Fuel Cell Technologies (FCT) Office's Fuel Cell program are warranted, as the presentation implies that the OEMs have solved many of the problems on which researchers continue to work.
- South Korea is mentioned as one of the countries from which data and insights are gained, but the results do not show much information relating to South Korea; they seem more geared towards the other countries.

### Question 4: Relevance/potential impact on advancing progress toward DOE research, development, and demonstration (RD&D) goals

This project was rated **3.4** for its relevance/potential impact.

- Having independent studies to point to is useful and helps corroborate other studies and boost arguments for FCEV and infrastructure. The data are very important.
- Understanding the costs and the international status of hydrogen and fuel cells is of high relevance to the DOE Hydrogen and Fuel Cells Program. This is an excellent summary of the current state of the technology.
- Gaining insight into technology progress, trends, and developing plans based on input from the major industry players and countries is key to calibrating modeling assumptions and to conducting effective analyses. Connections with these stakeholders should be kept on a continuous basis so that any developments that might have an effect on research direction and other decisions may be identified in a timely manner.
- The project provides a necessary evaluation of the status of fuel cell technologies and the prospects for FCEV commercialization. The project is aimed at understanding the current status of fuel cell technologies, which is important to DOE's understanding of where these technologies stand and what further research is needed. This project does not directly help achieve DOE's targets for fuel cell technologies, and further R&D will be needed to achieve these targets.

### Question 5: Proposed future work

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

- The proposed future work and reporting on this project are necessary and appropriate.
- This project could also try to identify/quantify the risks of not meeting deployment plans and targets.
- This project focuses on important issues for a hydrogen transition and the adoption of FCEV vehicles, including early market dynamics and the effect of international developments on FCEV adoption in the United States.

- This project mentioned two upcoming reports based on data, but it is not clear what other work will be done and how reports might be distributed to key stakeholders and publicized in conjunction with the introduction of FCEVs and hydrogen infrastructure stations.

### **Project strengths:**

- This project has good access to some stakeholders.
- This project provides a comprehensive assessment of the current state of fuel cell technologies for the transportation sector.
- This project is necessary to support vehicle/station rollout and increase the visibility and awareness of both with the public, lawmakers, and key stakeholders.
- This project addresses key barriers by providing knowledge on the current cost and performance status of hydrogen FCEV technology and projections. The international focus gives a full picture of the industry.
- This project highlights the status of technology, developing trends, and also where plans and projections do not match reality, all of which are useful insights affecting research.

### **Project weaknesses:**

- This project has no weaknesses.
- There was not much mention of the data on South Korea, even though that is stated as one of the countries investigated. It seems like the focus was more on the other countries.
- This project could do better promotion of the study and results, such as working with the groups involved to distribute information and make the public aware. This project should emphasize the corroboration with other studies and groups to build a case for vehicles/stations.
- Some of the information collected from OEMs seems to be in direct conflict with the U.S. DRIVE Fuel Cell Tech Team (FCTT), as well as with the research agenda of the FCT Office's Fuel Cell program (especially the information provided on slide 6). The state of the technology needs to be clarified with the FCTT and/or the FCT Office leadership.

### **Recommendations for additions/deletions to project scope:**

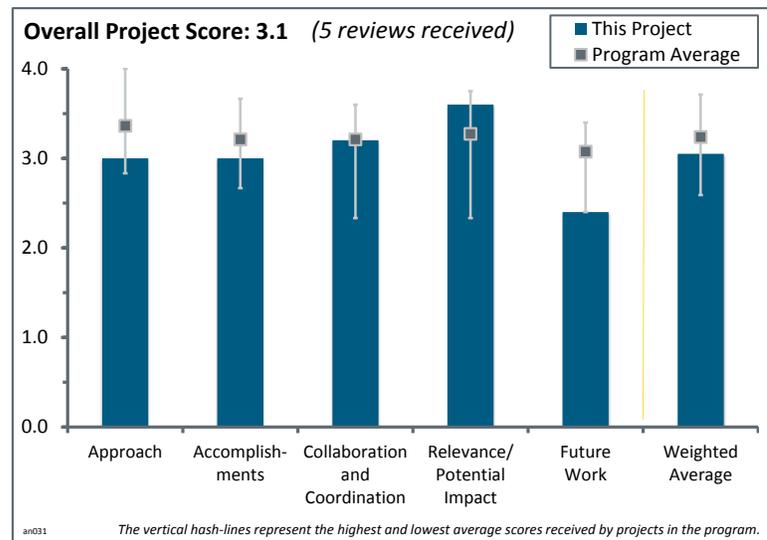
- There are no recommendations for this project.
- A discussion with U.S. DRIVE Tech Teams is necessary for this work to be relevant.
- This project should present the findings to other groups outside of fuel cells, such as The Society of Automotive Engineering, the Electric Drive Transportation Association, or other automotive groups.
- It would be good to modify and enhance the assumptions of various models used by the Hydrogen and Fuel Cells Program based on input from the major industry players and countries (to the extent that it is possible and feasible).

## Project # AN-031: Siting Strategies for Early Hydrogen Refueling Infrastructure in California: Learning from the Gasoline Experience

Michael Nicholas; University of California, Davis

### Brief Summary of Project:

Research in this project focused on determining the minimum number of hydrogen fueling stations necessary to serve the maximum number of fuel cell electric vehicle (FCEV) customers in order to reduce the capital investment needed for hydrogen refueling infrastructure. Strategies for placement, quantities, and network development of early hydrogen fueling stations were analyzed to provide fuel accessibility for an initial rollout of hydrogen fuel cell passenger cars based on studies of existing gasoline refueling behavior. Case studies were conducted for California using geographic information system-based analysis for station siting and convenience from the perspective of consumers. The research showed that an “anchor” station with a wide network of surrounding stations is a prerequisite for the consumer to purchase an FCEV.



### Question 1: Approach to performing the work

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

- It would be good to include a concise statement of the objectives, function, and data inputs in order to understand how this model is distinct from others. Overall, the approach is intuitively appealing and appears to be rigorous.
- The approach of clustering stations is good. This would provide redundant stations. If one station is down for maintenance or out of hydrogen, for example, drivers will have a nearby option. Placing stations at the exits of neighborhoods as they connect to highways is a good approach.
- The analysis methods are well designed and executed. The key shortcomings are identified, but potential solutions have not been explored. A key question is how to translate a particular configuration of station availability (type, size, and location) into a measure of consumer utility. The question of pricing hydrogen needs to be addressed from a policy perspective. The price of hydrogen will affect station economics, hydrogen demand, and consumer satisfaction with hydrogen vehicles. There needs to be a move towards an integrated analysis of these issues.
- The approach to this work seems reasonable, but it would have helped if the assumptions were explained in more detail and if additional information was presented on the other cited models.
- Development of the station siting network seems fairly generic. The project needs to better tie station siting and overall station needs to modeling of vehicle choice and expected FCEV purchases. It is not clear how station siting within clusters was accomplished. This project should tie station siting and travel distances to the households most likely to purchase FCEVs based on household market analysis (household income, education level, etc.). Given the breadth of hydrogen infrastructure, siting, and infrastructure rollout studies, the investigation should explicitly attempt to build on the findings of other available studies.

**Question 2: Accomplishments and progress toward overall project and U.S. Department of Energy (DOE) goals**

This project was rated **3.0** for its accomplishments and progress.

- The accomplishments and progress towards the goals seem to be on target. It would be clearer to provide an explanation of where the capital cost numbers presented came from, as well where the hydrogen cost figure of \$13/kilogram for 2015–2017 came from.
- This project has made excellent progress in developing the cluster concept and measuring its coverage. More attention needs to be paid to costs and benefits to identify and measure the trade-offs, and to the evolution of networks over time and the profitability of refueling outlets. This project has made good progress, but more needs to be done. At present, the project focuses on the first few stations, then assumes the market will take over. It is not clear if this is really true or how the economics work.
- Good progress has been made on the development of a conceptual siting approach. This project needs to progress beyond the conceptual, however, and refine station siting needs based on vehicle choice modeling and expected FCEV sales over time. At the same time, actual station siting should be developed based on census data relating to expected buyers of FCEVs (using metrics such as household income, education, etc). As there are a number of infrastructure rollout and siting studies, these investigations should compare and contrast them to other relevant studies and build on the growing base of knowledge.
- It seems like there should be better data than a survey from 1987; the 50% assumption needs justification or qualification. It is not clear how that results in new or relevant information. The principal investigator should restate the survey question on slide 16. It would be good to focus on new results.
- It was unclear what the new accomplishments were at this phase of the project. Good concepts of what is needed for station placements were presented, but maybe it is too early to see digested outputs from the analysis process.

**Question 3: Collaboration and coordination with other institutions**

This project was rated **3.2** for its collaboration and coordination.

- This project has an impressive list of collaborators. The NextSTEPS program appears to provide significant leverage of DOE funds.
- A significant list of collaborators and interactions were presented, and the fact that this work was conducted under the NextSTEPS consortium demonstrates that the interaction with industry is quite strong.
- This project has good collaboration. If possible, the retail fuel sector should be consulted more to see if they can help identify the appropriate business models. Benefit can be drawn from the research being done in Germany, Japan, Korea and other countries (e.g., Norway and Denmark), and vice versa.
- The reviewer has interfaced with California hydrogen developments. The work could be more visible in the California Fuel Cell Partnership forums. It would be beneficial to this project for California and the US Hydrogen Infrastructure project (H2USA) to communicate more frequently, such as by attending meetings and presenting to each other.
- This project lists good collaborations with California organizations, national laboratories, industry, and other academic researchers. While the list of collaborators is extensive, it is not clear how this work fits in with the other related research and modeling on both hydrogen infrastructure siting and deployments of FCEVs. The project should more explicitly build on research on likely FCEV purchases and vehicle choice modeling, and should more clearly coordinate with other researchers in this area to better ensure that station siting research is conducted in unison, not as individual, unrelated pieces.

**Question 4: Relevance/potential impact on advancing progress toward DOE research, development, and demonstration (RD&D) goals**

This project was rated **3.6** for its relevance/potential impact.

- This study is very relevant to the issue of infrastructure investment needs and market barriers.

- Given the status of FCEV in the world and the announcement of the H2USA organization, this analysis is of central importance.
- This project helps DOE better understand near-term deployment needs for hydrogen infrastructure. This project helps DOE understand the investment needs to develop the necessary hydrogen infrastructure to enable commercialization of FCEVs.
- This project provides a good regional analysis for early market hydrogen station placement, and this same analysis, expanded beyond California, will provide DOE with a good tool for analyzing early hydrogen market adoption in the United States.
- At this phase of transportation hydrogen technology proliferation, this is the most needed type of analysis. The analysis must, however, be digested quickly and disseminated to policy makers, investors, and the public in general. Hydrogen is a real winner in the technological realm, but it is severely suffering in public education and perception realms. Analysis of this type helps ground the public.

### Question 5: Proposed future work

This project was rated **2.4** for its proposed future work.

- The proposed work may need to be better defined.
- This analysis would benefit from detailed interaction with vehicle purchasing models. However, an approach to provide station availability to a majority of the market as fast as possible is appreciated.
- This project needs to focus more on the market impacts of station deployment to attempt to coordinate station deployment and vehicle market evolution. We need to develop more confidence that a given number of stations of particular types, deployed in a specific spatial consideration, will be sufficient to sell an appropriate number of FCEVs
- It would be good to refine the results of future work with respect to particular policy goals or industry partnership initiatives. Significant exploratory work has been done, and more focus seems appropriate at this point in time. It appears that the market hunting algorithm may be able to predict relative demand between stations, which could be useful in providing insight into investment risk.
- The investigator did not fully develop (or communicate) a plan for future work. The future work should include an assessment of the minimum number of stations needed in the early market (in specific build-out areas, such as southern California) based on evaluations of expected FCEV purchases. This evaluation should be conducted on a geographic basis to help DOE understand initial station usage levels and patterns over time and the potential need for government subsidization of station development and operation.

### Project strengths:

- Working under the NextSTEPS consortium is a strength of this project.
- The approach is robust and elaborate, and there is strong collaboration.
- This project is well focused on the most important barrier. It uses sound methodology and realistic data and assumptions. The geographic detail for station locations and markets and the inclusion of different types and sizes of stations are project strengths.
- This project helps DOE and California state government understand how hydrogen stations might be deployed during the early commercialization of FCEVs, which, in turn, will help government understand minimum station needs and the potential need for government support of hydrogen infrastructure.

### Project weaknesses:

- The approach could be more focused and relevant to particular policies or stakeholder decisions.
- This project needs to provide more detailed information on the assumptions and on the models cited.
- The project should more clearly tie hydrogen station needs to expected purchases of FCEVs. The project should more explicitly show how this investigation ties into and builds upon other research on hydrogen infrastructure siting and deployment, and the expected deployment of fuel cell vehicles.
- This project does not address the pricing of hydrogen during transition, the utility of stations to potential car buyers, and the effect on sales or customer satisfaction, except through coverage measures. This project

falls short of an integrated analysis of the evolution of an adequate hydrogen refueling infrastructure. This project needs to expand the scope, think bigger, and come up with new ideas and new methods..

### **Recommendations for additions/deletions to project scope:**

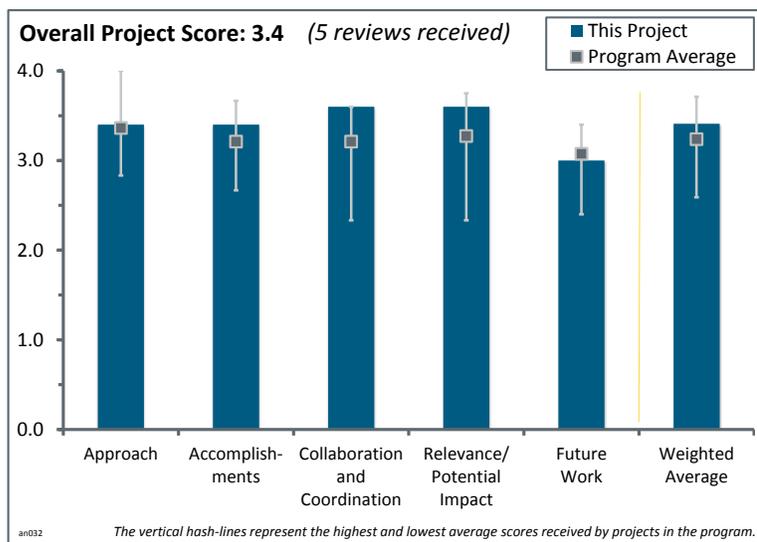
- This project should continue to pursue station size and relevance to investment risk. It should continue to pursue the value of networks to overall market growth rather than revenue for individual stations.
- This project should integrate with Professor Ogden's analysis of station economics and consider subsidy costs. It should also include measurement of consumer utility of stations and address dynamics of market evolution.

## Project # AN-032: Design and Economics of an Early Hydrogen Refueling Network for California

Joan Ogden; University of California, Davis

### Brief Summary of Project:

The objective of this project is to assess alternative strategies for introducing fuel cell electric vehicles (FCEVs) and hydrogen infrastructure in Southern California over the next decade to satisfy the zero emission vehicle regulation while taking into consideration station placement, quantity, size, and type. The analysis studies infrastructure economics from multiple perspectives: network, station owner, consumer. The project analyzed rollout strategies for FCEVs and hydrogen infrastructure in Southern California over the next decade through input and discussion with stakeholders in the auto industry, energy industry, industrial gas industry, state agencies, and national labs.



### Question 1: Approach to performing the work

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

- Evolution of station profitability over time is a very useful addition. This is an excellent first step in analyzing the economics of hydrogen refueling stations in a dynamic context.
- Analyzing the economics from several perspectives and including the station network and single-station owner is a good approach for this analysis work. It is also good that the work provided a comparison of several station types.
- It is reassuring that the approach has been vetted by project collaborators. Some additional analytics (sensitivities, perhaps) would be useful to better understand the relevance of different types of assumptions. It is difficult to judge how optimistic the cash flows are, for example, relative to the probable market outcomes.
- This study helps provide vital information on hydrogen station cost and infrastructure needs during the initial rollout of hydrogen infrastructure in California. Evaluations of infrastructure cash flows and break-even timing are crucial to understanding the necessary government role in developing a network of hydrogen fueling stations. This investigation should more explicitly attempt to build on the findings of other U.S. Department of Energy (DOE)-funded studies of hydrogen infrastructure rollout and hydrogen cost.
- This is great work in terms of considering multiple pathways of onsite refueling (liquid hydrogen [LH<sub>2</sub>], steam methane reforming [SMR], and electrolysis); however, there is a concern that SMR systems require a significant footprint, especially at the 1000 kg/day scale. The stations in the highest population density (first market) areas are very space-limited and overwhelmingly do not have room for SMR. In addition, SMR systems require significant onsite monitoring and maintenance; for example, gas-quality verification and maintenance. It is not clear if it is really feasible to consider this system type for early market forecourt applications. The upgradeability of SMR systems is also challenging. A station upgrading from 100 to 250 kg/day would need to replace the SMR because they do not stack gracefully; for example, the full footprint would be needed around the SMR to service components with a forklift.

**Question 2: Accomplishments and progress toward overall project and U.S. Department of Energy (DOE) goals**

This project was rated **3.4** for its accomplishments and progress.

- The overall incentives per station look comparable to expectations.
- This is a significant amount of work for the level of funding. NextSTEPS provides good leverage of DOE funds and enhanced the quality of this project through collaboration.
- This work showed good initial progress and accomplishments by providing some estimates for cash flow and a break-even year for different infrastructure build-out scenarios.
- The analysis is sound; however, the assumptions about the rate of increase in hydrogen vehicle sales are overly optimistic. More realistic scenarios need to be evaluated. It is also assumed that once the initial stations become profitable, future stations will be added by market demand. This may be the case, but it is not clear. The pricing of hydrogen needs to be considered in order to enable a practical policy analysis. Hydrogen price and station availability will strongly affect the willingness of consumers to purchase hydrogen vehicles. Thus, it is ultimately necessary to include consideration of consumer utility and vehicle choice.
- This project's initial findings will help DOE to understand near-term hydrogen infrastructure costs and the appropriate level of government support of infrastructure during early FCEV commercialization. The project provides estimates of the cost of both hydrogen fuel and the cost of a fueling network expected during the initial rollout of FCEV. The study should attempt to better link expected purchases of FCEV over time with station capacity utilization over time, considering the minimum number of stations expected to be needed during the early commercialization phase. Changes in station capacity utilization over time can then be tied to the expected hydrogen cost over time from these stations. This work seems to have been done in the context of station cash flow analyses, but it does not seem to be reflected in the reported levelized cost of hydrogen by year.

**Question 3: Collaboration and coordination with other institutions**

This project was rated **3.6** for its collaboration and coordination.

- NextSTEPS provides good leverage of DOE funds and enhanced quality through collaboration.
- This project involves excellent collaborations with California organizations, national laboratories, industry, and other non-profit and academic researchers.
- This project has extensive collaboration and interaction with industry by conducting this work under the NextSTEPS research consortium.
- Collaboration with a local business school will be invaluable.
- The principal investigator needs to collaborate with colleagues doing similar analyses in Germany and other places and should establish contacts with the fuel retailing industry.

**Question 4: Relevance/potential impact on advancing progress toward DOE research, development, and demonstration (RD&D) goals**

This project was rated **3.6** for its relevance/potential impact.

- This line of analysis is absolutely essential at this phase of hydrogen infrastructure rollout planning.
- A robust regional economic analysis for the initial rollout of hydrogen and FCEVs is a key contribution to DOE's goals and objectives.
- This project helps understand the cost of both hydrogen fuel and hydrogen infrastructure, as well as the investment needs to develop the necessary hydrogen infrastructure to enable commercialization of FCEVs.
- The approach would be improved with additional focus on probable outcomes or additional vetting of how optimistic the different model input assumptions might be compared to values that can be substantiated empirically.

- The subject addressed is of critical importance to the early evolution of the hydrogen vehicle market. It is the critical factor in original equipment manufacturers' decision making today when it comes to where and when to introduce FCEVs to the market.

### Question 5: Proposed future work

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

- The incorporation of other types of costs would be an improvement to the methodology.
- The proposed future work shows good direction towards the main goals for this project and towards addressing DOE barriers.
- The project suggests moving towards analyzing other regions and production pathways. More work should continue on the present analysis of southern California. The investigation should more clearly link to and compare to other DOE-funded analyses of hydrogen infrastructure in California. More work investigating the effects of low station utilization during the initial FCEV rollout is warranted, and the sensitivity analyses should be expanded. Additional work should be conducted on the underlying cost analysis assumptions to provide modeling validation. In particular, station cost assumptions relative to Hydrogen Analysis (H2A) mature market costs should be assessed and validated based on the current cost of stations sited in California, and based on literature and analyses related to the expected economies of scale cost curves and learning-by-doing improvements.

### Project strengths:

- The approach and collaboration are strengths of this project.
- This project has very strong collaboration and interactions with industry.
- This project uses solid knowledge of station economics, which are well represented in the model. The project considers the temporal dimension of station profitability, which is extremely important.
- This project helps with understanding the investment needed to overcome the "valley of death" until hydrogen infrastructure reaches a break-even level. This project helps DOE and the California state government better understand the potential need for government support of hydrogen infrastructure during early FCEV commercialization.

### Project weaknesses:

- This project needs to develop a more objective framework for comparing levels of optimism or pessimism for input assumptions.
- This project does not analyze hydrogen price strategies and policies. It does not include an integrated analysis of station economics and consumer response. The principal investigator needs to collaborate with colleagues in other countries that are considering similar problems.
- It is difficult to tell from the presentation, but the project might be repetitive with other DOE-funded techno-economic analyses of hydrogen infrastructure. The project should emphasize how it relates to and builds upon other DOE-funded research areas. The project needs more in-depth analyses of very early station deployments and of the effects on hydrogen cost of very under-utilized stations when relatively few FCEVs are deployed and consumer convenience requires a minimum number of station deployments.

### Recommendations for additions/deletions to project scope:

- It is strongly recommended that the project collaborate with a local business school. A finance graduate student could quickly add a lot more depth to the financial analysis.
- Some of the proposed future work topics have already been addressed. A more specific focus for each topic or a reduced list of topics is needed.
- This project should expand and consider multiple station types, sizes, and delivery pressures. Station economics should be integrated with vehicle choice and consumer satisfaction. At the very least, this project should consider alternative vehicle sales scenarios and economics beyond the initial station rollout.

Formal collaboration should be established with Germany's National Organization for Hydrogen and Fuel Cell Technology (NOW) and similar organizations in other countries.

## Project # AN-033: Analysis of Optimal Onboard Storage Pressure for Hydrogen Fuel Cell Vehicles

Zhenhong Lin; Oak Ridge National Laboratory

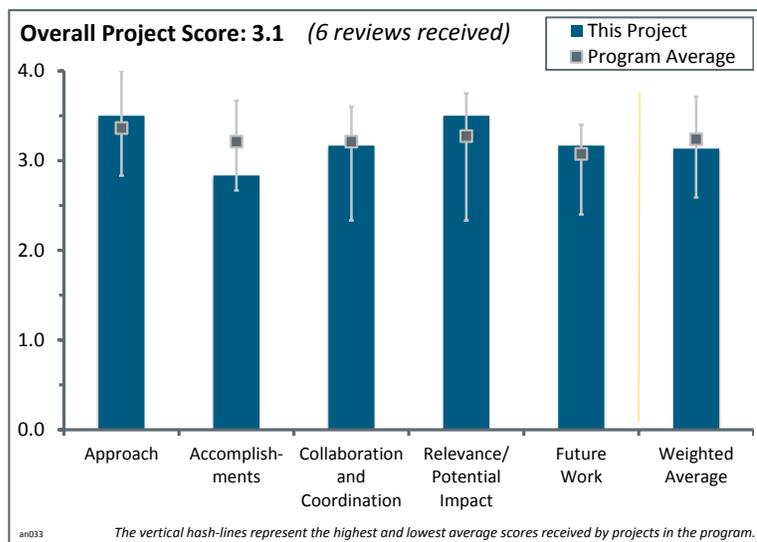
### Brief Summary of Project:

The goal of the project is to gain a better understanding of optimal delivered hydrogen pressure for refueling fuel cell electric vehicles (FCEVs). The project looks for a balance between storage and delivery pressure and quantity of stations to determine the best deployment of infrastructure to support consumer refueling needs. It offers an analytical framework for assessing the complicated relationships between onboard hydrogen storage pressure and range, costs, consumer acceptance, and industry risks.

### Question 1: Approach to performing the work

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

- This is a very good approach in investigating the optimal delivered pressure and understanding the tradeoff between the consumer refueling convenience and infrastructure costs. Assumptions and methodology of work are clearly stated.
- The approach provides good focus for the analysis. The initial approach has been set up very well, and the initial results are convincing, but completing the future work seems very important in order to fully address this research question.
- The approach to evaluate hydrogen fueling pressure (and hence range) to total consumer cost and consumer value is excellent and well needed. The project approach enables a better understanding of the interrelationship of storage pressure/range, infrastructure cost, hydrogen cost, and consumer value.
- The project addressed important barriers with respect to storage (cost and lifetime assessment) and market transformation (high capital cost of infrastructure for hydrogen FCEVs). The choice of hydrogen pressure (350 versus 500 versus 700 bar) is a concern, as hydrogen infrastructure rollout strategies are already being developed. The principal investigator considered direct costs of higher pressure on refueling stations and also consumer costs for the inconvenience of refueling as measured by the extra time for traveling to stations and refilling with low-pressure versus high-pressure hydrogen. The project looked at trade-offs between station costs and inconvenience costs at different pressures. The methodology for estimating consumer inconvenience could have been explained more fully. Also, it would have been good to understand the total spectrum of costs and benefits of high versus low pressure (including impacts on the vehicle cost and performance) in addition to station cost and driver inconvenience. Just optimizing with respect to station cost and the cost of consumer travel time may not be a true optimization unless other factors are accounted for. Automakers have already largely decided on 700 bar based on wanting a longer range. This should be considered in the framework of the study.
- In general, questions posed and parameters studied are good, but collaborating more with colleagues working on other station deployment-type analyses could provide better insights and different parameters to investigate.
- This project is generally effective for what it set out to do, but the goals are quite limited. The cost approach for system pressure comparisons is rational and straightforwardly executed. However, this approach does not, nor can it, account for the “annoyance factor” of having to refuel more often when at a low pressure. This factor may be significant, yet it is completely overlooked.



**Question 2: Accomplishments and progress toward overall project and U.S. Department of Energy (DOE) goals**

This project was rated **2.8** for its accomplishments and progress.

- This work has some good initial results, mainly on the method development and the case studies presented. It is good to see the sensitivity analysis and the parameters selected.
- The project has achieved significant progress towards understanding the consumer value of FCEV range versus refueling trips/time and also towards understanding optimal hydrogen fueling pressure. It would be good to see more modeling of hydrogen infrastructure clustering during the early FCEV commercialization phase. The project's modeling should be tied to consumer choice models of advanced vehicles to understand how changes in vehicle range can affect vehicle market penetration.
- The various trade-offs, sensitivities, and specific conditions were determined through this analysis, but results seem too conditional and uncertain. Perhaps a more in-depth look at some situations may help shed some more light.
- There is only modest progress in understanding the preferred pressure. The answer seems to be that it depends on a host of factors and pressure will increase with time/prevalence of FCEVs; hence, there is little actionable information in the results.
- Error bars on slides 9 or 11 might change the interpretation of the results. It was unclear if the influence on the rate of market growth was different for each type of marginal cost. This influence seems to be considered equivalent, or similarly relevant, given this comparison framework. It was unclear if the debt supporting higher delivered costs from more stations could be more easily serviced at a lower risk, with faster future market growth and the increased likelihood of future revenues. The typical patterns of interaction have been identified, but future work may change how these patterns are interpreted.
- The project has illustrated some interesting trade-offs between pressure, consumer convenience, and cost, but more remains to be done. It was difficult to tell what was being held constant and what was being varied in some graphs. It would have been helpful to tie these results to some actual plans, for example, a closer tie with California rollout plans. Using a cluster strategy like California's for the station rollout may eliminate some of the inconvenience issues raised. Also, some of the examples (e.g., 10% utilized stations) seem unlikely. Tying the work to actual plans might make it more realistic.

**Question 3: Collaboration and coordination with other institutions**

This project was rated **3.2** for its collaboration and coordination.

- This project has good collaboration with industry and other researchers.
- The project has a very good collaboration, including industry within the U.S. DRIVE Fuel Pathways Integration Tech Team, Argonne National Laboratory (ANL), and the University of California-Davis (UC-Davis).
- While not reflected in the analysis, the approach and results seem consistent with ANL and UC-Davis work, thereby suggesting adequate collaboration with those groups.
- Collaborating with colleagues working on other station deployment-type analyses would also be beneficial.
- Some additional input from industry on costs associated with modular expansion of station capacities would be useful. The sizes do not have to be fixed. The project could be improved by more input on financing options, or influence of station clustering strategies.
- This project has good collaboration with national laboratory researchers to understand varying station costs relative to dispensing pressure. The project has adequate collaboration with the fueling industry, but more collaboration with vehicle original equipment manufacturers (OEMs) is needed. The project would also benefit from more collaboration with researchers investigating initial hydrogen infrastructure rollout strategies.

#### Question 4: Relevance/potential impact on advancing progress toward DOE research, development, and demonstration (RD&D) goals

This project was rated **3.5** for its relevance/potential impact.

- The topic is highly relevant to understanding market barriers and research and development focus.
- Understanding the pros and cons of high pressure is a very important topic. With more realistic scenarios, this project could have even more value.
- As plans are made for early market infrastructure development, looking into factors such as required fueling pressures is important.
- This project provides vital information on station development and deployment, the consumer value of FCEVs relative to range, and the trade-offs between FCEV performance and cost necessary to lower the overall cost of FCEV ownership to consumers.
- This work is very relevant to DOE's objectives and will contribute to the understanding of what could be the optimal hydrogen fueling pressure in terms of infrastructure costs, energy usage, and consumer acceptance for the market penetration of FCEVs.
- Because of limitations in the approach and accomplishments, there is limited actionable information from this project.

#### Question 5: Proposed future work

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

- The proposed steps will moderately strengthen the project results.
- The proposed future work shows a good path towards the main goals and barriers of this project.
- The proposed work related to demand, risks, and financial parameters is important, as it will make the analysis more realistic and can provide significant insights.
- The proposed extension is good, especially for looking at the cluster strategy. Also, exploring other tradeoffs through a consumer choice model would be interesting.
- The proposed future work is appropriate. The project as explained should be expanded to model hydrogen infrastructure clustering in the initial rollout phase, and should be integrated with vehicle choice models.
- It is good to set up a logical framework to compare marginal costs. However, some additional consideration is needed on the large uncertainties and multivariate nature of consumer perception compared to financing options for station costs. Both types of costs can be managed in different ways, and the options for doing so seem relevant to this framework. Station costs can be financed and risks managed in various ways, perhaps through partnerships or contracts, while consumer behavior is highly variable and can also be "managed" or influenced in multiple ways. Given the different nature of these options, it seems fair to ask if this is really an apples-to-apples comparison of marginal costs. If some of these management options are easier to implement than others, or are inherently lower-risk, that should be reflected in this framework. Modeling cluster rollout strategies will require some estimate of the local density of early adopters. Variations in this density (or market depth) will be relevant to the station availability metrics, so it needs to be included explicitly in this future modeling effort.

#### Project strengths:

- The conceptual approach is on target.
- This project highlights the important trade-offs.
- This project addresses an important question with respect to choosing the best pressure.
- This work uses very good analysis tools and has very good interaction with its collaborators.
- The project provides a vital understanding of the consumer value of hydrogen storage pressure, and thus range. This work helps DOE better understand how hydrogen dispensing pressure can be optimized to increase consumer value and lower infrastructure needs and subsidies during the commercialization phase of FCEVs.

**Project weaknesses:**

- This project still has several uncertainties and key parameters to consider.
- It would be beneficial to this work if there is some input/feedback from the OEMs.
- More emphasis is needed on the initial FCEV commercialization phase and what the implications of this research are for DOE’s funding of hydrogen fueling infrastructure. The project needs more feedback from vehicle OEMs.
- The research question probably requires a more extensive analytic context to be addressed fully and to generate results that can be used to inform concrete policies. Additional work is needed beyond this phase (year) of the project to fully understand the analysis problem.
- The project approach does not account for the “annoyance factor” of having to refuel more often when at a low pressure (beyond the actual extra minutes spent in the station, if any). The conclusions are highly dependent on the number of FCEVs and the value of time. The first is a constantly changing number, and the second both is hard to quantify and differs from person to person.
- The framework for assessing the choice of pressure could be broader. The OEMs have already largely decided on 700 bar because they want a longer range, but this is not included in the analysis. This project should consider more realistic rollout cases, including clustering and station utilization that is reasonable over time.

**Recommendations for additions/deletions to project scope:**

- This project should broaden the framework.
- Although the initial project funding was relatively low, the proposed future plans will probably not strengthen the project sufficiently to be worth the additional expense.
- Results and insights from this study could be integrated into other infrastructure studies. This project should collaborate closely with the financial scenario analysis of deployment strategies investigated under project AN-042, Systems Analysis.
- The modeling cluster rollout strategies will require some estimate of the local density of early adopters. Variations in this density (or market depth) will be relevant to the project’s metrics for station availability, so they need to be included explicitly in this future modeling effort. There should be explicit inclusion of policies or financing options, and consumer convenience options, such as station clustering, onboard informatics, etc.

## Project # AN-034: Life Cycle Analysis of Hydrogen Onboard Storage Options

Amgad Elgowainy; Argonne National Laboratory

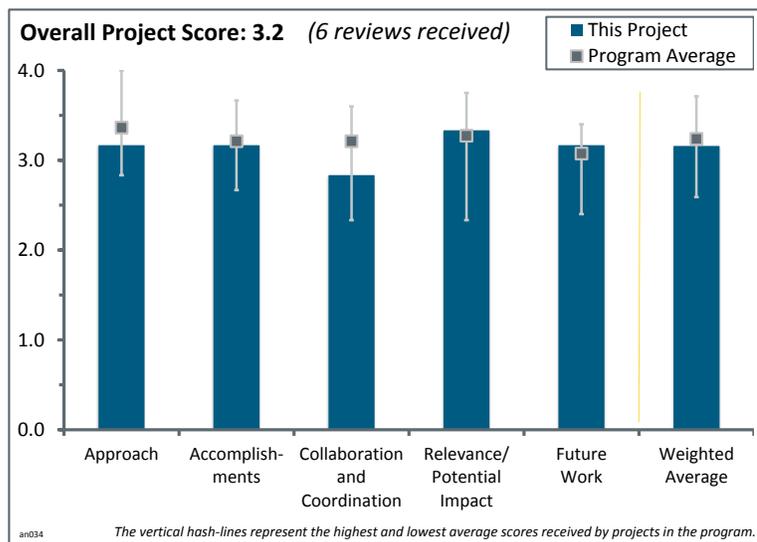
### Brief Summary of Project:

This project evaluated the impact of hydrogen storage technologies on energy and emissions for fuel cell electric vehicles (FCEVs). Onboard hydrogen storage contributes 15% to 23% of the vehicle manufacturing cycle and 3% to 5% of the total life cycle analysis (LCA) greenhouse gas (GHG) emissions. The data can be used to update the Greenhouse Gases, Regulated Emissions, and Energy Use in Transportation (GREET) model to evaluate emerging hydrogen production, delivery, and FCEV technologies.

### Question 1: Approach to performing the work

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

- This is a good approach using available data and appropriate sources, for the most part. The project needs to incorporate information obtained from additional technical teams.
- The utilization of the GREET modeling tool for this work provides an excellent approach for addressing project deliverables. The data sources used for the analysis are very appropriate for this work.
- The use of the GREET model is a good choice. The analysis has been carefully done. While the decision to use current practices for estimating life cycle impacts is understandable, it is probably misleading. By the time any of the pathways (with the possible exception of onsite steam methane reformers [SMR]) are actually implemented at a large enough scale to matter, the technology will be substantially different, and the energy sources and processes for manufacturing inputs will be less carbon-intensive (unless the project is not attempting to mitigate GHG emissions at all, in which case the project should not bother measuring them).
- The overall approach of the GREET model for LCA is excellent, and the GREET model is the de facto model for assessing transportation-related energy use and emissions. The approach for evaluating hydrogen storage systems, including literature assessments, simulation results, and interaction with storage researchers (particularly through the storage technical teams), is excellent. Likewise, the project team's approach to FCEV manufacturing using literature, simulations, and interactions with original equipment manufacturers (OEMs) is sound. Although the GREET model is an excellent tool for conducting fuel cycle (well-to-wheels [WTW]) evaluations of energy use and emissions in transportation, more interaction with U.S. Department of Energy (DOE)-funded analysts and modelers is needed to ensure consistent analyses of hydrogen-fueled fuel cell vehicles. In particular, the project team needs to ensure that assumptions used in their GREET modeling reflect DOE's standard assumptions, particularly as reflected in the Hydrogen Analysis (H2A) production model, H2A Delivery Scenario Analysis Model (HDSAM), and the Hydrogen Demand and Resource Analysis Tool (HyARC).
- The approach appears to be a standard LCA GREET approach.
- The approach is adequate and uses existing tools. There is a question as to the validity of the tools; it is unclear if they are validated. It would have been more convincing if a quick validation test was included.



**Question 2: Accomplishments and progress toward overall project and U.S. Department of Energy (DOE) goals**

This project was rated **3.2** for its accomplishments and progress.

- The incorporation of additional modules and functionality into GREET is progressing.
- This work improves existing comparisons of GHG pathways and should allow for good comparisons to battery electric vehicles and plug-in hybrid electric vehicles in terms of range.
- The preliminary results presented for several FCEV onboard options show very good accomplishments towards the main objectives of this work. The analysis of the comparison between these storage options will provide very valuable information to DOE's Hydrogen and Fuel Cells Program (the Program), mainly to its hydrogen storage R&D efforts.
- The task has been done well, but the premise of using the current practices will likely lead to misleading conclusions.
- Progress is good but could be better for the funds expended. Using the system for more cases would be cheaper each time.
- This project has made excellent progress towards evaluating the life-cycle energy and emissions intensity of various hydrogen storage systems. However, many of the findings are still cited as preliminary, and the evaluations need to be finalized. The WTW analysis conducted under this study appears to be more regional in scope, particularly regarding liquefaction emissions. The study should be expanded to include a national-level analysis, either by using a national-level electricity mix or by ensuring that appropriate delivery distances are used for potentially remote liquefaction plants. WTW analyses should be compared and contrasted to other DOE-funded WTW analyses. At the same time, the project should ensure that assumptions are consistent with DOE-funded analyses and modeling.

**Question 3: Collaboration and coordination with other institutions**

This project was rated **2.8** for its collaboration and coordination.

- There is good collaboration with the Hydrogen Storage Engineering Center of Excellence (HSECoE). In the future, it might be a good idea to show how each of the collaborators and partners contributed to the analysis work.
- The University of Michigan has significant LCA and automotive expertise.
- The industrial stakeholders are not described; otherwise, the only collaboration is with the National Renewable Energy Laboratory.
- This project needs to vet results with additional U.S. DRIVE Tech Teams. The lack of any impact on other parts of the vehicle (slide 14) cannot be correct. There must be an impact on, for example, vehicle structure for a storage system that weighs substantially more than another storage system.
- It is not clear which industry stakeholders were involved in this project or which industries were represented. The project relies on industry stakeholders for the development of storage and FCEV manufacturing emission factors. The project team needs to include more interactions with other DOE-funded researchers and modelers, particularly in regard to hydrogen fuel-cycle analysis, to better ensure that consistent assumptions are used in DOE's WTW analyses.

**Question 4: Relevance/potential impact on advancing progress toward DOE research, development, and demonstration (RD&D) goals**

This project was rated **3.3** for its relevance/potential impact.

- The GHG emission load of all the various components is valuable to know.
- The impact will be more significant in the context of comparing a total portfolio of options.
- The additional functionality and improved data will serve the GREET user community well.
- This project addresses a vital understanding of life-cycle energy use and GHG emissions associated with hydrogen and FCEVs.
- Providing an LCA for various FCEV onboard storage options is of great relevance to the Program's goals.

- This project would be more useful if it were based on the premise that FCEVs are likely to claim a significant market share after 2020, perhaps after 2025; that is the time frame and technological status to focus on. This likely requires scenarios, but so be it.

### Question 5: Proposed future work

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

- Continued improvements and added functionality are important for the GREET community.
- The proposed future work will provide a good expansion for the already robust GREET tool and will clearly be of great benefit in providing excellent LCA support to the Program.
- This project should include comparisons to cost estimates and “service” or “refueling experience” provided to consumers, where they exist.
- It would be good to see more examples of components and the methods applied to lots of other components that DOE is interested in. Plans for this are not specified.
- This work will get to future technologies next, which is where it should have started. This will require formulating scenarios or alternative technological and policy contexts. That needs some attention.
- The future work involving updates and improvements to the GREET model is necessary and appropriate. Technical support for DOE-funded researchers investigating transportation-related energy and emissions is crucial. The project team needs to work with other DOE-funded hydrogen researchers to ensure consistent analyses across the DOE Fuel Cell Technology Office.

### Project strengths:

- This project was carefully conducted and peer reviewed.
- The use of GREET as the modeling tool provides very credible results for this work.
- Comprehensive treatment has been given to this project, but it could do with a validation test.
- This project is consistent with the GREET framework, and its input assumptions are consistent.
- This project has a strong team with unique experience and good access to expert information.
- The GREET model is the de facto model for characterizing transportation-related energy use and emissions.

### Project weaknesses:

- It would be a good idea to show how each of the collaborators and partners contributed to the analysis work.
- This project has limited collaboration and vague plans to apply methodology to other situations.
- The pathway impacts today are not important compared to the pathway impacts for 20-plus years from now.
- This project needs a broader context of storage options for vehicles, but the funding level does not allow this.
- The assumptions of hydrogen pathways within the GREET model are not always consistent with other DOE-funded models.
- The lack of system-wide impact with changing storage systems is difficult to understand. In-depth analysis of the results is needed to confirm the results presented.

### Recommendations for additions/deletions to project scope:

- This project should extend to other applications and try to develop a methodology.
- This project should carefully develop a set of premises for future assessments based on when the market shares of FCEVs are likely to be large and when the stock of FCEVs is likely to be valuable. This project should consider policy contexts that are consistent with an effort to transition to low-carbon, low-petroleum vehicles.

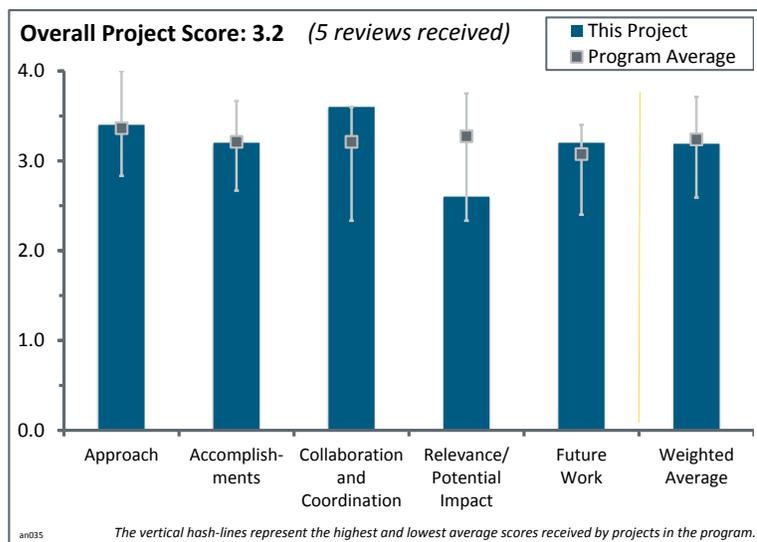
- Greater focus should be placed on operational dynamics and impacts on overall vehicle design, such as lightweighting, etc. This would be an important improvement. It seems like collaboration with other HSECoE vehicle modeling activities would be appropriate.

## Project # AN-035: Employment Impacts of Infrastructure Development for Hydrogen and Fuel Cell Technologies

Marianne Mintz; Argonne National Laboratory

### Brief Summary of Project:

This project provides a consistent platform to analyze employment and other economic impacts of alternative hydrogen and fuel cell investments and assist the U.S. Department of Energy (DOE) and stakeholders with data acquisition/validation and analysis to estimate the economic impact of deploying fuel cells and hydrogen infrastructure in early markets. The platform uses input-output economic modeling within the context of user-friendly tools—JOBS FC and JOBS H2—to calculate supply chain and induced employment, earnings, and economic output.



### Question 1: Approach to performing the work

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

- This provides a methodical look at jobs creation related to technology introduction and use.
- This project makes good use of a number of different models and tools from a variety of sources.
- This project uses an excellent and in-depth modeling approach to estimate hydrogen- and fuel cell-related job growth, and includes appropriate user feedback and linkages to design parameters and costs developed through other DOE research programs.
- Other than needing more real-world data, the approach is very sound.
- One reviewer did not enter a response.

### Question 2: Accomplishments and progress toward overall project and U.S. Department of Energy (DOE) goals

This project was rated **3.2** for its accomplishments and progress.

- A significant amount of work has been accomplished for the amount of funding provided by DOE.
- This project has made good progress, especially given the low funding level.
- The investigators have made excellent progress in developing the JOBS FC tool and evaluating the employment impacts of fuel cell deployments funded by the American Reinvestment and Recovery Act (Recovery Act). It would be great to see this model and approach applied to transportation-related fuel cell and hydrogen infrastructure deployments.
- The various components and structure of fuel cell and hydrogen infrastructure-related jobs have been modeled well and provide a good understanding of related jobs, but more granularity, such as the types of jobs, education levels needed, temporary/long-term nature, if we have the required workforce now, etc., would provide much more realistic and useful insights.
- This tool helps advance DOE goals to show the job/economic potential of fuel cells, although results are not that impressive (assuming an outsider's point of view). This project also supports Recovery Act spending. The project is still in the process of completing other major tasks, so there is more to be done before this project is complete. The hydrogen model will be very useful, particularly since infrastructure is so far behind fuel cell manufacturing right now.

**Question 3: Collaboration and coordination with other institutions**

This project was rated **3.6** for its collaboration and coordination.

- This project has an excellent set of relevant partners.
- This project has reached out to appropriate stakeholders for feedback.
- Efforts to interact with many relevant stakeholders should be continued.
- This project has good collaboration with groups, customers, companies, etc.
- The project included a wide range of national laboratory researchers in the development of the JOBS FC tool and received good input from industry and industry trade groups for data collection and model validation.

**Question 4: Relevance/potential impact on advancing progress toward DOE research, development, and demonstration (RD&D) goals**

This project was rated **2.6** for its relevance/potential impact.

- This could be a useful tool for local and state governments to use when evaluating the impacts of new industries.
- Hydrogen models will be tremendously useful to convince key stakeholders to install stations, which are much needed for vehicle rollout.
- While this project does not directly help DOE achieve progress towards its technical targets for fuel cell and hydrogen infrastructure, it is crucial that DOE evaluate the impact of these technologies on job creation to help the broader community understand the role fuel cell technologies can play in the U.S. economy. Showing the potential for job creation will help DOE be able to provide continued funding for fuel cell and hydrogen research and development (R&D). It would be useful if the investigators could apply the JOBS FC tool and methodology to transportation-related fuel cells.
- It is not clear how these results will be used to support end-user needs. There is some concern over using results inappropriately or out of context, but it is not clear how the researchers can compensate or manage this.
- The issues of job creation and related economic impacts are valid considerations, but the findings will likely not have a significant impact on R&D goals and objectives unless more granularity is provided and these analyses are tied closely to other modeling/analysis efforts and put into context (i.e., comparison with jobs in other sectors, including other clean energy sectors).

**Question 5: Proposed future work**

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

- The project has a good plan to complete work in a timely manner, dependent on receiving funds.
- So many avenues could be pursued to expand this model; this project needs to focus on the most valuable to move the industry forward.
- It sounds ambitious to include novel station options, training, and combined heat, hydrogen, and power, all within a comparable budget.
- As the model is expanded, the project could consider integrating the various modules (like fuel cell, hydrogen infrastructure, and other applications) so that these components are analyzed in a more integrated and holistic way and so that interactions can also be considered.
- This project definitely needs to be expanded to hydrogen station rollouts and transportation-related fuel cells, as the investigators suggested. It would be useful to use the JOBS FC tool and methodology to understand the potential for job creation that could occur under various scenarios for fuel cell vehicle commercialization (that is, use the JOBS tool to predict job growth for potential penetrations of fuel cell electric vehicles [FCEVs]; do not limit analyses to estimations of jobs created from actual fuel cell deployments).

**Project strengths:**

- This project has good collaboration with key groups.
- The connection to the analysis capabilities of RCF Economic and Financial Consulting, Inc. improves on the project's methodology.
- This is a methodical approach. The principal investigator has a good understanding of the intricacies of job creation impacts.
- The JOBS model and the project's estimations of job creation provide valuable information to the administration and to legislators to support and justify continued public funding of fuel cell and hydrogen technologies.
- This project can provide some insights and answers relating to employment and economic benefits when these types of issues are of focus and answers are needed. This project can enhance the explanation of benefits for developing a hydrogen fuel cell infrastructure.

**Project weaknesses:**

- This project needs more granularity to be able to provide more realistic and useful insights.
- This project needs better promotion of the tool to the right people, such as investors, fuel cell companies, and especially policy makers who could create favorable policies or initiatives to entice companies to build or expand facilities once they learn about job potential.
- It is not clear how the results can be used in the appropriate policy context, especially when comparing hydrogen to other technology options. Some concerns that results may be misused include the possibility that they are not conveyed in the appropriate context. The end-user tool needs to account/control for this somehow.
- The project should be expanded to estimate job impacts beyond Recovery Act-funded fuel cell deployments. The project should expand to include transportation-related fuel cell deployments and also evaluations of transportation-related fuel cell commercialization scenarios.

**Recommendations for additions/deletions to project scope:**

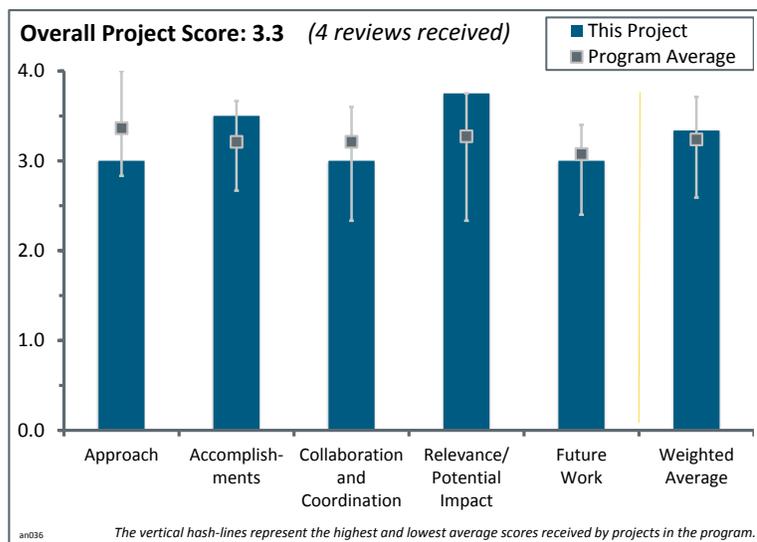
- The project should be expanded to include hydrogen infrastructure deployments and deployments of FCEVs.
- Factors such as the types of jobs, education levels needed, if jobs created are temporary or long-term in nature, if the required workforce is available now, etc. should be considered to provide granularity and depth to the results achieved. It would be beneficial to place the results found into context, such as showing how these numbers compare with other clean energy jobs or jobs created in other sectors.
- With Bloom Energy selling many megawatts of solid oxide fuel cells (SOFCs) to customers and expanding to the East Coast with a Delaware manufacturing facility, the tool should include SOFCs. It seems like it would add tremendous value to the JOBS tool since they are growing so much. SOFCs could also include smaller systems developed via the Solid State Energy Conversion Alliance (SECA) program and companies such as Delphi, Acumentrics, etc. for auxiliary power units and remote power. The project needs to do this first before other proposed work.

## Project # AN-036: Pathway Analysis: Projected Cost, Well-to-Wheels Energy Use and Emissions of Current Hydrogen Technologies

Todd Ramsden; National Renewable Energy Laboratory

### Brief Summary of Project:

The objective of this project is to conduct cost and life-cycle energy and emissions analyses of the complete supply chain of ten current-technology hydrogen pathways using the National Renewable Energy Laboratory's Macro-System Model (MSM) to evaluate hydrogen cost, energy requirements, and greenhouse gas (GHG) emissions. Detailed documentation of all input and output parameters and modeling results was developed by the project team and reviewed by industry partners. Detailed hydrogen costs and capital costs were developed for all hydrogen pathways; and upstream energy, feedstock usage, and GHG emissions were reported. The total fuel cell electric vehicle (FCEV) cost of ownership was analyzed, including fuel cycle and vehicle cycle.



### Question 1: Approach to performing the work

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

- The use of the MSM for hydrogen pathway analysis provides a very good approach towards this work, as that model is based on already well-established tools such as Hydrogen Analysis (H2A), the H2A Delivery Scenario Analysis Model (HDSAM), and the Greenhouse Gases, Regulated Emissions, and Energy Use in Transportation (GREET) model, which provide very credible data.
- This is a highly appropriate choice of models and analysis tools. The decision to analyze current production methods and costs makes the analysis hypothetical, since by the time there are significant quantities of hydrogen produced for vehicles to justify using most of the pathways, the current production methods and costs will likely not apply. Therefore, use of current technology may seem like the most concrete and realistic case, but it is actually a hypothetical case for these pathways. This detracts not from the accuracy of the analysis but from its usefulness. It does have usefulness as a reference point: no technological change, no additional regulation of emissions, etc. For technologies that are likely to be deployed in the early transition, the cost analysis is much more useful. The peer review by the U.S. DRIVE Fuel Pathways Integration Technical Team (FPITT) is an important validation and increases the value of the research.
- The study addressed important barriers to understanding hydrogen supply costs. The study focused on near-term hydrogen infrastructure technologies but also assumed that they were deployed at large scale (for example, large-scale biomass gasifier systems with pipeline delivery to a network of stations). This was somewhat of a contradiction since FCEV market penetration is unlikely to reach these levels until 2020 or beyond (i.e., beyond the near-term technology timeframe). Overall, the time frame of the analysis needs to be clarified. It is unclear how the near term is defined. Some important near-term supply routes, such as central steam methane reforming (SMR) with truck delivery, were not considered. This seemed like an important omission, as nearly all hydrogen transportation fuel for the next five years will probably come from this pathway. Also, it would be helpful to see how the various hydrogen pathways' GHG emissions compare to other fuels and electricity.
- The approach appears to be valid but perhaps not sharply focused enough. A concern is the results from the various modeling tools. It is not clear if the results are validated. The data sets are so diffuse it is somewhat

hard to see if the results might not be undermined by a simple spreadsheet error. It is not clear what the safeguards are.

### **Question 2: Accomplishments and progress toward overall project and U.S. Department of Energy (DOE) goals**

This project was rated **3.5** for its accomplishments and progress.

- The accomplishments of this work are very good, and the results for all the current hydrogen pathways have been reported in a very clear and detailed form.
- Although the final report is not yet published, progress towards the stated goals of the project is impressive and the report will undoubtedly will be published soon.
- Lots of work has been done, which is gratifying, but some validation tests would be more convincing.
- This study did examine costs and emissions for a variety of pathways at large scale. It would have been good to see comparisons of the results with other modeling efforts that have estimated the entire supply chain cost (for example, studies of the National Research Council of the National Academies on hydrogen, academic studies, etc.). It is unclear how the results compare to industry estimates.

### **Question 3: Collaboration and coordination with other institutions**

This project was rated **3.0** for its collaboration and coordination.

- It seems like there was a good review of assumptions through FPITT.
- It was very good collaboration to include national laboratory and industry feedback through FPITT.
- The collaborative activities are not clearly described. Collaboration is only with national laboratory sources. It would be better to use industry sources as well as government sources.
- There is good collaboration and good use of the FPITT for peer review. Different stakeholders have different views of what the status of the technology for each pathway will be by the time the pathway might be used in the future. These views need to be somehow systematically considered in deciding on the premises for the analysis.

### **Question 4: Relevance/potential impact on advancing progress toward DOE research, development, and demonstration (RD&D) goals**

This project was rated **3.8** for its relevance/potential impact.

- This is clearly very relevant, as it guides other research goal setting. Thus it needs a better validation test.
- The systematic evaluation of these pathways for cost and lifecycle emissions is critical to the overall systems analysis effort.
- Estimating the costs and emissions for different pathways is highly relevant to DOE's Hydrogen and Fuel Cells Program (the Program). This project combined models to accomplish this. The impact of the results could have been improved by a more careful definition of timeframe and focus.
- This work is very relevant to Program goals, as it provides a detailed cost and lifecycle energy and emissions analyses of several hydrogen pathways. This work will provide good guidance towards the initial rollout of FCEVs and hydrogen infrastructure.

### **Question 5: Proposed future work**

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

- The evaluation of pathways using future technologies is essential. There is also a critical need to understand how pathways will evolve and change during a multi-decade transition.
- It would be interesting to see results for future technologies. The principal investigator should also consider how the grid might be de-carbonized by then.

- The proposed work of including pathway analyses for advanced hydrogen technologies is a good complement for the actual work, but since the project is complete, it is not very clear how this will move forward.
- This question is not applicable as the project is completed.

**Project strengths:**

- This is a relevant and comprehensive study providing important information.
- The use of well-established modeling tools is a strength of this project.
- The choice of modeling tools, rigor of the analysis, and peer review are all strengths.
- This project combined well-developed existing DOE models via MSM to look at important problems.

**Project weaknesses:**

- As the project is complete, it is not very clear how the proposed work will move forward.
- The validation of methods and data is a weakness. It is not clear if the tools use spreadsheet methods and whether that could cause errors.
- The timeframe needs to be better defined. Some key pathways were missed (such as central SMR with truck delivery).
- The key focus should be on future technologies and the evolution of the system jointly with other energy supply and conversion systems and with manufacturing methods. The case in which an economy transitions to hydrogen-powered vehicles and greater use of fuel cells while failing to reduce GHG emissions from electricity generation and other key systems should be considered an unusual (probably illogical) scenario.

**Recommendations for additions/deletions to project scope:**

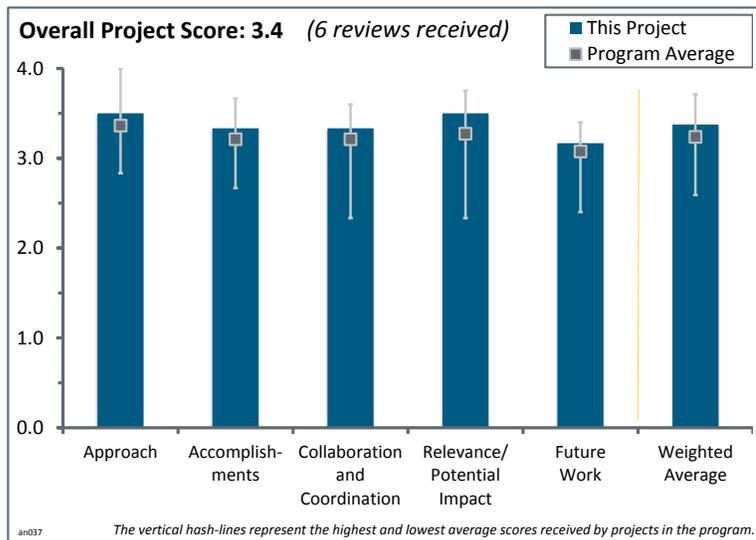
- This project concept should keep going and should give greater attention to advanced liquefaction pathways.
- There should be a comparison between well-to-wheels GHG results and other fuels/vehicles. Researchers should compare cost results with other studies.

## Project # AN-037: Hydrogen from Biogas: Resource Assessment

Genevieve Saur; National Renewable Energy Laboratory

### Brief Summary of Project:

This project addresses resource availability for renewable hydrogen, which provides alternatives to traditional sources of hydrogen, hedges against fluctuation in costs and demand for fossil fuels, and aids compliance with state policies for renewable fuels. The project updates prior studies on hydrogen from methane from wastewater treatment, landfills, and manure management, and expands analysis to include methane from industrial processes and organic food waste. Biogas has a diversity of geographic availability and can help support early market fuel cell electric vehicle rollout.



### Question 1: Approach to performing the work

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

- This project addresses the quantity and locations of biogas sources with estimates of vehicles that could be supported by the sources, and also includes economics and potential application models for future work.
- The inclusion of waste water treatment plants (WWTP), landfill gas, animal manure, industrial sources, and organic food waste for the resource assessment is a good approach. Also a good contribution to this work is the expansion of the analysis to include net availability by assessing resources currently in use.
- This is an important area to investigate; using waste for fuel solves many environmental problems on top of emissions, such as reducing solid waste, etc. Working with different government agencies to obtain data and final products has real-world value. It is key that animal waste as a source is part of the approach. This is a very targeted methodology and should yield accurate and useful projections.
- The project has a very clear approach to the problem of assessing biogas resources, with methods and data sources clearly stated. Geographic information system (GIS) tools are excellent for visualizing results. This is an excellent approach to helping understand this resource and addressing DOE Hydrogen and Fuel Cell Program (Program) barriers with respect to information on renewable resources for hydrogen production.
- Two reviewers did not enter a response.

### Question 2: Accomplishments and progress toward overall project and U.S. Department of Energy (DOE) goals

This project was rated **3.3** for its accomplishments and progress.

- This project appears to be on track to meet the proposed scope of work.
- The initial estimates presented show some good progress toward meeting the main work objectives.
- This project is moving along very well in terms of addressing its goal of assessing biogas as a resource. The methodology has been implemented for some cases. The presentation of the results was clear and concise. The project needs to establish that this is reasonable progress (30% complete) considering that the project ends in approximately two months. It is unclear if there was an issue with timely funding because of continuing resolutions or if there were other issues.
- Determining the net amounts of resource availability will result in a more accurate and complete estimate.
- The project is not complete, but it has made substantial progress so far with projections and mapping.

**Question 3: Collaboration and coordination with other institutions**

This project was rated **3.3** for its collaboration and coordination.

- This project has had good collaboration with key government agencies, such as the Environmental Protection Agency (EPA), U.S. Department of Agriculture (USDA), etc.
- There seems to be some good collaboration with EPA and USDA for the data sources.
- There is appropriate collaboration with DOE, national laboratories, USDA, and the industry.
- This project uses a variety of source data and partners, such as the USDA.
- This project has good awareness and utilization of data sets from other organizations. The audience pointed out opportunities for further collaborations.

**Question 4: Relevance/potential impact on advancing progress toward DOE research, development, and demonstration (RD&D) goals**

This project was rated **3.5** for its relevance/potential impact.

- This project has a very large impact. This is one of the areas that need to be focused on.
- Hydrogen from biogas is relevant to DOE, as it is one source of renewable hydrogen.
- Utilizing biogas resources provides a renewable hydrogen pathway while also serving as a value-add to waste management processes and environmental considerations.
- The project supports the concept of using waste as a hydrogen resource. The concept is highly appropriate; key information, analysis, and models to support decisions and specific applications are intended for future work.
- This project definitely supports DOE goals and could help alleviate the need to build hydrogen stations by utilizing WWTPs, landfills, and farms to generate hydrogen. This project also helps by acting as a showcase for using waste in a way that not only provides clean fuel for fuel cell electric vehicles but also eliminates costs and environmental problems associated with solid waste, burning or flaring gas, etc.
- This is an important and relevant topic to Program goals. Strictly on a resource basis, biogas appears to be a near-term renewable source for hydrogen that could fuel a percentage of the U.S. fleet if fuel cell vehicles were fueled with biogas-derived hydrogen. To judge the competitiveness of biogas and hydrogen, the quality of the hydrogen obtained and the costs still need to be assessed, but that assessment is not part of this project.

**Question 5: Proposed future work**

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

- The proposed techno-economic analysis and the cost and biogas quality implications will be very good additions to this current work.
- There is a good plan for follow-on work. Biogas availability might also be correlated with analysis of combined heat and power (CHP) and combined heat, hydrogen, and power (CHHP) options.
- The future work, including additional feedstocks, economic analysis, and costs, is appropriate and should be undertaken. The existing work is currently not sufficient to support decisions and applications.
- Looking into biogas quality requirements and related costs will aid in determining the feasibility of these pathways, while assessment of biogas from industrial processes and food waste will highlight other potential renewable hydrogen pathways. Both aspects are important to gaining insights which will be valuable to related research and development.
- This project has lots of potential for future work. Including lipids could open a new market with fast food restaurants. This project needs to publicize its findings and report them to key stakeholders and markets, such as industrial farming, etc.
- The project needs a better tie-in with competing sources. Clean-up costs need to be incorporated, but it seems like this is already in the plan, which is good. An analysis of pipeline-ready gas is also needed.

**Project strengths:**

- This is a very important project. The assessment seems sound.
- Biogas-to-hydrogen is relevant to DOE as a source of renewable hydrogen.
- This project is low cost and serves as a good first step to identifying the source, quantity, and locations of hydrogen feedstocks.
- This project highlights the potential of a resource that is normally a waste but can provide a renewable hydrogen production pathway.
- This project is innovative, showing how to create an opportunity from waste. This project is useful and necessary, especially with the gap in hydrogen infrastructure development.
- The methodology was well thought-out and executed. This project addresses important issues assessing near-term renewable resources for hydrogen production from biogas.

**Project weaknesses:**

- The limited funding restricts the scope of this project.
- The project should be sure that all relevant data sources are included.
- To be really useful, there should be a better assessment of how hard this source of methane would be to use as “dirty” gas. This gas could be burned, but it is unclear whether there are extra costs related to the conversion to hydrogen.
- There are still a lot of issues that need to be resolved in order to gain a full understanding, such as the cost of biogas clean-up, competing uses, net resource amounts, etc. Without these factors investigated, the full and real potential of this pathway cannot be defined.
- The existing work is limited and is not directly tied to future work unless additional funding is provided. Additional work should be considered for funding with the objective of providing analysis/creating economic models to support decision making. Additional work should also consider models that include the value of waste management, greenhouse gas (GHG) reduction, and applications for electricity and thermal energy for comparative purposes.

**Recommendations for additions/deletions to project scope:**

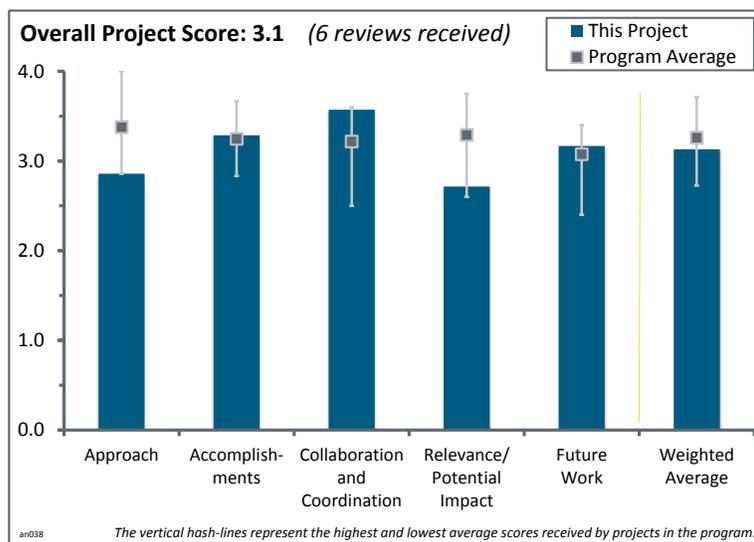
- The plans to incorporate cost are good.
- This project could also correlate biogas availability with regional analysis of CHP and CHHP options from biogas.
- This project should compare the costs of biogas clean-up, processing waste-to-hydrogen-to-removal (solid waste), and environmental clean-up (solid waste lagoons spilling into soil, water, etc.).
- This project could consider future trends in biogas availability. City population, waste resource availability and distribution, etc., should be considered. For example, as landfills fill up and waste treatment/handling methods change, population increases, etc., the nature of the availability and the quality of related feedstock for biogas will also change. It is important to also consider other competing uses of biogas.
- Additional work with the objective of creating analysis/economic models to support decision making should be considered. Additional work should also consider models that include the value of waste management, GHG reduction, and applications for electricity and thermal energy for comparative purposes. Also, the project may be of more value if additional clean-up systems (in addition to steam methane reforming) are considered and assessed within the project analysis.

## Project # AN-038: Global Hydrogen Resource Analysis (Hydrogen Implementing Agreement, Task 30A)

Tom Drennen; Sandia National Laboratories

### Brief Summary of Project:

This project aims to analyze potential hydrogen production and distribution pathways for countries participating in the International Energy Agency (IEA) Hydrogen Implementing Agreement (HIA) Task 30 (Global Hydrogen Systems Analysis), the overall goal of which is to perform comprehensive technical and market analysis of hydrogen technologies and resources, supply and demand related to the projected use of hydrogen in a low-carbon world. Another objective of Subtask A is to develop a user-friendly pathways analysis tool that allows users to understand the resource options and constraints to meeting future hydrogen demand for various fuel cell electric vehicle market shares, as well as to estimate potential petroleum savings and greenhouse gas emission reductions associated with various scenarios.



### Question 1: Approach to performing the work

This project was rated **2.9** for its approach.

- The study has a very comprehensive scope looking at hydrogen supply options in a diverse set of countries. The study sought information about future hydrogen supply within the context of each country, rather than imposing a standard view. This open-minded approach was good in that it was more likely to elicit country-specific information and give a more nuanced global view. The study did set up a single model, which optimized the system for low cost in each country separately. It appeared from the presentation that the constraints and policies were varied by country. This gives a more realistic view of which resources were most likely to be developed, which seems like a possible approach. But it did make the results more difficult to interpret, unless these constraints and policies were cataloged during the project. The study did address a key need for the DOE Hydrogen and Fuel Cells Program (Program) to know more about international markets and supplies of hydrogen, and the study filled in information gaps.
- Development of a hydrogen pathway analysis tool for consistent analyses coupled with country-specific data is a good approach to conducting multi-country hydrogen production and delivery evaluations. Development of a hydrogen analysis tool by leveraging the U.S. Department of Energy's (DOE's) work on Hydrogen Analysis (H2A), H2A Delivery Scenario Analysis Model (HDSAM), and the Macro-System Model (MSM) is an excellent way to reduce development time and costs and ensure consistency with hydrogen analyses conducted within the United States. There are a number of U.S.-specific analyses of resources available for hydrogen production, full hydrogen pathway costs, hydrogen pathway greenhouse gas emissions, etc. It would have been better if this investigation could tie into and build on those efforts rather than replicating them.
- This high-level modeling approach allows for international communication of goals and intentions for hydrogen production pathways. The approach is, however, missing a key near-term low-carbon pathway: steam methane reforming plus carbon capture and sequestration. Additionally, long-term carbon negative pathways, such as biomass/algae gasification plus carbon capture and sequestration, are not shown. The global impact of these two pathways may be critical for economic management of transportation carbon dioxide emissions.

- The approach needs to ensure greater rigor in methodology and consistency across inputs from different countries. The project should have integrated this work with an existing global energy model and existing global energy resource estimates, especially with such limited funds.
- The background on this project is not clear. It is unclear if this project's purpose is to simply keep track of what others are doing so that the United States does not miss anything, if the team is trying to do a global market assessment, or if this a case of "all boats rise with the tide."
- It seems this is chiefly a tool for facilitating dialogue and for satisfying the requirements of an IEA implementing agreement. However, this method is susceptible to inconsistencies in assumptions across various countries. The means of resolving such problems appears to be ad hoc dialogue. There appears to be no method for ensuring consistency in assumptions about competition for feedstocks. This results in a rating of only "fair," but there are probably institutional constraints that led to the adoption of this approach; however, these should have been explicitly stated. Nonetheless, this rating might be too harsh. The use of a "least-cost" approach, given the means of obtaining input data and the decision not to rigorously validate the data provided by countries, seems inconsistent. This is a "what-if" model in which countries can input whatever data and assumptions they wish without a mechanism for checking consistency across countries; thus, the meaning of a least-cost solution for each country is unclear.

### Question 2: Accomplishments and progress toward overall project and U.S. Department of Energy (DOE) goals

This project was rated **3.3** for its accomplishments and progress.

- The project seems to be accomplishing the goals it set out to do.
- The project has made good progress on a very challenging scope. A large amount of information on hydrogen supply has been organized into an optimization framework.
- The model has been developed and used in interactions with countries. Discussions have been held with the countries involved; however, many country-specific inputs have yet to be entered in the model.
- There appears to be significant progress but little reassurance about the quality of the tool, the fidelity relative to other models, or consistency in relative resource availability across countries.
- It is acknowledged that each country has a different mindset. The development of this model is a practical stride forward for anticipating global impacts from different hydrogen pathway choices.
- There appears to have been good progress on analyzing hydrogen production and delivery pathways for a number of countries (especially European Union countries). It is not always clear whether the pathway analyses were conducted by the project team or through parallel efforts by other IEA member countries. Though this is an effort to analyze hydrogen pathways across multiple countries, it would be good to see more U.S.-specific results so that these results can be compared to other similar DOE-funded analysis efforts occurring in the United States.

### Question 3: Collaboration and coordination with other institutions

This project was rated **3.6** for its collaboration and coordination.

- The project is all about collaboration, and it appears that this objective has been satisfied.
- The collaboration with other countries through the IEA seems very good. The process of working through the HIA seems robust and productive.
- This is obviously the project's strength. There may be almost too many partners, but that is to be expected with global scope.
- It is not clear how effective collaboration is accomplished across such a long list of international collaborators. It may be the right list of collaborators, but there is some concern about effective and clear communication.
- This project includes an impressive array of collaborations with other IEA member countries, indicating a high degree of coordination and leveraging of country-specific research and analysis efforts. More collaboration with researchers within the United States would have been preferable to ensure consistency with the modeling, assumptions, and findings of U.S.-led hydrogen research. Additional collaboration with

DOE-funded investigators in the United States would be useful to better leverage DOE's funding of hydrogen research.

#### **Question 4: Relevance/potential impact on advancing progress toward DOE research, development, and demonstration (RD&D) goals**

This project was rated **2.7** for its relevance/potential impact.

- The topic is highly relevant to the Program. A major “big picture” conclusion from the study was that resource availability is not a limiting factor for hydrogen production. This has been known for a long time through other DOE studies and other IEA studies. So what seems different about this study is the attempt to understand the different contexts within each country when doing an optimization.
- If resource availability is not a limiting factor and the least-cost analysis is not robust (i.e., high fidelity with other cost models), then it is not clear what the relevance or potential impact will be (positive or negative) of making this model available to the general public.
- It is difficult to understand what the final outcome will be. If it is to foster interaction and cooperation, then this is relevant, but from a technical point of view, the project does not result in a single tool, which makes results hard to harmonize and use.
- While this effort seems to have helped countries learn from each other and start to perform analyses on a more consistent basis, there are too many considerations/assumptions, differing values, policies, etc., and each country will follow its own path. While the effort aids in some learning, this project cannot make everything completely consistent across the countries, and this effort does not seem like it will have a critical impact/benefit on DOE's RD&D objectives.
- The presentation leaves one with the impression that this is largely an exercise required by an IEA implementing agreement and that not much of substance is expected to result. Of course, that impression could be incorrect. This makes the project difficult to rate on this criterion. If this impression is correct, there is still a need for such exercises in the context of international collaboration.
- Collaboration with international groups and researchers outside the United States is a vital component of furthering fuel cell commercialization and development of hydrogen infrastructure. Though international collaboration is needed, the project team did not provide a good understanding of how this effort would help overcome specific barriers and technical challenges listed in the Fuel Cell Technologies Office Multi-Year Research, Development, and Demonstration Plan (MYRDDP). The project team should help develop feedback mechanisms to better ensure that the findings of this project tie back into the MYRDDP to overcome challenges and barriers to widespread fuel-cell commercialization.

#### **Question 5: Proposed future work**

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

- The future work proposed seems appropriate.
- The project is wrapping up; the report and journal article will be peer-reviewed.
- Perhaps the best use of insights gained from this effort is in creating a place for hydrogen and fuel cells in the overarching analysis of the IEA, thus improving visibility.
- The proposed work is appropriate to bring the project to a close and disseminate the results within IEA. It would also be good to see some comparisons with other IEA work (for example, Energy Technology Perspective series or the Mobility Model). In addition, it would be great to catalog the different policy contexts in each country and discuss how this influences the choice of hydrogen pathways in different countries.
- Completing a final report on this investigation to share results and insights with IEA analysts and the hydrogen and fuel cell community overall is crucial. Final results should emphasize lessons learned and sensitivity analyses to better understand the requirements necessary for commercialization of fuel cell vehicles.

**Project strengths:**

- This project is highly collaborative and interactive.
- The project's international partners and good, broad look at the world are strengths.
- This project has strong international collaboration and cross-country analyses of hydrogen production and delivery pathways.
- The goal of "performing a comprehensive technical and market analysis" is admirable, especially in a global context and for a low-carbon future.
- This project is very comprehensive. This is an excellent attempt to gather information, project future hydrogen pathways, and organize findings into a useful tool. This project provided a good tool to stimulate discussion in the worldwide hydrogen community.
- Discussions amongst various countries/stakeholders and an attempt to follow similar/consistent methods can provide some learning and guidance, helping countries identify issues or factors they had not considered before.

**Project weaknesses:**

- There are not any real weaknesses, but making sense of the results in diverse countries may be challenging.
- The results may be hard to use.
- This project lacks validation and checks for consistency across countries.
- There are too many stakeholders and too many diverse assumptions and considerations.
- It is not clear why a stand-alone modeling approach was used to pursue the goal of the project. Multiple international energy market models exist. The scope of the project is very ambitious, and it would require significant resources to complete a high-quality product.
- This project needs to better integrate analysis efforts with similar efforts conducted within the United States and funded by DOE. This project seems to replicate a number of analysis efforts that have been conducted within the United States. The project should do more to leverage and build upon these efforts to better ensure consistent assumptions and findings. The project should provide better feedback to DOE to help understand where additional resources and research and development is needed within the United States to aid commercialization of fuel cell vehicles, and also to share lessons learned by other countries.

**Recommendations for additions/deletions to project scope:**

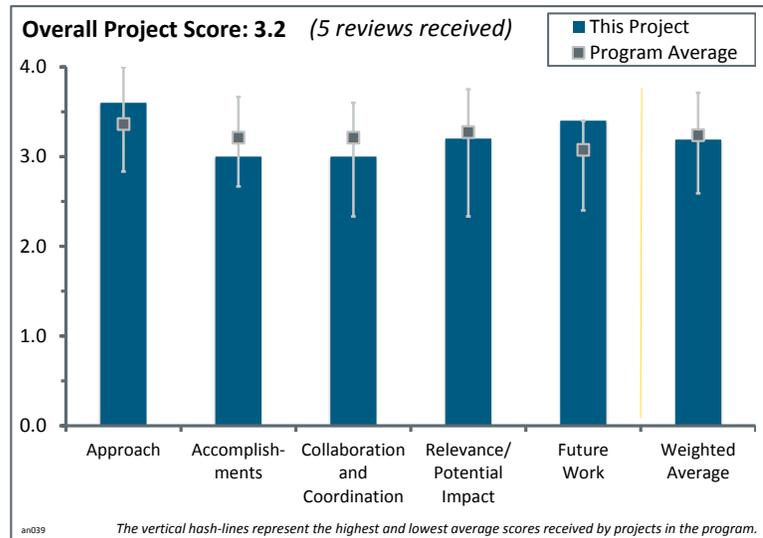
- The team should follow through with this project and wrap it up.
- This project should try to harmonize methods so countries are more comparable.
- The project should make sure all the value is extracted from the learnings in different countries. These should be written up as part of the final report. This should also be compared with the results of other, less granular global assessment models, such as IEA-MARKAL modeling.
- It would be very useful to include strategic implications of national hydrogen policies, for example, evaluating first-mover advantage/disadvantage. In light of global plans for hydrogen production, such implications should start to be visible.

## Project # AN-039: Life Cycle Analysis of Water Use for Hydrogen Production Pathways

Amgad Elgowainy; Argonne National Laboratory

### Brief Summary of Project:

The objectives of this project are to 1) establish a baseline of life cycle water consumption for baseline fuels and feedstock sources; 2) evaluate water consumption for hydrogen production processes; 3) assess the impact of feedstock sources on life cycle water consumption for hydrogen production; 4) identify major contributors in the upstream supply chain to water consumption of hydrogen pathways and identify improvements for more efficient water use; and 5) identify vulnerabilities with respect to resource availability by region for large-scale hydrogen production.



### Question 1: Approach to performing the work

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

- This project has a well-defined scope and clear approach.
- The project approach is quite simple: integrating a power water model into the existing analysis framework to track water consumption. This approach is very logical and economical (as it builds on existing models).
- The project addresses a critical issue for future energy, including hydrogen. It builds in a logical way on existing Argonne National Laboratory (ANL) water models and on the Greenhouse Gases, Regulated Emissions, and Energy Use in Transportation (GREET) model to address questions.
- The approach seems competent and adequate, but the project has not yet been implemented, so what is wrong is not yet evident. The approach should be refined as the project proceeds.
- It is a good approach to add water consumption to the GREET model for all fuels, but this project may only address water use for hydrogen production. Information and models for water consumption for all fuels are needed to support comparative analysis and decision making.
- It is unclear how well the model will handle regional issues. Using this model may require coupling with other information about regional water flows. This part of the approach could have been more fully explored (e.g., how to use this model).

### Question 2: Accomplishments and progress toward overall project and U.S. Department of Energy (DOE) goals

This project was rated **3.0** for its accomplishments and progress.

- Progress seems to be proceeding according to schedule.
- Progress is consistent but limited owing to a constraint and/or delay on funding.
- The project just started and thus has few accomplishments at this point.
- This is not really applicable because of the lack of funds. Accomplishments should be expected to roll in when funds arrive.
- The project has just been funded, so it is hard to assess progress so far. It seems like this project is off to a good start and will add value to the GREET model, and can help provide water use information to enable

regional life-cycle cost analyses as well. The initial evaluation includes plans to examine several hydrogen pathways that are major water users.

### Question 3: Collaboration and coordination with other institutions

This project was rated **3.0** for its collaboration and coordination.

- There is appropriate collaboration with DOE and ANL, and informal collaboration with the U.S. Environmental Protection Agency and the U.S. Department of Agriculture.
- It looks like there will be good collaboration within the ANL group. The project should look at the work of other groups in this area as well.
- The principal investigator and his team have lots of experience and a history of collaboration with many outside groups. The reviewer is confident there will be substantial collaboration and vetting of assumptions. However, the slides presented do not really make this case.
- Collaborations are not strongly evident in the presentation.
- There is not really enough information to judge, but it seems as though there is good collaboration with other institutions.

### Question 4: Relevance/potential impact on advancing progress toward DOE research, development, and demonstration (RD&D) goals

This project was rated **3.2** for its relevance/potential impact.

- Water availability is an often overlooked resource, and this is a timely and important study.
- Water use for energy is a highly relevant topic, and the proposed study should improve the utility of DOE's modeling toolkit.
- Inclusion of water consumption as one of the decision criteria in the GREET model is highly valuable for comparative analysis and decision making.
- The potential impact is unclear; water is an important issue.
- There is a need to comprehensively tabulate and compare water usage among production options. This program will do that in a thorough and complete way. However, a high degree of accuracy is not particularly needed, and thus a faster, less-accurate tabulation might achieve the same impact.

### Question 5: Proposed future work

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

- The plans look fine.
- Because the project has just started, virtually all work is in the future.
- The project has been planned but not yet implemented. There do appear to be several alternative scenarios accounted for as the project is implemented
- The proposed work is good, but all fuels, including hydrogen, must be assessed for water consumption and included in the GREET model for effective comparative analysis.

### Project strengths:

- The approach and plan appear to be sound, and the project is relevant and important.
- Water and energy are key topics. This builds on well-established ANL models, such as GREET and water models.
- The completion of a GREET model for water use for comparative analysis for all highly valuable fuels is a strength.
- A highly experienced team is conducting this project. It builds on existing analysis models and general GREET computational framework.

**Project weaknesses:**

- Progress is minimal owing to a lack of funding.
- There is a potential that the disruption of funding could result in gaps that challenge the effectiveness of the project for comparative analysis of all fuels.
- The project needs to show how the updated GREET with water modeling could be used in a regional context. The project does not need to actually do a regional analysis, but just indicate how it might be done.

**Recommendations for additions/deletions to project scope:**

- The project should add regionalization.
- The project team should see what happens once the funding has been used to implement the project.
- The project should increase or confirm the scope of work to include a water analysis in GREET for all fuels.

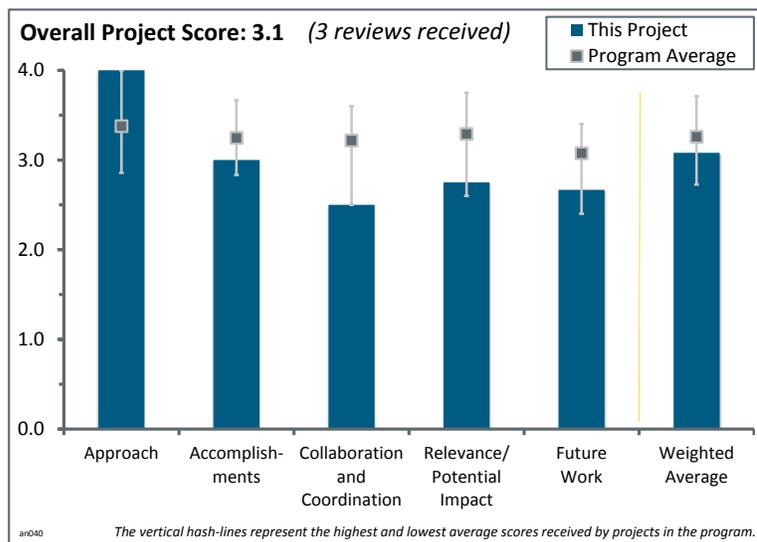
## Project # AN-040: Analysis of Fuel Cell Integration with Biofuels Production

Mark Ruth; National Renewable Energy Laboratory

### Brief Summary of Project:

Objectives of this project include reviewing biomass processing options being developed; identifying opportunities for fuel cell integration with a focus on combined heat, hydrogen, and power (CHHP) options; and estimating how integration of fuel cells into biorefineries may affect levelized biofuel cost in both CHHP and combined heat and power (CHP) configurations. Future benefits may include reductions in greenhouse gas emissions, hedging against market volatility, increased reliability, and improved resilience. Analysis focuses on the cost competitiveness of CHP and CHHP systems in fast pyrolysis biorefineries.

Other potential options for industrial use of fuel cells are also evaluated.



### Question 1: Approach to performing the work

This project was rated **4.0** for its approach.

- This project has a clear approach.
- This is a very thorough analysis, examining several possibilities. This project demonstrates the value of such studies very well.
- The project builds on existing analysis tools to explore a specific scenario (fuel cell CHP or CHHP in a fast pyrolysis plant). The approach and presentation are well organized and clearly presented.
- The project studied the potential application of natural-gas-fueled CHP and CHHP fuel cell systems in biorefinery applications. It has a clear problem statement. The project looked for a biorefinery process that required hydrogen as an input. The problem is interesting in terms of looking for possible markets for stationary fuel cells in an industrial setting.

### Question 2: Accomplishments and progress toward overall project and U.S. Department of Energy (DOE) goals

This project was rated **3.0** for its accomplishments and progress.

- The progress is good, as the project is almost complete.
- This project is now complete and provided good value for the funds expended.
- The project was well executed and logically organized and presented. Unfortunately, the results of the case study did not show a benefit of CHP or CHHP integration. Nonetheless, the analysis needed to be conducted to determine this result.
- The project made a detailed comparison of system performance and cost for a variety of input parameters. The results were not very promising for using fuel cells in this application. Only a few situations within a large parameter space showed an advantage for adding a fuel cell to the plant design. The explanation of the results could have been a bit clearer. In particular, it is unclear what the prospects are for processing hydrogen as part of the CHHP system as opposed to producing it in a steam methane reformer. It is not clear if there are situations where it is advantageous, likely, or unlikely.

### Question 3: Collaboration and coordination with other institutions

This project was rated **2.5** for its collaboration and coordination.

- This project has good coordination with other institutions within DOE.
- Good collaboration was demonstrated by using the existing national lab models and coordinating with the DOE Bioenergy Technologies Office.
- This project drew on earlier DOE work on biorefinery design. It is unclear if other collaborations were included. It might have been interesting to look at other groups doing biorefinery design.
- The collaborators are limited. The presentation mentioned other collaborators that are not listed in the slides. It is difficult to determine how well the coordination works.

### Question 4: Relevance/potential impact on advancing progress toward DOE research, development, and demonstration (RD&D) goals

This project was rated **2.8** for its relevance/potential impact.

- The good use of biomass is very relevant for renewable hydrogen. This topic is very important to the future of hydrogen credibility.
- This project is relevant but not critical to the DOE Hydrogen and Fuel Cells Program.
- This project merits a “good” rating with respect to relevance but only a “fair” rating with respect to the impact, as the pathway examined is not any better than the baseline approach.
- The study was a worthy analytic effort to explore the potential for fuel cell CHHP in a particular biorefinery process. The potential impact of a basically negative result is unclear. It is not clear if there are more general conclusions to be drawn or other situations where CHHP would be more promising.

### Question 5: Proposed future work

This project was rated **2.7** for its proposed future work.

- The proposed plans are general/non-specific.
- This question is not applicable, as the project is completed.
- This project could be focused more on other promising options. The examination of greenhouse gases is a good idea. The system analyzed used natural gas, but biogas as a feedstock could also be examined.

### Project strengths:

- This is an interesting case for hydrogen and power production.
- This project has a good approach and thorough analysis and was well presented.
- This is a logical, well-executed analysis. This was an investigation of CHP/CHHP integration where the result really was not known ahead of time.
- This project did a comprehensive technical economic analysis of a particular biorefinery process to assess the idea of adding fuel cell CHP and CHHP systems.

### Project weaknesses:

- This project did not have sufficient collaboration, and it was not clear how the biofuels producers will react to the results.
- It is not clear if general conclusions can be drawn about using fuel cells for CHHP in process plants. More promising designs and the larger meaning of this study need to be identified.

### Recommendations for additions/deletions to project scope:

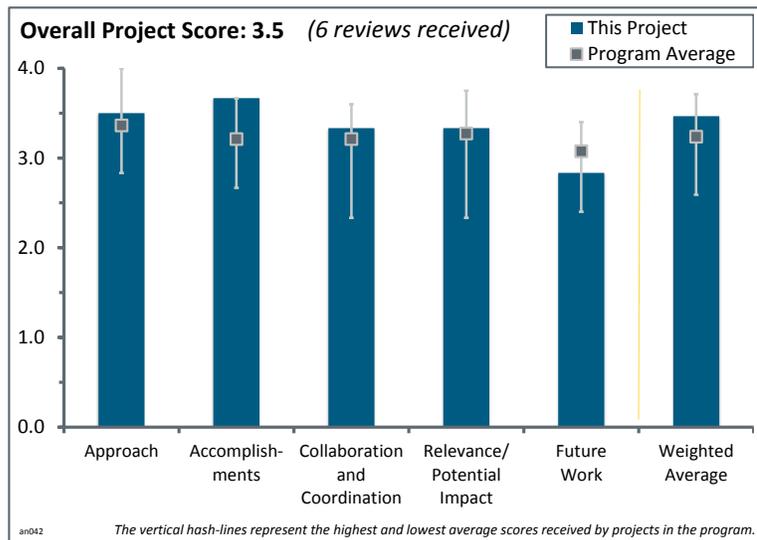
- No responses.

## Project # AN-042: Hawai'i Hydrogen Initiative (H2I) Financial Scenario Analysis

Michael Penev; National Renewable Energy Laboratory

### Brief Summary of Project:

This analysis helps identify opportunities and constraints for equity, debt, and public financing in the fuel cell electric vehicle (FCEV) market. The study considers vehicle adoption rates, determines infrastructure support requirements, evaluates a full range of operating expenses, applies a competitive revenue ceiling, performs accounting cycle analysis, and performs multi-year financing projections. The deployment and financial model indicates stations would need subsidies to support capital and operational expenses because of low capital utilization of early stations, and debt and equity investments will be critical to early market introduction and subsequent adoption.



### Question 1: Approach to performing the work

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

- This is a well-constructed program that explores a specific hydrogen infrastructure build-out (Hawaii) and uses existing tools to conduct scenario analysis.
- The approach to the Hawaii problem is excellent. One thing to consider is whether Hawaii is an appropriate case compared with the rest of the United States, as Hawaii has relatively short drive distances. The driving range per fill assumed for the model is not realistic at present for most FCEVs.
- This is an excellent approach that includes adoption rates, costs, revenues, incentives, financing, sensitivity analysis, cash flow, pricing, and revenue shortfalls. The model would provide flexibility to modify local input data. This approach would support planning for development and deployment in other areas.
- This project was well-designed and successfully addresses the business case for hydrogen fueling stations. The work is carried out using a solid techno-economic basis. It is not clear, however, how it addresses the stated barrier of “stove-piped/siloed analytical capability.”
- The approach seems appropriate given the scale of the project. It is integrated with other efforts. More information on the ADOPT sales model is needed to see how station siting and vehicle adoption are linked. It is unclear if this project addresses FCEV market competition with electric vehicles (EVs) or plug-in hybrid electric vehicles (PHEVs).

### Question 2: Accomplishments and progress toward overall project and U.S. Department of Energy (DOE) goals

This project was rated **3.7** for its accomplishments and progress.

- This project has made excellent progress on the problem. A thorough treatise is presented on the issues that need to be considered, and the models appear to work well.
- This project has made good progress. This is a nice case study, but it would be good to see how an island situation translates to a mainland situation.
- Analysis, model, and conclusions are appropriate and highly valuable for Hawaii and potentially for other regions.

- Significant progress was made toward understanding the hydrogen infrastructure as it might build out in Hawaii's non-standard situation. The project has many elements, which must be examined together. This makes the project challenging.
- The results make it clear that the business case for hydrogen fueling stations is very challenging. The results should help to make it clear that additional cost reduction for hydrogen production, delivery, and dispensing, together with subsidies and incentives, will be needed to make a case for private investment in hydrogen fueling stations.

### Question 3: Collaboration and coordination with other institutions

This project was rated **3.3** for its collaboration and coordination.

- This is excellent; the number and variety of the participating partners are impressive.
- The results from this analysis (and other regional analyses in the future) should be used in communicating with key decision makers and investors.
- The team seems to draw upon a diverse set of contributors.
- Some work from other institutions was incorporated.
- The collaboration is good, but additional input from other original equipment manufacturers (OEMs), gas suppliers, and regions would increase value.

### Question 4: Relevance/potential impact on advancing progress toward DOE research, development, and demonstration (RD&D) goals

This project was rated **3.3** for its relevance/potential impact.

- The approach is highly valuable and timely as auto and refueling OEMs consider rollout and the government considers program incentives.
- This project significantly advances understanding of the potential factors affecting FCEV use in Hawaii. This understanding clearly shows the need for incentives in the near term (and potentially in the long term, also).
- The relevance issue is obscured by whether the Hawaii case translates to the rest of the country.
- This is a nice end-to-end analysis, but how this relates to other non-island situations needs to be demonstrated more, even if this is just the modelers' estimations.
- As the eventual discussion needs to consider both technical and financial factors, this project is a step in the right direction. Until now, analyses had been too focused on only technological factors.

### Question 5: Proposed future work

This project was rated **2.8** for its proposed future work.

- The future work looks appropriate, but it would be good to see a little more work (or explanation) on the market uptake of vehicles and competition with alternatives.
- The additional refinements are appropriate, with input from OEMs, gas suppliers, regional coordinators/government, and financing/developers to test assumptions.
- The model developed and analysis conducted for Hawaii serves as a good structure and baseline to perform similar analyses in different regions of the country. The model will serve as a valuable tool in understanding what is needed for deployment elsewhere, and eventually nationwide.
- This project does not have any future work planned.
- The project is completed, but there are plans to develop other cases in more representative locations.
- The present study lays out the overall challenge. Any future work to further refine the model would provide little benefit.

**Project strengths:**

- This project presents a complex scenario in a logical fashion and uses existing models in an appropriate and logical manner to consider a Hawaiian scenario.
- This is a detailed and realistic analysis of a deployment scenario that could be replicated in other locations.
- This project incorporates financial factors, which is a critical element in planning deployments, making results more realistic, and making better guiding decisions.
- This project has thorough treatment of the issues and considers two good cases. The project could have been stronger with an intermediate scenario.

**Project weaknesses:**

- These project results are relevant only to Hawaii.
- The approach has yet to be tested with industry, including finance industry for deployment and development with expectations for return on investment.
- Care needs to be taken to ensure that the model is applicable on a wide platform, that it is not constrained by Hawaii-specific factors and assumptions, and that it is flexible and dynamic enough to benefit analyses of other regions.
- This project only considers delivered gaseous hydrogen and liquid hydrogen at a price that appears divorced from its actual value. The optimistic scenario models vehicle price incentives that continue indefinitely. A case should be considered in which these subsidies end. Too many service station sizes are modeled. While one wishes to explore the “optimal size” of service stations, the market would never develop 15 different sizes for sale. The number of service stations should be reduced to maybe 3 or 4 sizes and the model re-run. The “key findings” listed are weak. There are more conclusions to draw from the modeling results, but they are not made in the presentation.

**Recommendations for additions/deletions to project scope:**

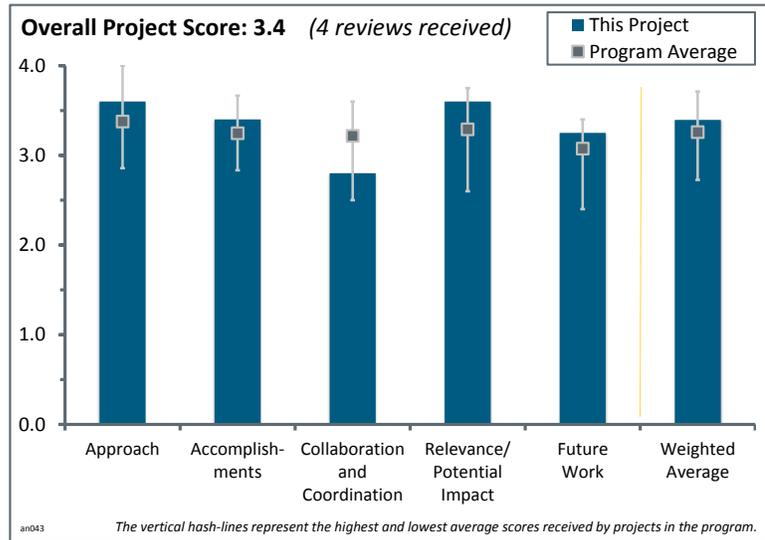
- This project should do more representative locations.
- This project could consider using a model to compare/contrast deployment plans in the United States versus other countries in order to gain an insight into what is working and why, what is not working, and what can be learned.
- This project should conduct testing/vetting with industry, expand and refine incentives and program options for incentives, consider increased OEM vehicle support within the sensitivity model, consider increased FCEV fuel efficiency and increased gasoline costs within the sensitivity model, and develop a *pro forma* model for individual refueling stations.
- The cost of hydrogen could be further explored. The source of the current “cost at the station” is unclear. A modified optimistic case in which vehicle subsidies are ended should be explored. This could indicate whether FCEV purchases plummet when subsidies end or if a tipping point has already passed. This project should reduce the number of station sizes and redo the analysis. The conclusions should be expanded to better reflect the analysis conducted.

## Project # AN-043: Analysis of Community Energy

Darlene Steward; National Renewable Energy Laboratory

### Brief Summary of Project:

This study evaluates the potential benefits of integrating renewable (photovoltaic [PV]) electricity generation with transportation fueling, building on a previous analysis of hydrogen for community-scale electricity storage. The project involves creating simulated hydrogen- and battery/electric-based PV refueling systems in the FCPower Model, establishing hourly building load profiles from empirical load data, applying empirical solar resource data, establishing vehicle refueling profiles, modeling system hourly energy flows, and calculating system electricity and fuel costs.



### Question 1: Approach to performing the work

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

- The premise and the research direction met with a reviewer’s approval. This was a discrete, nicely contained project.
- This was a very good approach to determine component sizes, assess costs, and compare options.
- This project was well-designed and successfully addresses the economics of excess PV output for vehicle refueling. The work is carried out using a solid techno-economic basis. It is not clear, however, how it addresses the stated barrier of “stove-piped/siloed analytical capability.”
- The approach is satisfactory, although it could be more comprehensive as noted in the future plans.
- One reviewer did not enter a response.

### Question 2: Accomplishments and progress toward overall project and U.S. Department of Energy (DOE) goals

This project was rated **3.4** for its accomplishments and progress.

- This project has made very good progress in assessing the concept and comparing the options for electric vehicles (EVs) and fuel cell electric vehicles (FCEVs). The project is valuable for assessing the utilization of community loads, available roof space, distributed generation (DG) to the community, load management, grid/utility interaction, and onsite vehicle refueling/recharging.
- The progress is satisfactory and adequate for the funds provided.
- This project showed the case, or lack of a case, for hydrogen refueling at the neighborhood level.
- The results indicate a hydrogen cost of \$11 to \$34/kg, depending on the size of the PV system. It is unclear how this shows progress towards the DOE hydrogen production cost goal of \$2 to \$4/kg. The study assumed a 20-year lifetime for the electrolyzer unit, but there is no evidence of that level of durability for electrolyzers. It is not clear to what extent the study assumptions reflect today’s technology or some idealized future projection of the technology. For example, today’s cost of electrolyzers is probably not \$600/kW.

### Question 3: Collaboration and coordination with other institutions

This project was rated **2.8** for its collaboration and coordination.

- Collaboration seems to be very good, but cost estimates would be stronger if the team employed industry review and citation.
- This project utilized models from other institutions with some collaboration.
- This project should also consider collaboration with different utilities and component suppliers.
- A project like this needs to have a wider variety of participants and potential stakeholders, plus more regional data sets to account for seasonal and geographic differences.
- The project could have benefited from greater collaboration with battery and EV experts. The selection of the zinc/air battery for excess generation storage may not be the best choice; current deployments of battery systems for grid energy storage suggest otherwise.

### Question 4: Relevance/potential impact on advancing progress toward DOE research, development, and demonstration (RD&D) goals

This project was rated **3.6** for its relevance/potential impact.

- This project and others that are working on distributed refueling/other energy storage have a potentially large role to play in effectively managing renewable power production at the local level.
- This investigation can help determine community-based deployment scenarios that may help with the build-out of infrastructure in a way that differs from conventional approaches, potentially uncovering more beneficial approaches while also benefiting communities and increasing technology visibility.
- This concept is futuristic but highly valuable to assess energy resource options for new or existing development with emerging technologies that could provide distributed resources directly to consumers and to utilities.
- This project provides a relevant demonstration but needs to be widened to more seasons and more locations.
- While the work is largely unbiased and technically sound, the results suggest that the work will have little positive impact on the use of electrolyzers/hydrogen storage for excess PV system output.

### Question 5: Proposed future work

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

- Inclusion of existing future incentives, methodology, and seasonal variation associated with PV production is appropriate.
- The proposal to look at seasons other than July is good, but the project needs to look at other locations with different weather patterns.
- Further project refinements were proposed, but they are not likely to change the results of the study or provide much additional value.
- More fine tuning of the cases by considering optimization, deployment of different technologies, and financial factors will provide further insights.

#### Project strengths:

- This is a good demonstration of the approach.
- This is a creative approach that goes beyond the typical boundaries/way of thinking, potentially opening up new pathways and opportunities.
- This is a comprehensive approach with comparative analysis for a community energy system.

#### Project weaknesses:

- This project needs to be applied to many more seasons and locations.

- The costs appear to be low, and the capacity factor needs to be confirmed for location. The level of operations and maintenance (O&M) and equipment durability is unclear. A comparative analysis with conventional fuels and vehicle costs would be valuable for financing and necessary for development.

### **Recommendations for additions/deletions to project scope:**

- After scenarios are fine-tuned with more detailed considerations, it would be good to look at what a community-based deployment in various parts of the country might mean for the overall development of infrastructure for the nation. It would be good to compare/contrast with typical deployment scenarios.
- This project needs an industry review and quotes on costs, capacity factors, vendor guarantee, O&M costs for long-term operation, and equipment durability. A comprehensive comparative analysis of baseline and individual scenarios (conventional fuels and grid power, PV with net metering and conventional fuels, PV with recharging, and hydrogen with refueling) would be valuable for decision making and the development of a *pro forma* for financing.

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## Program Comments Provided by Reviewers

### Hydrogen Production and Delivery Program Comments

#### Hydrogen Production

1. Was the 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 and/or session overview presentations of the program if appropriate.)
  - The Hydrogen Production program area was very well covered—the important issues (including material performance and capital costs for all production pathways) and challenges were clearly described and progress was shown on examples for all research fields (including novel hydrogen production methods) within the program.
  - The program area seemed to be adequately covered; however, based on a review of the PowerPoint slides, important issues and challenges were not clearly identified. Progress was reported, but there was little mention of previous years' successes, which would have served as a useful baseline.
  - Yes to all of the questions. The progress was usually presented as a status, which made it impossible to judge the progress in comparison to the previous year.
  - There has been some good work on perovskite compounds; this work is novel and may be a breakthrough.
  - Yes, issues and challenges were highlighted. It is not clear how progress was made compared to 2012 during the introduction; the main focus was on current achievements, which is good.
  - Yes, the program area did adequately address program goals and objectives. Current market cost analysis and near-term and long-term market cost expectations were clearly identified. Program technical goals and expectations were also clearly identified.
  - The program area was adequately covered, with important issues identified pathway-by-pathway. Not only were the previous year's accomplishments and progress covered, but they were covered in a multi-year context. Slides showing quantitative progress over an extended period of time juxtaposed with targets are more valuable than single-year snapshots and are appreciated.
  - Project benchmarks were well defined and adequately covered during the presentation. Challenges were defined in materials performance and capital cost with future targets established on electrolyzer and photochemical economic pathways. Progress over the past year's efforts were identified and analyzed. However, gaps identified across the three near-term areas may need additional work to be completely addressed. Use of the Small Business Innovation Research (SBIR) program to advance the basic research appears to be an excellent use of funds. Budget constraints may result in longer-term projects to address the identified issues and challenges.
  - The sub-program on biological hydrogen production using photobiological organisms and enzyme development seems to represent the core of the efforts. As such, the program has a dynamic group of investigators who have expertise in molecular biology, enzyme kinetics, and organism development. Progress has been made since the previous year. However, the group lacks concerted efforts and efforts on scaling reactions beyond bench scale. The group also lacks chemical engineering expertise. Also, the Fuel Cell Technologies Office (FCTO) is encouraged to broaden the investigation of organisms that can produce hydrogen biologically beyond photosynthetic bacteria and algae. There are other microbial organisms that have the potential to produce hydrogen at commercially relevant titers, including the archaeon *Thermococcus kodakaraensis* (see Thomas Santangelo's work at The Ohio State University). Such organisms are becoming more genetically tractable and may use mechanisms to generate hydrogen other than photobiological, which have the potential to reduce the capital costs involved with vessels, such as enclosed photobioreactors.
  - It is unclear if any of these technologies have been adopted by any of the demonstration projects in the United States to show that they can achieve some validated production cost targets.
  - This presentation seemed to be more of the same—same challenges, same barriers, and the same amount of progress. It would have been better to show, for example, what the capital cost and production cost of hydrogen is based on the electrolysis funding opportunity announcement (FOA) run in fiscal year (FY) 2007 with a \$300 cost goal. There was brief mention of progress made by Proton OnSite and Giner, Inc.,

but the description of the component improvements seemed short compared to the catalyst loadings. It is unclear if they made the \$300, if the operating cost came down with the capital, and if the production cost broke the relationship between electricity and hydrogen cost. If the catalyst loading came down, it is unclear what the yield was per plate. It is unclear if the energy efficiency improved or whether it was reduced.

- The photobiological work is not making much progress. It is good science, but even a five-fold increase in hydrogenase activity is minor and not much of an accomplishment considering the amount of time spent. There was no clear path presented for how to achieve the 2020 cost targets.

## 2. Are plans identified for addressing issues and challenges? Are there gaps in the project portfolio?

- The program overview addressed current technology, cost, hydrogen production methods, and challenges.
- Gaps are defined. However, the plans and pathways to address the issues and challenges within the identified gaps appear to be jeopardized by projected budgets constraints. The project portfolio appears to be aimed at addressing the gaps.
- Plans are in place for more research and development (R&D). There do not seem to be many gaps in the long-term portfolio, but one could argue that small steam methane reforming (SMR) technology is currently very weak and the potential for small tri-generation (combined heat, hydrogen and power, or “CHHP”) systems for home use is undeveloped due to the low demand for hydrogen vehicles. The U.S. Department of Energy (DOE) should consider providing support for small CHHP systems.
- The projects address the main issues and challenges very well. However, to achieve the DOE goals for hydrogen production costs, there seems to be a gap in demonstrating promising technologies. Budgets for such demonstrations seem to be limited. Joint actions as proposed by the International Partnership for Hydrogen and Fuel Cells in the Economy some years ago might help to achieve progress. Partners from abroad might be able to create synergy by bringing in infrastructure and knowledge that is presently not available within the program.
- The presentation clearly identified movement from distributed natural gas production to renewable distributed production and longer-term technologies, which is appropriate. The FY 2014 request has a significant amount of additional funding for distributed renewable production; the presentation did not indicate the direction of this funding (pyrolysis, aqueous reforming, or other). One assumes that other areas of major funding (high-temperature solar thermochemical, photoelectrochemical, biological) will continue the ongoing efforts reported in the presentation.
- Issues and challenges are expected to be addressed through FOAs issued over the next fiscal years. Overall gaps in project portfolio are not completely clear.
- The Hydrogen Production program area should consider more practical technologies for production of hydrogen. Due to near-term and long-term specific targets and goals, the program should focus more on practical technologies than “science projects.” Solar-thermochemical technology is one of those technologies that perhaps is very attractive on paper but in reality is not very practical. Solar energy generation technology can be coupled with water electrolysis stack technology to produce hydrogen at a much higher rate and smaller footprint. The program needs to reevaluate some of the technical approaches and spend funds on technologies that already have demonstrated hydrogen production in a large scale and are commercially available.
- It is unclear what the following statement in the presentation means: “Nearer term technologies being transitioned to Tech-Val portfolio and continue to be supported by SBIR Program.” What about near-term electrolysis development with regard to dynamic operation and capital cost decrease? Is DOE satisfied with current electrolyzer performance? It is unclear if there are considerations for new projects on upscaling electrolyzers for centralized production.
- While analysis is important to ensure the correct approaches are being taken, it was not clear which technologies or systems have been eliminated or reduced in priority due to funding constraints or limited R&D results. It seems the sub-element already has an approach for the next 7–10 years—improved SMR with lower greenhouse gas emissions and higher efficiencies—but there are not enough projects to jump start the applications. The biggest gap is how the individual program elements are coming together to meet the well-to-wheel expectations.
- The sub-program on biological hydrogen production could benefit from reactor engineering efforts. R&D to improve photobioreactor designs is being pursued in the DOE Energy Efficiency and Renewable Energy

(EERE) Bioenergy Technologies Office, the Defense Advanced Research Projects Agency (DARPA), U.S. Department of Defense/Air Force, and the National Science Foundation. The FCTO could be well-served by collaborating with these entities to share insights on R&D progress as well as techno-economic modeling analyses in terms of understanding the current progress toward cost barriers and remaining challenges specific to hydrogen production.

- No specific plans were shared, although vague key milestones and general future plans were presented. The portfolio seemed to have a glaring gap in electrolysis funding/research. The production goal and pathway strategies indicate that electrolysis is a significant near- and mid-term distributed and central technology, along with biomass; however, the hydrogen production budget for FY 2013 funds little research in biomass and electrolysis and the FY 2014 request is even smaller. This does not make sense based on the prior slides indicating that these are target near-term research areas.

### 3. Does the program area appear to be focused, well managed, and effective in addressing the DOE Hydrogen and Fuel Cells Program's needs?

- The Hydrogen Production program area appears to be effective, well focused, and well managed.
- There was a good overview of focus; more information could be given about management and effectiveness, although the individual project presentations did show the results.
- The program area appears to be well managed and focused, but focused on longer-term efforts (i.e., solar thermochemical, photoelectrochemical, and photobiological). The program would better suit its near- and mid-term goals if electrolysis was more heavily funded.
- The sub-program area on biological hydrogen production is very focused and well managed. The sub-program area could benefit from more funding in order to broaden the portfolio and lower risks associated with the single focus on cyanobacteria and microalgae.
- Yes, the program overview was focused and effectively addressed DOE Hydrogen and Fuel Cells Program (Program) needs. However, the Hydrogen Production program management team should consider looking into similar programs that are currently under development in other federal agencies—in particular, the National Aeronautics and Space Administration (NASA). NASA has a long history and extensive expertise on electrolysis technologies, cryogenic hydrogen, and oxygen storage and delivery.
- The work appears to be focused and well managed. Technical barriers and the scope of work to address the barriers and gaps are clear and well defined.
- The program area appears to be well managed, but it is not effective in addressing the overall Program's needs. If there are critical dates in 2015, more emphasis should be on the technologies needed to achieve those targets and less emphasis should be placed on pathways that require over 15 years to achieve any significant improvements. If there are no critical dates in the near term, such as to commercialize fuel cell vehicles, standalone auxiliary power units, or other applications that determine the success or failure of the Program, then working on incremental improvements is fine and will produce some good science and engineering.

### 4. Other Comments:

- The presentation featured good use of the rule of thumb of 1 minute per slide—it fit well into the 15 minutes available for the session introduction and the presenter did not appear rushed.
- Very good progress has been made on the scope of work. Validation testing may need to be considered. It is unclear what the table on slide 10 from the University of Colorado is showing. It is unclear if future SBIR grants are a viable option.
- The requested budget for FY 2014 shows funding decreases for electrolysis technology but significant increases for photoelectrochemical and solar thermochemical technologies. Does DOE think that these two technologies will be ready to meet hydrogen production and cost targets by 2020? Is it feasible for solar thermochemical technology to reduce the cost of hydrogen production by 75%—from \$14.80 in 2015 to \$3.70 in 2020, or for photoelectrochemical technology to meet its 2020 cost targets?
- The DOE goals for hydrogen production cost are very ambitious. This is the right strategy and important to accelerate the fast and sustainable introduction of hydrogen in the economy. However, it seems to be difficult to achieve the goals based on the carried-out projects alone. Because this is an issue all over the

world, there might be synergy with other R&D programs that could be leveraged to improve the program area's output through joint efforts.

## Hydrogen Delivery

1. Was the 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 and/or session overview presentations of the program if appropriate.)

- The presentation was well done, but there was far more material than could be adequately covered in the time allotted.
- Definitely yes to all of the questions. The progress was usually presented as “status 2013” compared to targets (see the table on slide 3). It was not possible to judge the progress in comparison to the previous year in most cases.
- The Hydrogen Delivery program area was presented very well. The important issues and challenges were identified and discussed clearly. Progress was also described. Measuring the progress was rather difficult—it might be more appropriate to evaluate this only at the end of the projects.
- The presentation adequately addressed program goals and objectives. Current market cost analyses along with near-term and long-term market cost expectations were clearly identified. Program technical goals and expectations were also clearly identified.
- The program area was adequately covered and key challenges to addressing future targets were addressed up front. The 2013 progress reports were described, including major accomplishments and highlights, but there was little comparison to previous years' accomplishment besides the 2012 status table. It would have been nice to include this information so that the recent accomplishments could be put into perspective.
- The Hydrogen Delivery program area was adequately covered, apparently incorporating content of the new *Fuel Cell Technologies Office Multi-Year Research, Development, and Demonstration Plan* and workshop learning. Key issues and challenges were identified. Single-year accomplishments were presented, but of greater value were the descriptions of progress over time relative to targets. For example, commendably, slide 14 graphically portrayed progress on current density from 2007–2013. It was not as apparent on slide 14 the period over which parts the count was reduced; this could guide expectations regarding further reductions.
- The presentation was very good and the program was well covered and important issues and challenges were identified. The high cost of hydrogen compression is identified as an area where more research is needed.
- Central delivery targets were well defined and adequately covered during the presentation. Critical issues and challenges were identified and discussed. Advancements in technology through analysis and modeling were clearly presented and future work necessary to meet program goals and objectives were presented.
- All projects within this program area were covered; however, the time available for the introduction is so short that DOE Hydrogen and Fuel Cells Program Annual Merit Review (AMR) management should consider advising introductory speakers (overall, including this presentation) to avoid getting into details about session projects due to time constraints. Instead, they should mention the project title, the presenter, and one sentence about highlights of a specific presenter/project, and then move on. This would also leave the opportunity for the principal investigators to share their key findings with the reviewers and audience during their session presentations. Important issues and challenges were identified, but they could be presented in a more general way for all projects as a group since specific project presenters will get into more detail. Specific 2013 progress compared to 2012 was not clearly identified.
- The presentation identified all of the barriers as it has in the past, but it did not clearly address which issues do not have adequate solutions or resources available to address them in the R&D plans. Progress was addressed only marginally and, other than talk about high market penetrations needed for cost reduction, a clear path for improving the near-term market was not identified. Most of the information presented was only analysis and it was not clear how it was validated or if industry agrees with the assumptions and conclusions. For example, with regard to compression, storage, and dispensing cost (CSD) reduction by using tube trailers and a cascade system, it is unclear which current hydrogen delivery companies reviewed the results and agreed this was a reasonable approach for focusing limited research and development funds.

## 2. Are plans identified for addressing issues and challenges? Are there gaps in the project portfolio?

- The plans are satisfactory.
- The projects carried out under the subtopic are clearly within its key areas and are able to achieve the goals.
- There are good plans to address the roadblocks identified in the new roadmap.
- Plans and funding described in the presentation indicate that the Hydrogen Delivery program area has prioritized its challenges and directed 2013/2014 funding accordingly. The prioritization seems appropriate given the issues and their time frames (i.e., the nearer-term, higher-priority issues, such as forecourt CSD, are receiving relatively greater emphasis).
- Yes, but there was not enough time to get into each item. For example, metering has extensive challenges, but there was no time to mention it, much less get into detail.
- There was minimal coverage due to time limitations, which occurred because too much detail was presented about each project. Gaps are hard to identify due to the significant amount of information presented during the session introduction.
- Yes, a coherent plan appears to be in the works, although funding for a planned funding opportunity announcement (FOA) needs to be allocated, and federal support for early stations that deploy 700 bar fueling systems for the first 1,000 fuel cell electric vehicles (FCEVs) from each manufacturer appears to be essential because the commercial business case will not exist until there are many hundreds of stations.
- Plans are identified, although there appears to be a lack of projects/activities aimed at near-term R&D topics (e.g., reliability and cost of gaseous compression). Maybe some new projects will develop as a result of the CSD workshop. Also, the topics of hydrogen quality and hydrogen metering should be addressed.
- Technical targets are well defined along with the plans necessary to address the challenges. Scientific gaps and the metrics necessary to reach the gaps were included in the discussion and slides. The lack of discussion on collaborative research by other federal agencies was not discussed regarding transmission/delivery/storage and distribution. Some work appears to be more focused toward a paper-based study on cost analysis to meet the targets instead of a research-/data-based analysis.
- Yes, the program overview did address current technical, cost, and hydrogen delivery methods challenges. The program should consider looking into high-pressure electrochemical electrolysis technology; although it was briefly mentioned in the program overview, it needs more consideration. Currently, NASA's high-pressure static feed electrochemical water electrolysis SBIR program is developing an electrochemical system that can produce hydrogen or oxygen up to 413 bar without any mechanical compression. This technology currently is being developed for production of high-pressure oxygen for NASA's life support program.
- There are plans to achieve the targets identified in the *Fuel Cell Technologies Office Multi-Year Research, Development, and Demonstration Plan*, but the relationship of the plans to what has been experienced already, for example, in the California Fuel Cell Partnership, was not explained. The program funding is limited, so even if a FOA is released in late 2013, it is unclear what anticipated achievements will be made and if there are any plans to use the existing demonstrations as real test beds. While analysis is a good tool, fuel cell cost has not been reduced as the analysis indicated, so it is unclear why the forecourt should also reduce as drastically, especially if reliability and product liability are key for new systems and components.
- Specific plans are not identified, but general short- and long-term goals and strategic plans are described. The portfolio seems solid; however, three of the six key milestones from "today -2015" are focused on liquid hydrogen delivery yet only one liquid delivery seems to be funded. More projects that investigate liquid storage and pumps seem to be in order.

## 3. Does the program area appear to be focused, well managed, and effective in addressing the DOE Hydrogen and Fuel Cells Program's needs?

- Yes, the work is targeted at the biggest hurdles to reduce the cost of delivered hydrogen at the forecourt.
- The Hydrogen Delivery program area appears to be appropriately focused, well managed and effective. It has a good balance between support of analysis and component development, as well as between emphases on forecourt CSD versus delivery.
- The program area is focused on addressing what the researchers' analysis indicates are the major cost barriers. It is managed as well as could be expected with limited resources.

- The Hydrogen Delivery program area is very well managed and focused on the key issues and challenges that need to be addressed.
- Yes, except for liquid hydrogen storage and pumps.
- Yes, although a key metric going forward should be the actual deployment of these technologies. That would be the real test of success.
- The program area appears to be focused, well managed, and effective, but this mainly becomes clear when listening to individual project presentations. The program introduction should focus more on management, highlighting the impact on progress toward goals and future steps to address the goals from a project management perspective.
- Yes, the program overview is focused and effective in addressing the overall Program's needs. However the Hydrogen Delivery program management team should consider looking into similar programs that are currently under development by other federal agencies—in particular, NASA. NASA has a long history and extensive expertise in cryogenic hydrogen and oxygen storage and delivery.

4. Other Comments:

- The learnings from the recent CSD workshop at Argonne National Laboratory were reflected in the presentation.
- It will be good to attend the international workshop on infrastructure topics at the end of June in Berlin.
- The presentation used a lot of abbreviations that were not always explained. For the unfamiliar listener, this may have led to confusion. Overall, it was a good presentation.
- Overall this was a good presentation, but presenting 21 slides within 15 minutes is too much. A good rule of thumb is 1 minute per slide, with a limited and concise amount of information on each slide (which appears to be a challenge for all DOE presenters).
- There is good progress toward the goals...on paper. However, it is not clear if the solutions are practical for real-world deployment. Many of the technologies developed are not in day-to-day use nor are there plans for them to be so in the foreseeable future. It is unclear why this is the case and whether this throws doubt on the actual results.
- Connections with other funding opportunities were mentioned (e.g., European Union programs). It would be helpful for the participants to know more precisely what these possibilities are because it is very complicated to find the right links in Europe without a deep knowledge of the various programs, but the benefit especially in codes and standards are immense if work could be carried out jointly.

## Hydrogen Storage Program Comments

1. Was the 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 program if appropriate.)
  - Yes, the presentation gave a good overview of the program area.
  - This program area continued its tradition of having a very good presentation that describes issues, challenges, and progress related to moving forward toward achieving the program’s RD&D goals in hydrogen storage.
  - The program area is comprehensive and carefully planned. The presentation was well organized and provided sufficient detail to allow a good understanding of approaches, progress, and plans in each technology area.
  - The program area was well covered with enough breadth and depth to clearly understand the challenges, degrees of progress, areas of priority, and the reasons for the priorities. The degree of barriers were shown clearly (with the help of spider charts) to allow qualitative comparisons among the various projects.
  - The Hydrogen Storage program area was well covered. The presentation stated that its main goal is to develop and demonstrate viable hydrogen storage technologies for transportation, stationary, material handling, and portable power applications; clearly identified the volumetric density limitation and cost challenges of the near-term incumbent compressed gas technology; and identified the need for better materials for the longer term technologies to enable them to meet all of the technical targets. The results from the Hydrogen Storage Engineering Center of Excellence (HSECoE) were very valuable in identifying the issues and challenges of material-based storage and will help direct and focus materials development. The progress relative to the previous year was clearly presented via spider chart illustrations and pathways via waterfall charts.
  - The program area was well covered by presenting well-refined charts and emphasizing and re-emphasizing important points and takeaways. Important issues and challenges were identified, such as the following, which is difficult to categorize but was mentioned as “Note: there are ~20 specific onboard storage targets that must be met simultaneously.”
  - The program area was covered in a concise and very clear manner. Progress in individual projects, and the program as a whole, were clearly presented and are being well managed by the program managers.
  - The approach to divide the program area into “near-term” and “long-term” options is very productive and will likely, soon, lead to applications using hydrogen. It may likely prove highly relevant to focus on improving the more “low-tech” solution, i.e., high-pressure gas storage, by reducing the cost for carbon fiber and increase the tensile strength to be used to develop new high-pressure storage tanks. There is clearly significant progress within most programs and several solutions fulfill most of the targets set by DOE; only a few out of the 20 targets need to be further improved. The focus in the research program is broad, covering engineering and materials science with a focus toward the most challenging target, mobile applications. But, also, shorter-term applications are covered, such as materials-handling forklifts, single-use portable applications, and stationary applications.
  
2. Are plans identified for addressing issues and challenges? Are there gaps in the project portfolio?
  - Yes, plans were identified for addressing issues and challenges.
  - There are no gaps in the project portfolio.
  - The portfolio does a good job of covering gaps. The program has made good use of limited funding.
  - Plans for addressing challenges have been presented and are being managed within the limitations of the program’s current budget.
  - Plans with key milestones were presented for physical storage and material-based storage: mainly, to reduce the cost of carbon fiber precursors, improve materials properties, and prove design concepts and feedback materials development. The addition of non-automotive storage activities filled a gap in the storage portfolio.
  - The issues and challenges related to attaining appropriate materials properties were well discussed and described. While there are no glaring gaps in the materials strategy, the upcoming funding opportunity announcement (FOA) may be able to address any small adjustments in the portfolio.

- Plans were identified for addressing issues and challenges both on a detailed and generalized scale: general motivation was provided in the “Goal and Objectives” slide followed by specific quantitative metrics, followed by strategies, then overviews of projects to address challenges, and finally how the discussed approaches would translate in a solution.
- The plans going forward were described to provide a general understanding; deeper plan descriptions are necessary within the specific project presentations.
- There is clearly a need to discover novel materials that could come closer to fulfilling all of the DOE targets. Increased focus on fundamental materials science within hydrogen-containing materials would be good. Liquid hydrogen is previously known to have low energy efficiency. It would be very interesting to obtain an estimate of the energy efficiency for the liquid cryopump technology, which allows the direct fueling of supercritical hydrogen.
- The HSECoE is facing serious challenges in the development of a prototype engineering system that meets or exceeds DOE targets. Those obstacles were not described in much detail in this presentation. Consequently, it is difficult to fully assess the status of the project/program. The ever-increasing complexity that seems to be accompanying the development of a prototype engineering system based on ammonia borane (AB) is especially disconcerting. In addition, efficient, cost-effective off-board regeneration of the AB system is highly problematic. If AB is going to serve as a surrogate material for prototype system development, it seems that a more careful examination of the many issues that impact the regeneration process must be considered.

3. Does the program area appear to be focused, well managed, and effective in addressing the DOE Hydrogen and Fuel Cells Program’s needs?

- The Hydrogen Storage program area appears to be very focused, well managed, and effective.
- The program area is as focused and well managed as it ever has been. Every year, the focus on addressing DOE needs is improved.
- The program area is very well managed and is focused on critical technology issues. The DOE management team is doing an excellent job of interacting with all program participants and informing the technical community in a timely and straightforward way about the overall status of the program and upcoming funding thrusts and opportunities.
- The storage team continues to be very focused on the RD&D needs and goals of the program. The program area is well managed by the DOE Headquarters/Golden Field Office team, as is the tradition.
- The program area is compellingly focused, as is DOE’s approach. The program is also well managed by a program manager and a team that is thinking critically, yet aimed at moving forward. The team comprises an effective leader and members who are experts in addressing DOE Hydrogen and Fuel Cell Program’s needs.
- The Hydrogen Storage program area is well focused on achieving the program’s targets, and it appears to be well managed. It is well balanced; however, the level of funding may not be sufficient to advance the technologies performance in a timely manner to achieve DOE targets.
- There has been a realignment with the inclusion of near-term niche markets, which are in the purview of the DOE Hydrogen and Fuel Cells Program and is an important addition for program continuity and success in reaching longer-term hydrogen storage goals.
- The program area clearly has strong and visible coordination and organization. The Hydrogen Storage program manager appears to stay in close contact with all programs and is a very competent leader. The speaker mentioned in his presentation that the ideal hydrogen storage material should meet 20 specific onboard storage targets defined by DOE, simultaneously, to meet the demands for a broad range of vehicles. This is clearly challenging. Therefore, it may be fruitful (as proposed in the *Fuel Cell Technologies Office Multi-Year Research, Development, and Demonstration Plan*) to put some focus on the more “low-tech” approaches of high-pressure hydrogen gas storage. This is possibly the most focused and efficient research program dedicated toward hydrogen energy storage, worldwide. A major focus is technological and engineering aspects and improving known technology, but there is still room for some fundamental science research as well, which may provide completely new approaches for hydrogen storage and novel “long term” solutions.

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#### 4. Other Comments:

- The Hydrogen Storage program area is very focused on automobile applications and targets for automobile applications.
- The program manager is effective in fostering an encouraging yet sobering environment to present and discuss ongoing research with him and his team. Each team member appears to work independently but with common goals to help SBIR researchers remain focused on DOE metrics. The responsiveness of the program manager and his team supports constructive and iterative feedback.
- The attention to non-automotive applications is a welcome improvement. Real commercialization will see evolution of these technologies within both automotive and nonautomotive applications. DOE's focus on both is consistent with how technical products actually evolve in the marketplace, which can only benefit the overall storage improvements for both.
- During the course of a research program, it usually comes out that some materials or systems may not fulfill the defined targets. These materials or systems might still have potential for other applications but cannot be investigated any more. Such a program should leave 0%–20% of the budget to be spent in the second half of a project or program on promising materials or systems for spin-offs in order to increase the probability of finalizing developments for potential applications.
- High-pressure hydrogen gas storage (tank) has some advantages compared to known solid-state storage materials (e.g., fast refueling). It was suggested that perhaps materials may be developed that could be introduced into the storage tank and improve the volumetric storage density.
- In future reviews, it is suggested that all presenters be required to explicitly state the major problems and challenges in their specific approaches and then discuss a plan for mitigating those risks. Without that information, it is very difficult for the reviewers to fully understand the context in which the future plans are being formulated (it also forces the principal investigator [PI] and team to be brutally honest about the status of their project).
- In materials discovery programs of the future, ensuring the proposers have the equipment or will have the equipment in very short order to achieve their proposed goals needs to be closely examined. Two projects in the Storage program did not have the critical high-pressure characterization equipment in year-one to carry out the R&D proposed. Another project did not have the laboratory capability to study pressure reactions at a pressure relevant to DOE requirements after a two-year project. The results of the latter project are of little value to the Storage program. Good progress is being made in most projects, and the community in attendance at the DOE Hydrogen and Fuel Cells Annual Merit Review (AMR) was, in general, an attentive audience. Attendance was good, and those in attendance asked good questions indicating that the general level of interest is still high within the storage community. There are a few outlier projects that are struggling, but those are likely to be identified through the AMR peer review process. One project that will be perceived to be failing is indeed not likely to meet its goals. But the project is really a success, because it set out to validate a very unusual claim in the literature that, if true, could provide a breakout opportunity for hydrogen sorption. The PI on this project is very meticulous and well respected and cannot repeat the literature claims. This is highly valuable information for DOE to obtain, even if it is negative evidence, because now the community knows that this is a direction that does not need to be revisited. The PI is to be congratulated on his candor. The two post-doctoral programs appeared to result in an excellent multidisciplinary experience for the post doctorates. DOE should track their careers to examine its return on investment.

## Fuel Cells Program Comments

1. Was the 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 and/or session overview presentations of the program if appropriate.)
  - Yes, the Fuel Cells program area was adequately covered, important issues and challenges were identified, and progress was clearly presented.
  - The presentation was excellent. It gave a complete overview of past progress and what important challenges need to be addressed.
  - Important issues were identified and progress was reported in a clear and concise way.
  - The program area was well covered with a clear view of and approach for addressing the different challenges that need to be overcome. The template for each project presentation enables reviewers to understand the targets aimed for and evaluate the progress made. The program was well covered with a clear view and approach of the different challenges to overcome, in particular for the program presentation. The template enables, for each presentation, to evaluate with a clear positioning of the subject addressed, the target to reach and the progress made.
  - There was a good overview and discussion of a few specific examples of technical progress. More comparison to the previous year would be interesting. More detail on the upcoming year would be useful, if possible.
  - The main issues were covered well. There was a lot of emphasis on modeling and analysis and not much on research thrusts for the upcoming year, as is typically heard at this AMR meeting. Perhaps this is because DOE is in a period of transition as a new Secretary is being selected.
  - The program area was well covered. The presentation was very well structured and combined messages of the approach and examples of detailed research very well. The presentation made the idea behind the program very clear. The progress was adequately presented as far as it is possible in such a short time frame.
  - The presentation was well done and described the current fuel cell technology program well. The targets are totally clear, and the overall program is focused and well managed. The emphasis tends to be on the light duty automobile applications, but it was also clearly stated that other commercial applications are also moving onto the DOE screen.
  - The presenter did an excellent job with a complex subject in a short period of time. The reviewer learned a lot and will distribute the presentation to his company. Important issues and priorities were well described for the past year. The presenter's knowledge and thoroughness were evident.
  - The Fuel Cells program area was fairly accurately covered. The stated emphasis did not completely match the projects presented, with little or no membrane, membrane electrode assembly (MEA) integration, and balance of plant projects. Also, several of the catalyst projects seem to have overlapping scopes. With most projects ending in 2013, it will be a short fuel cell session next year. Also, cost projections are leveling off, with no clear path presented to bridge the gap.
  - Yes, the program area was well covered, including the important issues and challenges. Progress in this area was not explicitly compared to where things stood in 2012, but the sweep of program progress was clearly presented.
  - Basically, yes; but the current cost breakdown and technical scenario with a bar chart to achieve the future target should be shown in the slides, as was presented at the 2012 AMR. That can be quite helpful for the reviewers.
  
2. Are plans identified for addressing issues and challenges? Are there gaps in the project portfolio?
  - Yes, plans were identified for addressing issues and challenges, and there are no gaps in the portfolio.
  - The proposed plans are appropriate. The project portfolio and the budget allocation are adequate with the main cost drivers identified, particularly for the stack. Nevertheless, regarding the cost breakdown, a new focus on metallic bipolar plates may be needed because they represent the second highest cost component for high-volume production. Actually, developing durable stamped metallic bipolar plates (with a lifetime of more than 10,000 to 20,000 hours) might open the material handling equipment (MHE) market, or even

some stationary markets. This may then lead to manufacturing and operation feedback for R&D actions to overcome issues in automotive applications

- The focus areas have been identified; however, the details of the plans are vague.
- The present projects were explained and plans for these were clear. Plans for innovation were not dealt with. Perhaps this is because DOE is in a period of transition as a new Secretary is being selected.
- Forward funding is causing a temporary gap in the project portfolio's robustness.
- Several projects need to have the roles reversed, with industrial partners taking the lead and the national laboratories providing the needed resources, as R&D developments transition into actual products and systems.
- Plans were properly addressed. One possible gap is that more attention needs to be given to problems that are appearing at high current density in hydrogen/air at low platinum loadings. Better fundamental understanding of possible interfacial oxygen transport problems may be needed to allow the progress that has been made in increasing kinetic oxygen reduction reaction (ORR) activity with lower platinum loadings to be realized in practical fuel cells.
- The Fuel Cells program area does an exceptional job; however, there are constant challenges that arise due to funding limitations and changes in priority. Currently, the projects on membranes have largely been completed but underrepresented in the portfolio; further materials advances could be beneficial. Work in portable power, while not a significant part of the current portfolio, is not particularly valuable and could be even further de-emphasized.
- The presentation described plans for addressing issues and challenges well. One gap is the reduced focus on transportation. Other than batteries, fuel cells can provide propulsion for vehicles on a basis that is very similar to today's convenience and flexibility. It is recommended to sharpen the focus on transportation, especially on propulsion of vehicles.
- Some of the biggest challenges are not even listed and were not addressed at all in the future plans. One of the biggest gaps was between the status and the target in the thermal heat rejection (Q/delta T) requirement. This was not highlighted as an issue and no projects are specifically addressing it. New materials for stacks and humidifiers will be required to achieve this. Cost projections, for the third straight year, are based on nanostructured thin film (NSTF), which is an extremely risky technology. Also, addressing the challenge of high current density performance of low-loaded electrodes requires a much greater focus. There are also major gaps with a complete lack of membrane, gas diffusion layer, plate, and seal projects. The challenge remains: encouraging automotive original equipment manufacturers to market technology in direct competition with their present commercial base. In other places, Japan, for example, the government facilitates such a transfer. For instance, Osaka Gas, a huge utility, sells both natural gas and "appliances" that burn natural gas (e.g., water heaters). It was natural to add a new appliance, a combined heat and power (CHP) fuel cell system, to that market. The program might search for similar opportunities in the United States. Fuel cells have admirable low emissions. The evidence about particulate matter/human health is overwhelming. It seems like a strong emphasis on "clean air now" might add strength to the fuel cell technology message [cancer and heart disease costs hundreds of billions each year] -- fuel cells in urban environments are game changers.

### 3. Does the program area appear to be focused, well managed, and effective in addressing the DOE Hydrogen and Fuel Cells Program's R&D needs?

- Yes, the Fuel Cells program area is focused, well managed, and effective in addressing the DOE Hydrogen and Fuel Cells Program's needs.
- This program area is very well focused, well managed, and effective compared to other government programs. The program manager clearly has a good sense of where the value points are and how to spend the taxpayers' money most efficiently.
- Yes to all; this program is a role model for DOE.
- The program area is very well managed. The high technical competence of the DOE project officers is key to this success.
- The entire activity is exceptionally focused and driven by targets. The management team is fully functional and exceptional as well.
- The program area appears to be well focused, well managed, and effective in addressing the Hydrogen and Fuel Cells Program's needs. However, some points may be addressed:

- MEA studies appear too focused on the same manufacturer. A potential risk is that not all of the associated project outcomes will be applicable for other types of MEA production.
- System modeling is done well, but stack data used for performance and near-future durability are actually only single-cell data. This may have an impact on the results' accuracy. Therefore, some single cell/stack data comparison will be welcome.
- The program area manages its existing project portfolio well. However, it seems that little vision is applied to the innovation that will be needed to meet the DOE Hydrogen and Fuel Cell Program's needs. The Program did some reaching out to stakeholders for inputs on future areas of R&D needs, which is good.
- The program area is fairly well focused. Many of the less productive and poorly managed projects from last year have been cancelled, which is very encouraging. Most remaining projects have proven valuable or still have the potential to provide value.
- Because many systems are hybridized with batteries, it could be interesting to introduce this hybridization into the system modeling. Actually, the system control balance will significantly impact either the fuel cell system's durability or the global system's efficiency. Many of the projects are at the point where they need critical evaluation as to their potential for commercialization. If ready, the projects should be turned over to industrial partners; if not, a decision should be made to further develop or drop the project.
- There is room to improve the management of the Annual Merit Review. Many project presentation files about the programs seem to have almost the same slides as those of previous year, depending on the programs. If you instruct the PI to show what is updated/changed compared with the previous year, then it would be easier to understand and review the programs.
- The program area is not adequately focused; the ratio of money spent does not seem to proportionally match the focus areas. Further, new projects are being funded using proposals submitted three years ago, and new learnings in areas such as membrane durability and system mitigation for start-stop means that projects on improving membrane and carbon support durability are irrelevant.

#### 4. Other Comments:

- The DOE Hydrogen and Fuel Cells Program has helped accelerate progress in automotive fuel cell technology significantly over the last decade.
- The Fuel Cells program area has exhibited typically fine performance over the past year.
- This was a good, concise summary of a good program.
- A new "scorecard" may be useful, detailing DOE fuel cell projects that have enabled commercialized products.
- Overall, this is a tough job at this time. It seems that a lot of projects are wrapping up, and the next steps are not clear. Hopefully new solicitations and finalizing the selection of DOE's top leadership at the top of DOE will get things back on track.
- The unaddressed issue is that, despite all the progress of the Fuel Cell program area, DOE seems to be ignoring the fact that the cost projections are becoming asymptotic at about \$45/kW and there are not any projects on the horizon to bridge the gap to \$30/kW. New step-out ideas and funding are needed to keep the momentum going.
- As shown on slides 4 and 5, given that catalyst costs are 46% of the cost of making a polymer electrolyte membrane (PEM) fuel cell stack at a production rate of 500,000 units per year, it is imperative that DOE continue fundamental work in catalyst development. The promise afforded by the 3M roll-to-roll processing technique will set the stage for the next generation of high-performance, low-cost catalysts. The Ni<sub>7</sub>Pt<sub>3</sub>-NSTF materials show what promise can be realized by a first-principles materials design approach. The outstanding kinetics of the Ni<sub>7</sub>Pt<sub>3</sub> alloy are unfortunately combined with a nickel-dissolution rate that will prevent them from being deployed on a large scale. The advantage of the 3M approach is that complex multicomponent alloys can be synthesized in a large-scale commercial setting. This technique can be applied to non-NSTF high-surface-area supports. Advanced alloys with high ORR kinetics and low-platinum loadings and that are also stable in acid electrolytes have been developed by the Jet Propulsion Laboratory, and these new alloy classes could set a new paradigm for future fuel cell catalysts. None of these achievements would have been made possible without the DOE Office of Energy Efficiency and Renewable Energy (EERE) funding targeted to catalyst development. Therefore, it is hoped that DOE will continue to support this area, either in the EERE or the DOE Basic Science offices, because these new materials are key to the future.

- The fuel cell activity is now approaching a transition between development and commercialization. Most R&D money in the private sector is spent in the commercialization phase; however, much of that R&D is typically proprietary. Getting the correct balance in a public R&D program is challenging, but doable. The Fuel Cell program team needs to think more about market creation. Right now, some of the Japanese and Korean combined heat and power (CHP) units should be evaluated in U.S. laboratories. The question should be, “Given these ‘components,’ how can such hardware be integrated into a new system?” For example, given a clean sheet of paper, what would a house look like with a CHP system? How would you manage a group of CHP-deployed houses to form a mini-grid? And so on, with all other commercialization opportunities.

## Manufacturing R&D Program Comments

1. Was the 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 and/or session overview presentations of the program if appropriate.)
  - Yes, the Manufacturing R&D program area was adequately covered. However, it is unclear if the key issues have been identified yet.
  - The program area was well described. Prior successes were also described, helping attendees to appreciate the program's value.
2. Are plans identified for addressing issues and challenges? Are there gaps in the project portfolio?
  - It was helpful to learn about the Manufacturing R&D program area's funding opportunity announcement (FOA) and the Clean Energy Manufacturing Initiative. The future plans were clear.
3. Does the program area appear to be focused, well managed, and effective in addressing the DOE Hydrogen and Fuel Cells Program's R&D needs?
  - Yes, the program appears to be focused, well managed, and effective.
  - The objective of the Manufacturing R&D program area should focus on manufacturing cost, enabling the design of choice, and reducing the cost of producing the design.
4. Other Comments:
  - The funding should focus on alternate manufacturing and quality control techniques that lower the cost of producing any design of choice.
  - DOE should consider the addition of support for improved design for manufacture and assembly (DFMA) that is directly relevant to PEM and SOFC fuel cell stacks and advanced stack assembly methods. Hopefully the FY 2014 appropriation will be the same as the DOE request.

## Technology Validation Program Comments

1. Was the 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 and/or session overview presentations of the program if appropriate.)
  - The Technology Validation program area was adequately covered, important issues and challenges were identified, and progress was clearly presented.
  - The program area was well presented and complete. The structure of the Fuel Cell Technologies Office, as shown on slide 2, can be readily understood and the placement of the program within the Office is clear. Slide 3, in combination with the rest of the program manager's presentation, provided a succinct summary of the program's goal to assess technologies and provide feedback for the benefit of other DOE Hydrogen and Fuel Cells Program areas. Slides 6–11 provided an excellent summary of progress and set the stage well for the individual project reviews. It is unclear whether the specific objectives listed on slide 3 comprise all of those associated with the program or whether they are a selected subset; that should be clarified in the slides and/or oral presentation. Some of the equipment included in the program (e.g., buses, MHE, and backup power) is not reflected in the objectives cited. On slide 4, another challenge could be: "Determining priorities for expenditure of Technology Validation program resources."
  
2. Are plans identified for addressing issues and challenges? Are there gaps in the project portfolio?
  - Yes, plans were identified for addressing issues and challenges. No, there are no gaps in the portfolio.
  - The bulk of fiscal year (FY) 2014 Technology Validation program resources will evidently be for projects resulting from proposals submitted in response to an upcoming funding opportunity announcement (FOA). Given the topics identified on slide 12, it appears that ongoing "core" program activities, such as data collection on light-duty-vehicle and bus performance, will continue with FY 2013 funds, however, this was not (to this reviewer's knowledge) stated directly during the program manager's oral presentation. Reviewers should be assured that new topics planned for the portfolio, such as fuel cell hybrid-electric medium-duty trucks and rooftop installations of fuel cell backup power systems, will not be initiated at the expense of continual support for "core" program activities.
  - One Technology Validation program goal is to demonstrate 50,000 hour life of 100 kW–3 MW stationary fuel cell systems, but that would take 5.7 years of continuous testing, and it is unclear if there is any evidence that such a test has even been planned for such large fuel cell systems, let alone started. Fuel cell auxiliary power unit durability is 15,000 hours or 1.7 years; again, there was no indication that such a test has been planned. In some circumstances, one can propose accelerated life testing, such as increasing the repetition rate of equipment that must be cycled on and off or increasing the radiation striking a photovoltaic panel, for example. No means of conducting accelerated life testing of fuel cell systems was presented.
  
3. Does the program area appear to be focused, well managed, and effective in addressing the DOE Hydrogen and Fuel Cells Program's R&D needs?
  - The Technology Validation program area appears to be well focused, well managed, and effective.
  - Overall, the program area is important and well managed. Its partnership with, and dependence on, the National Renewable Energy Laboratory's (NREL's) outstanding data collection/analysis team is key to the success of its efforts and to achieving its goals and objectives. The line of demarcation between the Technology Validation and Market Transformation programs is not completely clear. A case could be made that the H2Pump project, with eight demonstration systems, is within the purview of the Market Transformation program area. The planned funding opportunity announcement (FOA) topics include demonstrations. (Given that, both demonstrations and data validation of the demonstration project(s) results are important and need to be closely linked.)
  - For the most part, yes. However, two other fueling station components need attention. Certainly, compressors should be a top priority, given their high failure rate. The Technology Validation program should consider the development of gas pre-cooling refrigeration systems for 700 bar dispensing; current refrigeration systems are too costly, which could impede early market introduction. Similarly, hydrogen

dispensers are too expensive, and the program should consider the development of low-cost 700 bar dispensers, including the development of durable and accurate flow meters.

4. Other Comments:

- Future Technology Validation program overview presentations should include a brief statement on how decisions are made regarding projects to be funded by the program. For example, it would be helpful to have some insight into the merits of the H2Pump project and rooftop installations of fuel cell backup power systems, relative to other opportunities. One guess is that the total amount of hydrogen that can potentially be produced by H2Pump's technology is small compared to current hydrogen demand—and very small relative to demand in a “hydrogen economy.” If the analysis of its potential has not been done, it should be considered for inclusion in the Systems Analysis program and accomplished before more funds are committed to hydrogen recycling projects. DOE’s funding decisions should reflect analysis that identifies technologies capable of providing a significant portion of the demand for hydrogen and that address a robust market for fuel cells.
- The electrochemical pump program should be redirected. The current focus on recovering hydrogen from metal annealing furnaces is a niche market that will not advance the Hydrogen and Fuel Cell Program’s mission of expediting the commercialization of fuel cell electric vehicles (FCEVs) and stationary fuel cells. The recovered hydrogen is needed in the annealing furnace and cannot be used as a fuel for FCEVs, for example. Instead of capturing hydrogen from furnace exhausts, the program should be redirected to developing an inexpensive electrochemical hydrogen compressor to replace mechanical compressors, with twin goals of lower capital cost and vastly improved durability and low maintenance.

## Safety, Codes and Standards Program Comments

1. Was the 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 and/or session overview presentations of the program if appropriate.)
  - Yes, the Safety, Codes and Standards (SCS) program area was adequately covered, important issues and challenges were identified, and progress was clearly presented.
  - Coverage of the SCS program area was very good. The range of projects discussed was consistent with the program and the projects to be discussed later. The presenter discussed the issues and challenges and described how these were being addressed in the research and other ongoing projects. Progress was described well, including standards approved, training materials and coverage, and lessons learned. Also described well were the research results and how they were being fed into the regulations, codes, and standards activities and disseminated to the public and other users. The new “app” for Apple products is very exciting, as are plans to expand the app to other applications.
  - While some issues and challenges were identified and progress was clearly presented in comparison to the previous year (e.g., progress related to safety [jets and flames, emergency response training, information products, etc.]), there are key issues that do not appear to be a priority with DOE.
  - No. There were statements made by some of the presenters that were challenged by the audience. There is still so much that needs to be completed before one can truly state that risk can be identified and quantified. The first round of standards has been published and some realistic preliminary economic targets have been established. Product and system innovation will now follow to meet the commercial requirements that are being set forth by industry. Funding and support is now critical to ensure that industry takes on the risk and starts investing in this market space. The plan to manage this transition (hand off) was not clearly articulated.
  
2. Are plans identified for addressing issues and challenges? Are there gaps in the project portfolio?
  - The program plans seem very well thought out, with much work this year focused on developing data and tools that will address known issues and challenges. Meetings and webinars that targeted specific issues, such as hydrogen fueling protocols and materials issues, were also developed and conducted. The program is always seeking feedback to identify gaps as they are discovered and to begin to address them. It may be worthwhile to consider revisiting the national template and international template to update and validate future plans that meet the anticipated priorities of industry and other stakeholders.
  - While the overview presentation stated that the execution of high-priority R&D is a necessary and integral part of the SCS activity, the topics for future R&D work and the approach that will be taken for implementing this R&D are not identified.
  - There are limited plans. There seems to be a disconnect in what DOE is doing to support the hydrogen industry in the transition period. Hydrogen as a transportation solution is very much still driven by DOE funding. If funding were to be stopped, hydrogen would not go forward in the United States. The hydrogen champions that were critical in driving the industry are now passing the batons to the next group. This group is not driven by the same passion and search for technological solutions, but rather by finding commercial solutions that can leverage the benefits of hydrogen as a fuel. The current commercial environment is not supportive of hydrogen when compared to other fuels, such as compressed natural gas and electricity. DOE needs to better realize and develop plans to support a hydrogen transition. Outreach and support to teach and help quantify and mitigate the commercial risk is most important. The signal of reduced DOE funding for the Hydrogen and Fuel Cells Program (the Program) has had a large, negative impact in the private sector. As a result, it seems that the hydrogen economy is always looming on the horizon, but only after another technical hurdle is overcome. There are still many technical showstoppers that this industry must tackle before it will be ready for the mass public: achieving accurate fuel metering, achieving component reliability, managing thermal issues, developing low-cost materials that are compatible with long-term hydrogen exposure at in-service conditions, and developing new and novel fueling station designs that are cost effective and allow infrastructure to be profitable. These are examples of issues that still need to be resolved and need to be tackled by a joint public-private enterprise. A reduction in funding for the Program drives the private sector to question the viability of this fuel as an alternative when placed beside the others, such as natural gas vehicles, electric vehicles, biofuels, etc.

- The planning on the slides for the SCS program area ended in 2012; this is very shortsighted. Yes, there were some big issues not covered in the presentation:
  - Through California Senate Bill (SB) 76, SAE J2719 has become law in California. The detection limits can be measured by expensive laboratories; however, since the standards for detection are not complete there are inadequate appropriate testing means. Though the priorities regarding the testing of single cells to appropriate loadings, CO detection, are important, they are not even close to the importance of finishing the detection methods.
  - Field Testing: (continuation of laboratory tests) Fueling standards should be further validated at a designated development station to show the positives and negatives (for instance SAE J2601 versus the MC Method, etc.). This station could also be a basis for metering and hydrogen quality testing.
  - Regarding CSA standards on dispenser components, the hose, breakaway, and connectors standards have not *been tested before becoming ANSI approved*; this should be investigated with data.
  - SAE J2578 /J2579 need data to be validated. Topics like stress rupture are inadequately covered in those documents.
  - Setback distances need to be aligned between the ISO and SAE world. This should be a coordinated data effort with the Japanese and European Union (EU) counterparts.
  - The hydrogen sensor work is obsolete because the industry has solutions in its production vehicles and stations. This project should be halted.
  - Hydrogen metering: Hydrogen metering is being evaluated through the National Renewable Energy Laboratory (NREL), and there is already an additional funding opportunity announcement (FOA) to investigate this. However, there needs to be a follow-on project that incorporates testing flow meters not only in the laboratory, but also in the field until a commercially acceptable flow meter is found to get within 2% accuracy.

3. Does the program area appear to be focused, well managed, and effective in addressing the DOE Hydrogen and Fuel Cells Program’s R&D needs?

- Yes, the SCS program area appears to be well considered, with regular feedback mechanisms to remain effective. Despite personnel changes, the program remains well managed.
- Yes. In particular, there are two major strong points in the SCS program area: (1) the direct interaction of researchers in the program with standards development organizations is very useful and highly contributes to the effectiveness of the program and (2) the active dissemination and outreach to ensure access to safety-relevant information for other stakeholders (authorities having jurisdiction) and the wider public.
- The program area has been able to achieve very strong results with limited funding. The management team should be commended for its courage in prioritizing research and cutting the projects that are less essential. The only challenge is that the program funding continues to drop and, as a result, its ability to benefit society is threatened. More focus on outreach is needed or all of the good that is being achieved with the Program’s funding will never be realized.
- The program area is well focused and well managed, but not effective in meeting their previous goals for the DOE Hydrogen and Fuel Cells Program. However, lack of input from industry on the latest needs illustrates a large gap (as outlined in the response to Question 2) and should be addressed to facilitate the commercialization of fuel cell electric vehicles and hydrogen infrastructure.

4. Other Comments:

- The importance of the international efforts is clear in the SCS program presentation, but this is less clear in presentations of the overall Hydrogen and Fuel Cells Program or in many of the project activities funded by the SCS program area. It is unclear if internal communications could be improved on this point.
- Suggestions: create a “Near-Term R&D Needs” list for codes and standards by canvassing industry members at ASTM/CSA/SAE needs, etc. to develop a roadmap; be a part of “accelerating key” industry codes and standards; and delete all hydrogen sensor work—this is not valuable to the industry at all.
- Parts of the underpinning research for the SCS work are carried out in a number of national laboratories. It may be worthwhile to try to better exploit synergies with non-U.S. activities (e.g., EU, Japan) when performing this R&D. It may be useful to identify a number of performance indicators (metrics of success) with associated targets and propose evaluators to assess the degree of achievement of these targets during the review.

## Market Transformation Program Comments

1. Was the 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 and/or session overview presentations of the program if appropriate.)
  - Yes, the Market Transformation program area was adequately covered, important issues and challenges were identified, and progress was clearly presented.
  - The program manager did a great job in his presentation.
  - Given the time allowed and the purpose, the presentation and material delivered were just about right. It might be worthwhile to explore some ways to better show how targets have trended over time. For instance, one could plot the increasing deployment of material handling equipment (MHE) funded by DOE, and then because that is virtually complete, reflect how that has spurred and helped catalyze the market and show how commercial deployment has progressed during and after those DOE-funded deployments. It would be helpful to capture how the activity in the program has supported the broader and more robust introduction in the marketplace. It is unclear whether that type of metric clearly comes through.
2. Are plans identified for addressing issues and challenges? Are there gaps in the project portfolio?
  - It looks like there is a “road map” for leveraging program resources for the next 4–6 years. One would think one of the major challenges that fuel cells must address over the next few years is keeping pace with battery improvements, so being agile in study and demonstration may be essential over that time frame.
  - It would be good to see significantly more resources allocated for the Market Transformation program area. It is time to get serious about this.
  - No, plans for addressing issues and challenges were not adequately addressed.
3. Does the program area appear to be focused, well managed, and effective in addressing the DOE Hydrogen and Fuel Cells Program’s R&D needs?
  - Yes, the Market Transformation program area appears to be focused, well managed, and effective.
4. Other Comments:
  - There is a good variety of projects with strong, important markets.
  - In addition to providing trending charts, as suggested in Question 1, it is recommended that some “market” metrics be introduced or discussed in the program overview or for each project. For instance, for micro-CHP, if the potential market is small commercial buildings, it should be defined what the characteristics of the buildings are, how many are located around the country, how much energy they use, etc. One would think that these types of metrics would help define priorities for the R&D and investment.

## Systems Analysis Program Comments

1. Was the 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 and/or session overview presentations of the program if appropriate.)

- Yes, the Systems Analysis program area was adequately covered, important issues and challenges were identified, and progress was clearly presented.
- Yes, however some interesting projects from last year were not reviewed. Evaluation of the Systems Analysis program area is best done across multiple years, given the broad portfolio of topics.
- There was a good summary of overall objectives and plans to implement the Assistant Secretary's new initiative, H2USA.

2. Are plans identified for addressing issues and challenges? Are there gaps in the project portfolio?

- Yes, plans for addressing issues and challenges were identified.
- Yes, plans and gaps were identified and addressed. The issue of funding continues to be a concern.
- A good adjustment in parameters was made within models to address fast-changing resource availability and costs, as well as consumer demand.
- A greater emphasis on near-term market barriers is warranted, given the status of fuel cell vehicles and the challenges with infrastructure deployment. A major gap is the lack of analysis of policy options to incentivize actors and finance infrastructure, but it appears that future work on H2USA may address this need.

3. Does the program area appear to be focused, well managed, and effective in addressing the DOE Hydrogen and Fuel Cells Program's R&D needs?

- Yes, the Systems Analysis program area appears to be focused, well managed, and effective.
- Yes, the program area appears to be focused, well managed, and effective. The manager is articulate and clear in his presentation of the program.
- Interactions between types of analysis and applications were illustrated with examples. There were good flowcharts to describe the process. The main focus is on analysis rather than model development.
- Yes, except for the gap of near-term market focus.

4. Other Comments:

- The Systems Analysis program area has moved logically from model development to model use to producing analysis for prime clients (other Fuel Cells Technologies Office programs and upper DOE management, as well as other stakeholders).
- The program should continually be assessed for direction and effectiveness if supply chain, manufacturing, and export of product become priority areas.

## Project Evaluation Form

This evaluation form was used for the following program panels: Hydrogen Production and Delivery; Hydrogen Storage; Fuel Cells; Manufacturing R&D; Technology Validation; Safety, Codes and Standards; Market Transformation; and Systems Analysis.

### Evaluation Criteria: U.S. Department of Energy (DOE) Hydrogen and Fuel Cells Program Annual Review

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*Provide specific, concise comments to support your evaluation and write clearly, please.*

#### 1. Approach

To performing the work – the degree to which barriers are addressed, the project is well-designed, feasible, and integrated with other efforts. (Weight = 20%)

**4 - Outstanding.** Sharply focused on critical 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.

- 4 - Outstanding
- 3 - Good
- 2 - Fair
- 1 - Poor

**Comments on Approach to performing the work:**

#### 2. Accomplishments and Progress

Toward overall project and DOE goals – the degree to which progress has been made and measured against performance indicators, and the degree to which the project has demonstrated progress toward DOE goals. (Weight = 45%)

**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 toward objectives or any barriers.

- 4 - Outstanding
- 3 - Good
- 2 - Fair
- 1 - Poor

**Comments on Accomplishments and Progress toward overall project and DOE goals:**

### 3. Collaboration and Coordination with Other Institutions

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 significantly improved.

**1 - Poor.** Most work is done at the sponsoring organization with little outside collaboration; little or no apparent coordination with partners.

4 - Outstanding

3 - Good

2 - Fair

1 - Poor

**Comments on Collaboration and Coordination with other institutions:**

### 4. Relevance/Potential Impact

The degree to which the project supports and advances progress toward the Hydrogen and Fuel Cells Program goals and objectives delineated in the Fuel Cell Technologies Office Multi-Year Research, Development & Demonstration Plan. (Weight = 15%)

**4 - Outstanding.** Project is critical to the Hydrogen and Fuel Cells Program and has potential to significantly advance progress toward DOE RD&D goals and objectives.

**3 - Good.** Most project aspects align with the Hydrogen and Fuel Cells Program and DOE RD&D objectives.

**2 - Fair.** Project partially supports the Hydrogen and Fuel Cells Program and DOE RD&D objectives.

**1 - Poor.** Project provides little potential impact on advancing progress toward the Hydrogen and Fuel Cells Program and DOE RD&D objectives.

4 - Outstanding

3 - Good

2 - Fair

1 - Poor

**Comments on Relevance/Potential Impact:**

## 5. Proposed Future Work

The degree to which the project has effectively planned its future in a logical manner by incorporating appropriate decision points, considering barriers to its goals and, when sensible, mitigating risk by providing alternate pathways.

Note: if a project has ended, please leave blank. (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.

4 - Outstanding

3 - Good

2 - Fair

1 - Poor

**Comments on Proposed Future Work:**

**Project Strengths:**

**Project Weaknesses:**

**Recommendations for Additions/Deletions to Project Scope:**

### List of Projects Not Reviewed

Project ID	Project Title	Principal Investigator Name	Organization
PD-004	Distributed Bio-Oil Reforming	Stefan Czernik	National Renewable Energy Laboratory
PD-013	Electrolyzer Development for the Copper-Chlorine Thermochemical Cycle	Michele Lewis	Argonne National Laboratory
PD-016	Oil-Free Centrifugal Hydrogen Compression Technology Demonstration	Hooshang Heshmat	Mohawk Innovative Technology
PD-017	Development of a Centrifugal Hydrogen Pipeline Gas Compressor	Frank Di Bella	Concepts NREC
PD-021	Development of High-Pressure Hydrogen Storage Tank for Storage and Gaseous Truck Delivery	Don Baldwin	Hexagon Lincoln
PD-027	Solar High-Temperature Water Splitting Cycle with Quantum Boost	Robin Taylor	Science Applications International Corporation
PD-030	PEM Electrolyzer Incorporating an Advanced Low-Cost Membrane	Monjid Hamdan	Giner Electrochemical Systems, LLC
PD-031	Renewable Electrolysis Integrated System Development and Testing	Kevin Harrison	National Renewable Energy Laboratory
PD-033	Solar Hydrogen Production by Photoelectrochemical (PEC) Water-Splitting: Advancing Technology Through the Synergistic Activities of the PEC Working Group	Thomas Jaramillo	Stanford University/National Renewable Energy Laboratory
PD-048	Electrochemical Hydrogen Compressor	Ludwig Lipp	FuelCell Energy, Inc.
PD-052	Photoelectrochemical Materials: Theory and Modeling	Muhammad Huda	University of Texas at Arlington
PD-053	Photoelectrochemical Hydrogen Production	Jian Hu	MVSystems/Hawaii Natural Energy Institute
PD-056	Critical Research for Cost-Effective Photoelectrochemical Production of Hydrogen	Liwei Xu	Midwest Optoelectronics, LLC
PD-065	Unitized Design for Home Refueling Appliance for Hydrogen Generation to 5,000 psi	Timothy Norman	Giner Electrochemical Systems, LLC

Project ID	Project Title	Principal Investigator Name	Organization
PD-067	Hydrogen by Wire Home Fueling System	Luke Dalton	Proton OnSite
PD-071	High-Performance, Low-Cost Hydrogen Generation from Renewable Energy	Katherine Ayers	Proton OnSite
PD-076	Metal Oxide Semiconductor Nanotubular Arrays for Photoelectrochemical Hydrogen Generation	Dev Chidambaram	University of Nevada, Reno
PD-090	Low-Cost, Large-Scale PEM Electrolysis for Renewable Energy Storage	Katherine Ayers	Proton OnSite
PD-091	Bio-Fueled Solid Oxide Fuel Cells	Gokhan Alptekin	TDA Research
PD-093	Polymer and Composite Material Performance in Hydrogen	Chris Moen	Sandia National Laboratories
PD-096	Electrolyzer Component Development for the HyS Thermochemical Cycle	William Summers	Savannah River National Laboratory
PD-097	Photoelectrochemical Material Synthesis at Los Alamos National Laboratory	Todd Williamson	Los Alamos National Laboratory
PD-098	Low-Noble-Metal-Content Catalysts/Electrodes for Hydrogen Production by Water Electrolysis	Katherine Ayers	Proton OnSite
PD-099	Next-Generation Silicon Microwire Array Devices for Unassisted Photoelectrosynthesis	Shane Ardo	California Institute of Technology
ST-014	Hydrogen Sorbent Measurement Qualification and Characterization	Phil Parilla	National Renewable Energy Laboratory
ST-018	Biomimetic Approach to Metal-Organic Frameworks with High Hydrogen Uptake	Joe Zhou	Texas A&M University
ST-034	Aluminum Hydride: the Organometallic Approach	Jim Wegrzyn	Brookhaven National Laboratory
ST-040	Fluid Phase Hydrogen Storage Material Development	Benjamin Davis	Los Alamos National Laboratory
ST-048	Hydrogen Storage Materials for Fuel Cell Powered Vehicles	Andrew Goudy	Delaware State University

APPENDIX D: PROJECTS NOT REVIEWED

Project ID	Project Title	Principal Investigator Name	Organization
ST-067	Neutron Characterization in Support of the Hydrogen Storage Program	Terry Udovic	National Institute of Standards and Technology
ST-095	Low-Cost, Metal Hydride-Based Hydrogen Storage System for Forklift Applications (Phase II)	Daniel Brayton	University of Hawaii
ST-105	Ultra-Lightweight, High-Pressure Hydrogen Fuel Tanks Reinforced with Carbon Nanotubes	Dongsheng Mao	Applied Nanotech, Inc.
ST-109	Low-Cost Integrated Nanoreinforcement for Composite Tanks—"LINCT" (Small Business Innovative Research Phase I)	Terrisa Duenas	NextGen Aeronautics
ST-110	Optimizing the Cost and Performance of Composite Cylinders for Hydrogen Storage using a Graded Construction	Andrea Haight	Composite Technologies Development
FC-028	Transport Studies Enabling Efficiency Optimization of Cost-Competitive Fuel Cell Stacks	Robert Dross/Amedeo Conti	Nuvera Fuel Cells
FC-040	High-Temperature Membrane with Humidification-Independent Cluster Structure	Ludwig Lipp	FuelCell Energy, Inc.
FC-049	Development of Micro-Structural Mitigation Strategies for PEM Fuel Cells: Morphological Simulations and Experimental Approaches	Silvia Wessel	Ballard
FC-079	Improving Fuel Cell Durability and Reliability	Prabhakar Singh	University of Connecticut Global Fuel Cell Center
FC-102	New High Performance Water Vapor Membranes to Improve Fuel Cell Balance of Plant Efficiency and Lower Costs	Earl Wagener	Tetramer Technologies, LLC
FC-105	Low-Cost PEM Fuel Cell Metal Bipolar Plates	C.H. Wang	TreadStone Technologies, Inc.
FC-106	Rationally Designed Catalyst Layers for PEM Fuel Cell Performance Optimization	Deborah Myers	Argonne National Laboratory
FC-107	Non-Precious Metal Fuel Cell Cathodes: Catalyst Development and Electrode Structure Design	Piotr Zelenay	Los Alamos National Laboratory
FC-108	Advanced Ionomers and Membrane Electrode Assemblies for Alkaline Membrane Fuel Cells	Bryan Pivovar	National Renewable Energy Laboratory
MN-005	Adaptive Process Controls and Ultrasonics for High-Temperature PEM Membrane Electrode Assembly Manufacture	Dan Walczyk	Rensselaer Polytechnic Institute

Project ID	Project Title	Principal Investigator Name	Organization
MN-008	Development of Advanced Manufacturing Technologies for Low-Cost Hydrogen Storage Vessels	Mark Leavitt	Quantum Fuel Systems Technologies Worldwide, Inc.
TV-001	Fuel Cell Electric Vehicle Evaluation	Jennifer Kurtz	National Renewable Energy Laboratory
TV-017	Next Generation Hydrogen Infrastructure Evaluation	Sam Sprik	National Renewable Energy Laboratory
TV-023	Data Collection and Validation of Newport Beach Hydrogen Station Performance	Michael Kashuba	California Air Resources Board
TV-024	California State University, Los Angeles Hydrogen Refueling Facility Performance Evaluation and Optimization	David Blekman	California State University, Los Angeles
TV-025	Performance Evaluation of Delivered Hydrogen Fueling Stations	Michael Tieu	Gas Technology Institute
SCS-015	Hydrogen Emergency Response Training for First Responders	Monte Elmore	Pacific Northwest National Laboratory
SCS-020	International Program for Hydrogen and Fuel Cells in the Economy – Regulations, Codes and Standards Working Group	Jay Keller	U.S. Department of Energy Consultant
H2RA-002	Solid Oxide Fuel Cell Diesel Auxiliary Power Unit Demonstration	Dan Hennessy	Delphi Automotive
H2RA-003	Highly Efficient, 5kW Combined Heat and Power Fuel Cells Demonstrating Durability and Economic Value in Residential and Light Commercial Applications	Jim Petrecky	Plug Power
H2RA-007	Accelerating Acceptance of Fuel Cell Backup Power Systems	Jim Petrecky	Plug Power
H2RA-012	Use of 72-Hour Hydrogen PEM Fuel Cell Systems to Support Emergency Communications	Kevin Kenny	Sprint
BES-001	Computer Simulation of Proton Transport in Fuel Cell Membranes	Gregory Voth	University of Chicago
BES-002	Fluoropolymers, Electrolytes, Composites, and Electrodes	Stephen Creager	Clemson University

Project ID	Project Title	Principal Investigator Name	Organization
BES-003	Gas Transport Across Hyperthin Membranes	Steven Regen	Lehigh University
BES-004	Theory-Guided Design of Nanoscale Multimetallic Nanocatalysts for Fuel Cells	Perla Balbuena	University of Texas
BES-005	Structure-Property Relationship in Metal Carbides and Bimetallic Alloys	Jingguang Chen	Columbia University
BES-006	Nanostructured Catalysts for Hydrogen Generation from Renewable Feedstocks	Abhaya Datye	University of New Mexico
BES-007	Fundamental Structure/Property Studies of Gas Separation Membrane Polymers	Benny Freeman	University of Texas-Austin
BES-008	Precisely Tunable High Performance Carbon Molecular Sieve Membranes for Energy Intensive Separations	William Koros	Georgia Tech
BES-009	Nanoporous Membranes for Hydrogen Production: Experimental Studies and Molecular Simulations	Muhammad Sahimi	University of Southern California
BES-010	Structure/Composition/Function Relationships in Supported Nanoscale Catalysts for Hydrogen	Peter Stair	Argonne National Laboratory
BES-011	Metal and Metal Oxide-Supported Platinum Monolayer Electrocatalysts for Oxygen Reduction	Radoslav Adzic	Brookhaven National Laboratory
BES-012	Active Sites and Mechanism for the Water-Gas Shift Reaction on Metal and Metal/Oxide Catalysts	Jose Rodriguez	Brookhaven National Laboratory
BES-013	Fundamentals of Catalysis and Chemical Transformations	Steve Overbury	Oak Ridge National Laboratory
BES-014	Activation of Small Molecules with Bi-Functional Ambiphilic Catalyst Complexes	Thomas Autrey	Pacific Northwest National Laboratory
BES-016	Bio-Inspired Molecular Catalysts for Oxidation of Hydrogen and Production of Hydrogen: Cheap Metals for Noble Tasks	Morris Bullock	Pacific Northwest National Laboratory
BES-017	Platinum Group Metal Substituted Complex Oxide Catalysts	Ram Seshadri	University of California-Santa Barbara
BES-018	Porous Transition Metal Oxides: Synthesis, Characterization, and Catalytic Activity	Steven Suib	University of Connecticut

Project ID	Project Title	Principal Investigator Name	Organization
BES-019	Understanding the Effects of Surface Chemistry and Microstructure on the Activity and Stability of Pt Electrocatalysts on Non-Carbon Supports	William Mustain	University of Connecticut
BES-020	In Situ NMR/Infrared/Raman and AB Initio DFT Investigations of Pt-Based Mono- and Bi-Metallic Nanoscale Electrocatalysts: From Sulfur-Poisoning to Polymer Promoters to Surface Activity Indexes	YuYe Tong	Georgetown University
BES-021	Investigation of the Nature of Active Sites on Heteroatom-Containing Carbon Nano-Structures for Oxygen Reduction Reaction	Umit Ozkan	The Ohio State University
BES-022	Oxide-Metal Interactions Studied on M@Oxide, Core-Shell Catalysts	Raymond Gorte	University of Pennsylvania
BES-023	Fundamental Studies of the Steam Reforming of Alcohols on PdZnO and Co/ZnO Catalysts	John Vohs	University of Pennsylvania
BES-024	Theoretically Relating the Surface Composition of the Pt Alloys to their Performance as the Electrocatalysts of Low-Temperature Fuel Cells	Guofeng Wang	University of Pittsburgh
BES-025	Nanoscale Surface Chemistry and Electrochemistry of Clean and Metal-Covered Faceted Substrates: Structure, Reactivity and Electronic Properties	Robert Bartynski	Rutgers University
BES-026	Correlation of Theory and Function in Well-Defined Bimetallic Electrocatalysts	Richard Crooks	University of Texas
BES-027	Metal-Ion Sites on Oxide Supports as Catalysts for the Water-Gas Shift and Methanol Steam Reforming Reactions	Maria Flytzani-Stephanopoulos	Tufts University
BES-028	Hydrocarbon Oxidation, Dehydrogenation and Coupling over Model Metal Oxide Surfaces	David Cox	Virginia Tech
BES-029	Atomic Level Studies of Advanced Catalysts for Hydrodeoxygenation	S. Ted Oyama	Virginia Tech
BES-030	Atomic-Scale Design of Metal and Alloy Catalysts: A Combined Theoretical and Experimental Approach	Manos Mavrikakis	University of Wisconsin

## 2013 Annual Merit Review Survey Questionnaire Results

Following the 2013 Hydrogen and Fuel Cells Program Annual Merit Review (AMR), all participants were asked for feedback on the review process and meeting logistics. This appendix summarizes the results of that feedback, and is organized by type of respondent, as follows:

1. All Respondents
2. Responses from “Attendee, neither Reviewer nor Presenter”
3. Responses from Reviewers
4. Responses from Presenters.

### 1. All Respondents

#### 1.1. What is your affiliation?

	Number of Responses	Response Ratio
Government agency directly sponsoring the program under review	10	4.4%
National/government laboratory, private-sector or university researcher whose project is under review	54	24.2%
Non-government institution that received funding from the program(s) under review	44	20%
Non-government institution that does not receive funding from the program(s) under review	39	17.4%
Government agency with interest in the work	4	2%
National/government laboratory, private-sector or university researcher not being reviewed	45	20.1%
Other (see listing below)	19	8.5%
No Responses	8	3.5%
<b>Total</b>	<b>223</b>	<b>100%</b>

#### “Other” Responses

- Manufacturer in the energy sector
- Contractor to a government agency interested in the work of the U.S. Department of Energy (DOE) Hydrogen and Fuel Cells Program
- Business development in an energy technology company
- Non-government institution that did receive funding, but is not under review
- Private company
- DOE contractor
- Financial sector representative
- Private consultant
- University funded by the DOE Basic Energy Sciences program
- University of Maryland
- University of China
- Canadian university
- Retired scientist
- International Energy Agency member from Germany (previous reviewer)

1.2. Purpose and scope of the Annual Merit Review were well defined by the Joint Plenary Session (answer only if you attended the Joint Plenary on Monday).

The top number is the count of respondents selecting the option. The bottom percentage is the percent of the total respondents selecting the option.

Highly Disagree	Disagree	Neutral	Agree	Highly Agree
1	1	8	55	53
1%	1%	7%	47%	45%

*12 Comments*

- The Joint Plenary Session (Joint Session) was excellent.
- The presentations were outstanding.
- The overview was good, but rather short.
- The instructions provided for the merit review process were very clear.
- The guidance and summary provided by Assistant Secretary for Energy Efficiency and Renewable (EERE) Energy David Danielson was excellent. This is evidence of great leadership.
- The Joint Session was extremely valuable as a high-level overview and provided context for the DOE Hydrogen and Fuel Cells Program and program area overviews. It was helpful to understand DOE's overall objectives regarding energy efficiency and how the programs fit into those goals.
- It seemed that DOE is in a period of transition because many comments were vague.
- The purpose of the AMR did not seem to be discussed in-depth during the Joint Session.
- There were not any specifics in any of the presentations, so only a qualitative estimation can be given, not a quantitative estimation.
- The Joint Session needs to focus more on breakthroughs and highlights from the last year instead of laying out the whole program. That is what the program websites are for.
- The Joint Session's graphics were too complex. The Session should have had only the Assistant Secretary speak about the Administration's policies and how these policies are promoting energy efficiency and renewable technologies.
- The presentations were interesting. The Basic Energy Sciences presentation focused too much on program structure; more scientific results would have been highly appreciated.

1.3. The two plenary sessions after the Joint Plenary Session were helpful to understanding the direction of the Hydrogen and Fuel Cells and Vehicle Technologies Programs (answer only if you attended either the Hydrogen and Fuel Cells or Vehicle Technologies plenary sessions on Monday).

The top number is the count of respondents selecting the option. The bottom percentage is the percent of the total respondents selecting the option.

Highly Disagree	Disagree	Neutral	Agree	Highly Agree
0	0	11	64	40
0%	0%	10%	56%	35%

*9 Comments*

- The plenary sessions were outstanding.
- The plenary was very valuable and covered, at a high level, the full scope of the Vehicle Technologies Office (VTO) programs.
- The VTO plenary session was useful in promoting understanding of the structure of the Office's programs and its overall goals, particularly because this was this participant's first Annual Merit Review (AMR).

- These were interesting sessions about the major results. It would have been nice to have some focus on global strategies for hydrogen, fuel cells, and vehicle technologies with regard to other types of energy and applications. There was more information than fit the presentation times.
- As in the Joint Session, DOE seems to be in a period of transition because many comments were vague.
- A special session at the end of the review for discussing the directions of the programs would be helpful.
- The plenary sessions were helpful, but there was a lot of duplication (many of the same slides) in the plenary sessions, the session introduction presentations, and the actual project presentations.
- The VTO plenary session provided useful program overview and program direction information.
- The Hydrogen and Fuel Cells Program plenary session was not as engaging as it could have been. The slides looked like a written report that had been forced to fit a presentation, and while this makes for a useful reference, it does not make for a useful presentation. The presenters should consider using simpler slides in the plenary session, with more detail available on a CD or online.

1.4. Program overviews were helpful to understanding the research objectives. (Answer only if you attended one or more program overviews.)

The top number is the count of respondents selecting the option. The bottom percentage is the percent of the total respondents selecting the option.

Highly Disagree	Disagree	Neutral	Agree	Highly Agree
1	2	7	85	74
1%	1%	4%	50%	44%

15 Comments

- The overviews help to put the research in perspective.
- The overviews were very useful because they gave highlights of the current research.
- The Vehicle Technologies Office merit reviews were conducted very well.
- These were interesting sessions that presented details about the targets and the major results.
- The program overviews helped this participant to better appreciate how the pieces fit together.
- The program overviews should highlight some of the past successes/projects that are influencing the current suite of projects or the direction of the programs.
- The program managers in each of the programs were very knowledgeable about the various projects and did a great job putting the work in perspective. The project highlights and progress toward meeting DOE goals were well presented.
- The program overviews always occur as part of the AMR meeting since they allow for a recap of the programs each year. They also allow for further detail on how the program works within the overall office.
- The program overviews were redundant if one attended the plenary overview sessions.
- The program overview for Vehicle and Systems Simulation and Testing did a good job of categorizing the work that would be presented in the following sessions.
- Many of the same slides were used in all of the overviews. It would have been better to have different slides used.
- The program overviews were somewhat repetitive with the Hydrogen and Fuel Cells Program plenary.
- More explicit identification of the multi-year research, development, and demonstration plan (MYRDDP) targets specific to the program would have been a nice reminder. There should have been bulleted points identifying them as goals, e.g., “these research projects are expected to address...”
- Because reviewers were generally limited to attending only a subset of the program sessions during the week, the plenary sessions on the first day were valuable in promoting understanding of what the other programs within the Offices were doing.
- A few people questioned why DOE is pursuing research on both plug-in hybrid electric vehicles (PHEVs) and internal combustion engine vehicles (ICEs), saying that if DOE is interested in a non-fossil-fuel-based approach for transportation, then the focus should be solely on PHEVs. In this reviewer’s opinion, DOE should focus on both PHEVs and ICEs.

- 1.5. What was your role in the Annual Merit Review? Check the most appropriate response. If you are both a presenter and a reviewer and want to comment as both, complete the evaluation twice, once as each.

	Number of Responses	Response Ratio
Attendee, neither Reviewer nor Presenter	106	47.5%
Presenter of a project	66	29.5%
Peer Reviewer	42	18.8%
No Responses	9	4.0%
<b>Total</b>	<b>223</b>	<b>100%</b>

## 2. Responses from “Attendee, neither Reviewer nor Presenter”

- 2.1. The quality, breadth, and depth of the following were sufficient to contribute to a comprehensive review:

The top number is the count of respondents selecting the option. The bottom percentage is the percent of the total respondents selecting the option.

	Highly Disagree	Disagree	Neutral	Agree	Highly Agree
Presentations	0	2	9	50	40
	0%	2%	9%	50%	40%
Question and answer periods	2	1	12	51	34
	2%	1%	12%	51%	34%
Answers provided to programmatic questions	0	1	11	57	30
	0%	1%	11%	58%	30%
Answers provided to technical questions	0	3	9	63	26
	0%	3%	9%	62%	26%

### 12 Comments

- The review was well controlled. The chairpersons in the meeting were good.
- The DOE manager in the VTO fuels section did a nice job of moderating.
- Not all of the presenters and presentations were of the same caliber, but, in general, all were appropriate for the scope of the review. Several presenters focused on a large number of separate efforts. While this can be nice, it does not allow significant depth on the aspects of the project that are working better and are clearly of more relevance.
- The scientific aspects of the results and discussion should be emphasized more.
- Although the time and presentation template is limited, more in-depth technology description should be included in the presentation.
- There should be more time for questions for non-reviewers.
- It was not clear if programmatic questions were asked.
- It was not clear if the “Answers provided...” referred to the individual project presentations or the program overview presentations.
- There was not enough in-depth discussion. The quality of reviewers’ questions is often low.
- There is still too much emphasis on the programmatic elements, and too little on the technical elements.
- There is an inherent difficulty in reviewing technical content in this format. Providing reviewers with some one-on-one time with the principal investigators would greatly improve the technical content of the reviews.

- It was hard to gauge when a project was in trouble. After reviewers started asking questions, it was clear that a few projects were in trouble. The presenters should be up-front and honest about the status of the project and not glaze over hard topics.

2.2. Enough time was allocated for presentations.

The top number is the count of respondents selecting the option. The bottom percentage is the percent of the total respondents selecting the option.

Highly Disagree	Disagree	Neutral	Agree	Highly Agree
0	4	13	44	40
0%	4%	13%	44%	40%

6 Comments

- The timing is perfect. There is plenty of time to cover the details of the technical program and assess the progress.
- It is a tightly packed schedule, but overall it is efficient.
- In some cases it was enough time, but not in all.
- There were some more complex projects that seemed to need more time, although in general it was enough.
- The time was generally enough, but there are several presenters that go over the allotted time year after year. Something needs to be done about that.
- The 20-minute time limit is enough; however, some of the presenters should have been more prepared and have a better understanding of how short that time actually is.

2.3. The questions asked by reviewers were sufficiently rigorous and detailed.

The top number is the count of respondents selecting the option. The bottom percentage is the percent of the total respondents selecting the option.

Highly Disagree	Disagree	Neutral	Agree	Highly Agree
1	5	24	48	23
1%	5%	24%	48%	23%

9 Comments

- The reviewers are experts in their field and it shows.
- Some improvements could be made in this area; however, overall these questions are very good.
- Many of the reviewers were very impressive. They asked thoughtful questions that brought value to the review.
- In some cases the questions were good, but in others the reviewers did not seem familiar with the work at all.
- There were some very good questions raised by reviewers, but some were lacking technicality. Additionally, some questions, though mostly asked by audience members, were ego-driven due to conflicts of interests.
- Some reviewers appeared unprepared.
- Some questions were more of a comment disguised as a question.
- Most of the reviewers' questions were fairly superficial.
- Because it is in a public setting, the questions never seemed to be too rigorous.

#### 2.4. The frequency (once per year) of this formal review process for this Program is:

	Number of Responses	Response Ratio
About right	88	39.4%
Too frequent	2	<1%
Not frequent enough	6	2.6%
No opinion	6	2.6%
No Responses	121	54.2%
<b>Total</b>	<b>223</b>	<b>100%</b>

##### 4 Comments

- One a year is perfect.
- The frequency is good. Having the meeting more frequently would be too costly, and less frequently would not allow participants to interact with other performers frequently enough.
- Twice a year would be better so that basic changes to direction could be made.
- Some projects require a lot of time to develop in terms of receiving equipment, constructing the laboratory, etc. In most cases, receiving equipment takes about a year. Running the equipment after safety reviews takes an additional 1–2 months. The frequency should be taken into account by considering the scope of the project.

#### 2.5. Logistics, facilities, and amenities were satisfactory.

The top number is the count of respondents selecting the option. The bottom percentage is the percent of the total respondents selecting the option.

Highly Disagree	Disagree	Neutral	Agree	Highly Agree
0	4	5	34	58
0%	4%	5%	34%	57%

##### 18 Comments

- The area chosen for the meeting was very accessible.
- This is an excellent venue. It is great to be close to a metro station and the airport.
- The meeting rooms were comfortable with good ventilation. The lunches were fine and had good service.
- A longer lunch time would have been nice. The food was great.
- It would be better if there was just one venue instead of two. Otherwise, it was great.
- There was only one microphone feedback incident; otherwise, the logistics were well handled.
- For the most part the logistics, facilities, and amenities were satisfactory. On Thursday, presentations in the Alexandria Room were somewhat difficult to see for non-reviewers because the screen was not sufficiently high enough to view in its entirety—other attendees' heads were in the way.
- The food should have been left out throughout the presentations and not just during the break times.
- The hotel could have been better at keeping coffee and cream supplied.
- There needs to be more seating in the foyer and hallways outside of the presentation rooms.
- Washington, DC is on the expensive side.
- The venue was not very nice or comfortable.
- The air conditioning was too cold.
- The walk between hotels was a barrier to attending the presentations.
- The hotels are too far from each other to allow switching between the sessions.
- The hotel removed much of the congregating furniture and made it difficult to have conversations outside of the review meetings.
- It is not clear why the review was held in Washington, DC. It seems the total spending could be decreased if this meeting were held elsewhere.

- It is too expensive to travel to Washington, DC. It should be done at a less expensive location near Argonne National Laboratory (ANL), keeping in mind that the largest participant group traveling from a single organization might save some money.

2.6. The visual quality of the presentations was adequate. I was able to see all of the presentations I attended.

The top number is the count of respondents selecting the option. The bottom percentage is the percent of the total respondents selecting the option.

Highly Disagree	Disagree	Neutral	Agree	Highly Agree
2	3	9	44	44
2%	3%	9%	43%	43%

11 Comments

- *From five respondents:* The font was too small and many presenters put too much information on one slide.
- Sitting in the front allowed for no trouble seeing the screen.
- The monitors in the individual rooms were good. There were not enough screens in the banquet hall for all to see clearly.
- A larger screen with better resolution was needed. Those in the back could not see anything.
- In the large rooms it was difficult to see the presentations. Also, during lunch half the audience faced away from the screens. It would be helpful to have screens on the other side of the room.
- The standard pastel backgrounds with white fonts were very difficult to see. A minimum font size (16 point) should be recommended.
- In every room the projected image was larger than the screen, causing information to be cut off. Someone should have checked this out prior to the meeting. Also, the transition from PDFs to PowerPoints and back was not flawless. One slight distraction during the transfer leads to pushing one wrong button, resulting in much delay in finding one's way back. There needs to be a better process for going from one presentation to another.

2.7. The audio quality of the presentations was adequate. I was able to hear all the presentations I attended.

The top number is the count of respondents selecting the option. The bottom percentage is the percent of the total respondents selecting the option.

Highly Disagree	Disagree	Neutral	Agree	Highly Agree
0	0	1	49	49
0%	0%	1%	49%	49%

5 Comments

- The audio people were excellent. It is not clear why there was an ORISE person in each room.
- People need to be sure to use the microphones. The microphones are critical in the banquet hall.
- Aside from a few glitches, it was mostly OK. The lunches were an exception; the volume needs to be increased during those presentations.
- There was one presenter who could not be understood and it was entirely the individual's fault.
- Too many speakers wandered away from the microphone, especially when answering questions. Additionally, when sitting near the back of the presentation rooms, the audience was continually interrupted by the conversations in the lobby when people entering or leaving do not shut the door.

### 2.8. The meeting hotel accommodations (sleeping rooms) were satisfactory.

The top number is the count of respondents selecting the option. The bottom percentage is the percent of the total respondents selecting the option.

Highly Disagree	Disagree	Neutral	Agree	Highly Agree
1	1	19	37	24
1%	1%	23%	45%	29%

8 Comments

- *From five respondents:* The meeting hotel was too expensive.
- It was a very nice hotel.
- The hotel was a little noisy at night with trucks making loud beeping sounds when backing up to make deliveries.
- For those that could not get a room (due to the hotel being booked up), there were many other options nearby.

### 2.9. The information about the Review and the hotel accommodations sent to me prior to the Review was adequate.

The top number is the count of respondents selecting the option. The bottom percentage is the percent of the total respondents selecting the option.

Highly Disagree	Disagree	Neutral	Agree	Highly Agree
0	0	6	45	47
0%	0%	6%	46%	48%

1 Comment

- It would be better to know the paper titles in each session and not just the category.

### 2.10. What was the most useful part of the review process?

63 Responses

- *From 14 respondents:* The opportunity to network and/or brainstorm with researchers.
- *From 10 respondents:* The oral technical presentations.
- *From 8 respondents:* Learning about the technical progress and status of the various projects.
- *From 5 respondents:* The question and answer session for reviewers.
- *From 4 respondents:* The ability to see the entire breadth of DOE activity on a single place over just a few days.
- *From 3 respondents:* The plenary sessions, which provided a good overview.
- *From 3 respondents:* The poster sessions and the ability to interact more with researchers during these sessions.
- *From 2 respondents:* The ability to learn about similar research projects was very useful, since it generated a greater understanding of related R&D as well as ideas for future research areas.
- *From 2 respondents:* The energy storage session.
- Getting an update on the fuel cell industry as a whole, and the background on general adoption plans for the general public.
- Information transfer, networking, and adherence to the schedule.
- The presentations that showed progress towards the DOE goals and multi-year R&D plan targets.
- Gaining a better understanding of what the national laboratories are currently focusing on.
- Seeing how well the projects are doing and how they are helping DOE meet its goals.

- The list of presentations and presenters, which allowed participants to network with them off-line without having to look for people in the halls.
- The fact that the slides and information were provided as a reference during the meeting.
- Grouping the proposals by subject area and content was very useful. The poster sessions were not as effective as the oral presentations.
- The same format for each presentation made it easy to follow from one program to another and get an idea of the program's health.
- The ability to see a clear technology development path, associated challenges, and plans to address them. It was easy to see good progress.
- Being able to ask questions directly to the presenters and having them all together at the same time.

### 2.11. What could have been done better?

#### 37 Responses

- *From 3 respondents:* Nothing could have been done better.
- *From 2 respondents:* More time is needed for questions and answers.
- The presentations need more technical details.
- The cost of the hotel room could be reduced.
- The venue and access to the internet could have been better.
- There should be more collaboration between fuel cells and batteries.
- There should be more innovative approaches and new faces.
- There should be more sleeping rooms available at the conference hotels.
- There could have been more information on the DOE budget and funding opportunities.
- The luncheon food was so-so.
- The food and beverage service at the poster session could have been better announced.
- The break area was way too small. Something needs to be done to move people away from the small area.
- There should be a longer lunch time and longer poster sessions, because there were so many nice results.
- Overall, it was very well done. The hotel space was a bit crowded and made it difficult at times to move around.
- The components of each program were reviewed satisfactorily. The same rigor on the overall program could make it better.
- There could have been more in-depth technology information and better presentation rooms. The AMR could also be in a different location—another area besides Washington, DC.
- Overall the meeting was well organized. The AMR should consider limiting attendance from foreign entities (e.g., universities from China and entities from Japan can easily attend now).
- The presentations should be on a USB drive rather than a CD. This participant wanted to read about presentations that he could not attend, but his computer does not have a CD drive.
- There should be less duplication of information between the plenary, the introductions, and the actual presentations.
- The review is already good enough. It would be better if the lunch provided vegetarian options that attendees can select online before going to the meeting.
- All of the speakers on a single topic should be put in one session; for example, ANL presenters on voltage decay of layered cathode materials.
- Outstanding results could be presented in the form of exhibits in addition to oral/poster presentations, where applicable.
- Examples from overviews at the beginning could have focused more on a particular successful current or past project.
- The AMR should consider adding a red/yellow/green status for quickly gauging the health of a project (is it meeting technical objectives, cost targets, etc.).
- There should be more time allowed for networking. This is a rare event for industry experts to get together, so at least one non-working lunch or just time set aside for networking could be beneficial.

- The AMR should get higher-quality reviewers (maybe they should be reimbursed.) There are too many industry/government reviewers. While this review process is necessary, the nature of the review displaces scientific discussion. Also, specific to this year, there were way too many “overview” presentations.
- The projects could have been grouped under different sections; for example, basic research and development (R&D), applied technology, and industrial projects could have been reviewed in different sessions.
- The time allocated for presentations should be strictly enforced and sufficient time should be allowed for questions and answers. Also, the AMR should pick reviewers so that the question-and-answer period is utilized effectively.
- There need to be more vegetarian options at the AMR lunch events—this is also more sustainable. A cereal-based vegetarian entree choice (e.g., pasta or rice) would be preferred to only an all-vegetable dish.
- Not all of the session chairpersons kept the presenters to a strict schedule. Some presentations started late and others started early. This caused significant problems when going from one hotel to the next for presentations that were scheduled right after one another. There were several times when this respondent missed a major part of the presentation due to this.
- The summary and future directions were almost nonexistent for many presenters. The presenters had a summary slide, which they typically glossed over, but had little else. On future directions, presenters often said just a few words about what was moving forward without much detail on why or how. The presenters indicated their goals and achievements in a clear fashion and should also do so for the future work.
- The chairs of the sessions need lessons in notifying the speaker when the time is up. In one session, the chair failed to draw the attention of the speaker to the cards that alerted the time remaining. The chair did not speak up or try any other approach to get the speaker’s attention. The chair was then obviously frustrated and was rude to the speaker.
- There could be better networking opportunities. The hallway outside of the meeting rooms was crowded during the break. It was difficult to get the drinks and network.
- There could be color-coded badges for different divisions; for example, people attending fuel cell presentations will have one color badge and people attending battery presentations will have a different color. That way people are easier to spot and network with.

## 2.12. Overall, how satisfied are you with the review process?

The top number is the count of respondents selecting the option. The bottom percentage is the percent of the total respondents selecting the option.

Highly Disagree	Disagree	Neutral	Agree	Highly Agree
0	1	3	46	47
0%	1%	3%	47%	48%

### 5 Comments

- *From 2 respondents:* The AMR is a great meeting.
- The review process was excellent.
- It would be hard to see something like this happening in the other countries.
- This has become an excellent technical meeting for the scientific community and complements the Directions in Engine Efficiency and Emissions Research (DEER) conference very well.

2.13. Would you recommend this review process to others, and should it be applied to other DOE programs?

	Number of Responses	Response Ratio
Yes	94	42.1%
No	2	<1%
No Responses	127	56.9%
<b>Total</b>	<b>223</b>	<b>100%</b>

9 Comments

- This is the example for how it should be done.
- In spite of some hiccups, this review is still the best that DOE offers.
- A consistent application of this type of review across the Office of Energy Efficiency and Renewable Energy programs would be welcome.
- The process is well run and helps performers exchange information, as well as provides a public face for the reviews.
- Except for the frequency (only once per year), the format is fine.
- The review process is too large.
- Smaller reviews with more reviewer/principal investigator one-on-one time would provide a better technical review. The format used in the current AMR process is excellent for providing the interested public with a good overview of the program.
- The review process is good, but it is unclear whether any funded projects ever really get terminated if peer reviewers find they do not meet the requirements for sustained program funds.
- It is a pretty good system, but conflicts of interests cannot be eliminated with this review model—they can only be mitigated. It would also be nice to add a summary from the program manager on the goals right before the technical session to remind everyone of the reason for the target numbers and objectives presented in many of the talks.

2.14. Please provide comments and recommendations on the overall review process.

12 Responses

- Supplying all presentations on a CD at registration was very much appreciated.
- This participant likes the AMR peer review process and is thinking of implementing a similar process for R&D project review in his company.
- As a PhD student in the fuel cell field, this participant is interested in participating as a peer reviewer. Students would definitely learn a lot by being a part of this process.
- Hearing the specific presentations and talking with the presenters afterward was interesting; meeting several presenters at one time was advantageous.
- Considering how many projects had to be reviewed, the process seemed to be more effective than has been seen in many other programs.
- The overall review process was satisfactory and provided the attendees with a good chance to get to know each other.
- It is hard to believe that most of the projects are on schedule and on budget.
- The reviewers should ask about the commercial relevance and the potential for commercial success. For too many of the funded projects it is unclear how useful the project outputs will be.
- The presentations should be more structured. An overview slide that mentions all of the subprojects of the principal investigator (PI) with the bulk of the presentation focused on just one or two efforts that are meeting project goals would be useful. Also, a slide that addresses the approach for meeting the future goals was lacking.
- The PIs need lessons in “SMART” (specific, measurable, attainable, relevant, and time-bound) milestones. Many milestones listed were simply tasks, such as “measure such-and-such property.”

- A major error by the AMR planners was setting the AMR to be the same week as the Electrochemical Society meeting, whose date was set years in advance.
- The starting time of the event could be improved. When travelling from the West Coast, it is impossible to get to the event by the start of the plenary if one leaves on Monday morning. It does not make a lot of sense to pay for an extra hotel night to travel on Sunday and only have a half-day event on Monday. Please start later on Monday.

### 3. Responses from Reviewers

#### 3.1. Information about the program(s)/project(s) under review was provided sufficiently prior to the review session.

The top number is the count of respondents selecting the option. The bottom percentage is the percent of the total respondents selecting the option.

Highly Disagree	Disagree	Neutral	Agree	Highly Agree
0	3	2	16	19
0%	8%	5%	40%	48%

10 Comments

- *From 4 respondents:* The information on the programs and projects under review was provided sufficiently prior to the session.
- It was useful to have the slides ahead of time.
- It is essential to have the project materials ahead of time to help formulate questions in advance.
- Due to confidentiality issues, many projects could not provide certain technical details.
- Providing the program summaries a week or two before the review would have been helpful.
- After resetting my password and getting access to the system, on the day before my sessions my password was no longer active and I could not see the slides in advance.
- It would have been good to have been able to read more about each project prior to the presentations. Including the abstracts in the meeting agenda would be helpful. It would be great if more information about each project were available online (other than through the PeerNet system).

#### 3.2. Review instructions were provided in a timely manner.

The top number is the count of respondents selecting the option. The bottom percentage is the percent of the total respondents selecting the option.

Highly Disagree	Disagree	Neutral	Agree	Highly Agree
1	0	0	16	23
3%	0%	0%	40%	58%

3 Comments

- Yes, instructions were provided through webinars and again at the meeting.
- There were two webinars in advance instructing the reviewers on how to use the PeerNet system and the criteria by which the research projects were to be judged.
- Even though this reviewer signed up as a reviewer in February, he did not receive any review assignments and had to work this out with the individual program managers during the meeting, which was a frustration.

#### 3.3. The information provided in the presentations was adequate for a meaningful review of the projects.

The top number is the count of respondents selecting the option. The bottom percentage is the percent of the total respondents selecting the option.

Highly Disagree	Disagree	Neutral	Agree	Highly Agree
1	2	4	29	4
3%	5%	10%	73%	10%

*14 Comments*

- The presentations provided adequate information for reviewers to prepare questions to the presenters.
- The backup slides and the specific slides for the reviewers are really useful for better evaluating the level of work performed.
- A 20-minute presentation with a 10-minute question-and-answer period is a short time to present all of the relevant information about projects with a broad scope. However, the presenters did a good job under this time constraint, and the program managers did a good job of enforcing it.
- The quality of the material varied in some cases.
- For the most part, the information provided was adequate to give a meaningful review. For one of the newer projects, information protection issues prevented the principal investigator (PI) from disclosing much at all about the chemistry being used, which made it difficult to provide a meaningful review.
- Some presentations have more useful information in the text than others.
- This year, many projects had less to present due to the delayed funding availability.
- There should be an option to present more detailed slides on the accomplishments if they were achieved.
- The “reviewer only” information was helpful; plus, looking back at prior reviews (on the DOE website) by and/or about the same person/team was also helpful in evaluating the projects.
- The presentations are quite short. Some of the pro forma material (such as the barriers addressed) tends to be less useful; more information on the technical approach/results would have been useful.
- The “proprietary” dodge to full disclosure is a handicap in too many projects. Often this is used a full year after the start of a project and discovery of an effect. This should be discouraged.
- The projects funded at \$15 million were allocated the same time for review as those allocated \$0.5 million. The time allocated has to be equitable, or else this review is not very effective.
- Some of the presenters continue to give presentations that only they themselves and possibly a few other highly specialized experts in the world can understand.
- Several of the presentations did not have the reviewer-only slides and some presenters did not respond to reviewer comments from previous years. These reviews are only as useful as the PIs make them.

### 3.4. The evaluation criteria upon which the review was organized (see below) were clearly defined.

The top number is the count of respondents selecting the option. The bottom percentage is the percent of the total respondents selecting the option.

	Highly Disagree	Disagree	Neutral	Agree	Highly Agree
Relevance	0	0	1	22	17
	0%	0%	3%	55%	43%
Approach	0	0	1	24	14
	0%	0%	3%	62%	36%
Technical Accomplishments and Progress	0	1	1	21	16
	0%	3%	3%	54%	41%
Technology Transfer and Collaboration	0	0	5	22	12
	0%	0%	13%	56%	31%
Proposed Future Research	0	1	4	22	12
	0%	3%	10%	56%	31%

#### 13 Comments

- The evaluation criteria provided a good template for review.
- The criteria for evaluation were clear and concise. The criteria are an effective assessment of the progress and the future of the program being rated.
- There was an absence of some specifications.
- These criteria are rather general and difficult to quantify.
- The mention of “new results” used in some presentations should be generalized.
- It might help if the criteria for the approach and the proposed future research are described in more detail.
- The topic of future research was interesting. Because some projects were ending, it was not clear how to score this field.
- It was occasionally challenging to evaluate projects that were either completed or highly specialized, with respect to DOE’s overall goals.
- It would be useful to provide a reminder for the reviewers of how the research components address specific components in the DOE multi-year research, development, and demonstration plan.
- The technology transfer and collaboration sections were hard to judge. Most of the principal investigators just provided a list of organizations, without specifying what degree of technology transfer or collaboration occurred.
- Regarding collaboration, not only the names of collaborators and the actions, but also the collaboration scheme should be mentioned to describe what kind of network/relation exists there.
- Collaboration was a mixed bag. In some cases, a large company has the people and resources needed in-house. In others, quality leverage is useful and appropriate. In some cases, a partner seems to be there just so it can claim collaboration. Some refinement of these criteria might be useful.
- The technical criteria are geared toward projects that take place in laboratories and do not reflect the efforts required by technology validation projects that are fielded in a community and require a whole range of different challenges, such as getting legal agreements, permitting, and codes and standards requirements in place. There is more to many projects than just working in a laboratory under a defined structure.

3.5. The evaluation criteria were adequately addressed in the presentations.

The top number is the count of respondents selecting the option. The bottom percentage is the percent of the total respondents selecting the option.

	Highly Disagree	Disagree	Neutral	Agree	Highly Agree
Relevance	0	2	6	23	9
	0%	5%	15%	58%	23%
Approach	0	1	4	24	10
	0%	3%	10%	62%	26%
Technical Accomplishments and Progress	0	1	4	24	10
	0%	3%	10%	62%	26%
Technology Transfer and Collaboration	0	2	9	21	6
	0%	5%	24%	55%	16%
Proposed Future Research	0	1	7	25	
	0%	3%	18%	66%	13%

8 Comments

- The presenters know the criteria and tend to emphasize them.
- The researchers were generally pretty good about making it clear what belonged in each category.
- Most of the presenters were careful to structure their presentations around these criteria in order to make the reviewers' jobs easier.
- This was good for the most part, but not across all projects. Special recognition should be given to Oak Ridge National Laboratory. Its presentations were well organized and contained all of the required information.
- In some cases, it was difficult to evaluate a project on one or more criteria due to insufficient information.
- Sometimes progress is being made in a very meaningful way despite not necessarily meeting evaluation criteria. That is the nature of R&D. DOE should be flexible here.
- Technology transfer was barely addressed. The proposed future research was addressed, but it was kind of an afterthought in most cases.
- In most cases the industry/market relevance is not obvious. The slide on collaborations at the end of the presentations is often not talked about in detail.

3.6. The right criteria and weightings were used to evaluate the project(s)/program(s).

The top number is the count of respondents selecting the option. The bottom percentage is the percent of the total respondents selecting the option.

	Highly Disagree	Disagree	Neutral	Agree	Highly Agree
Relevance	1	1	4	24	10
	3%	3%	10%	60%	25%
Approach	0	0	5	25	10
	0%	0%	13%	63%	25%
Technical Accomplishments and Progress	0	1	5	26	8
	0%	3%	13%	65%	20%
Technology Transfer and Collaboration	1	1	9	22	7
	3%	3%	23%	55%	18%
Proposed Future Research	0	0	5	27	8
	0%	0%	13%	68%	20%

4 Comments

- The relevance category is confusing—the research contracts should have been awarded because the research will lead to the displacement of oil. Weighting this by 20% is a “gimme,” which means that everyone gets at least 20%. Also, sometimes the collaborations felt a bit like checking boxes, like the collaborators were listed, but they did not seem integral to the research program.
- The technical criteria are geared toward projects that take place in laboratories and do not reflect the efforts required by technology validation projects that are fielded in a community and require a whole range of different challenges, such as getting legal agreements, permitting, and codes and standards requirements in place. There is more to many projects than just working in a laboratory under a defined structure.
- Because technology transfer and collaboration was given a 10% weight, some of the teams added universities that did not play a real role. To satisfy this requirement, the presenters were showing group photos to support their team collaboration. The weight should be reduced to 0%.
- In terms of one particular project, this reviewer wonders how much the reviews are really taken into account. Based on the scores and the reviewer comments from the past 3 years, it is not clear how this project has continued. This is very frustrating for a reviewer.

3.7. During the Annual Merit Review, reviewers had adequate access to the Principal Investigators.

The top number is the count of respondents selecting the option. The bottom percentage is the percent of the total respondents selecting the option.

Highly Disagree	Disagree	Neutral	Agree	Highly Agree
0	1	6	19	14
0%	3%	15%	48%	35%

6 Comments

- The location, breaks, and lunches are perfect to have access to principal investigators (PIs) and many other people.
- The single most valuable part of the AMR was the ability to meet and talk with the PIs.
- There were a few presentations that had the typical stand-ins as presenters. Though, in general, those presenters were adequately informed about the project at hand.
- The question and answer time was too short to get into much detail.
- It was good that the moderator required the peer reviewers’ questions to be asked first.

- It would be a good idea if there was a chance for some breakout sessions where only reviewers and PIs were present, preferably each evening that a presentation is made. There could also be a side room next to the posters.

3.8. Information on the location and timing of the projects was adequate and easy to find.

The top number is the count of respondents selecting the option. The bottom percentage is the percent of the total respondents selecting the option.

Highly Disagree	Disagree	Neutral	Agree	Highly Agree
0	1	3	17	19
0%	3%	8%	43%	48%

3 Comments

- The schedule was easy to follow.
- The review was well organized as usual.
- Kudos to the session managers for ensuring the timing was maintained.

3.9. The number of projects I was expected to review was:

	Number of Responses	Response Ratio
Too many	1	<1%
Too few	9	4.0%
About right	30	13.4%
No Responses	183	82.0%
<b>Total</b>	<b>223</b>	<b>100%</b>

8 Comments

- Reviewing about 20 projects over the 3 days of the AMR was just fine.
- This reviewer only had three projects to review, but others had more.
- This reviewer reviewed two projects and had been expecting to review more.
- Reviewing four projects was good—many more than that would have impacted the ability to participate in other activities at the AMR.
- It was fine to review 10 projects, but reviewing 8 technical projects in one poster session was a bit too much. The last two projects did not receive the same degree of attention that the first few did.
- This reviewer was present all week, but was only asked to review Thursday and Friday. One of those days all of the sessions were back to back. It would be nice to spread the evaluations apart a bit more.
- This reviewer had one project this year, compared to the previous years when he reviewed 4–5 projects—this seems questionable. Even though the reviewer was travelling from Germany, 3–5 projects would be reasonable.
- This reviewer would have preferred to review more presentations and was frustrated that he was not able to do so.

### 3.10. Altogether, the preparatory materials, presentations, and the question and answer period provided sufficient depth for a meaningful review.

The top number is the count of respondents selecting the option. The bottom percentage is the percent of the total respondents selecting the option.

Highly Disagree	Disagree	Neutral	Agree	Highly Agree
0	3	5	21	11
0%	8%	13%	53%	28%

#### 11 Comments

- This was a nicely run program review, as usual.
- This was this reviewer's first AMR, and overall it was an excellent experience. A lot was learned about the current DOE research in the reviewer's areas of interest.
- This reviewer only did posters so he was able to ask the principal investigator questions as necessary.
- For some of the large projects, the time is very compressed.
- The reviews were much more meaningful when the meetings were smaller and in-depth.
- The question-and-answer part of the sessions was inadequate to delve deeply into a project's progress.
- Every project submits an annual report to DOE; access to these reports prior to the review would be useful for reviewers to familiarize themselves with the projects.
- This reviewer could have provided a more meaningful review if the presenters expressed key factors in a readily intelligible way for non-experts.
- The time allocated for presentations should be scaled up for larger projects.
- This is very project dependent. Some of the larger projects are quite diverse with many activities, and it is difficult to discuss the accomplishments in the time or slides allotted. A longer presentation time or perhaps a more detailed report of progress in the supplemental slides for these projects would make for a more meaningful review.
- Yes, except for the "proprietary dodge" by some presenters and some things falling through the cracks when the application of performance criteria is too rigid. Regarding falling through the cracks, it is good to remember that the goal is to learn how to improve, not to sell a specific idea. Incremental improvement at the expense of revolutionary change is not the way to go.

### 3.11. Please provide additional comments.

#### 11 Responses

- The AMR is a very well-run exercise and is essential to the process of evaluating progress in the Vehicle Technologies Office and Hydrogen and Fuel Cells Program.
- Specifications for each project should be submitted to reviewers in confidence and a few days before the presentations.
- There would be more focus on the Vehicle Technologies Office if its reviews were separate from the Hydrogen and Fuel Cells Program's reviews. The reviewers do not seem to overlap all that much, and the very large number of people present is a barrier to effective networking.
- Some projects are on "core technology" and it would be nice to know if that technology was being developed further or just "put on the shelf." For those projects that are exploring available core technology, it would be nice to know their success in having that technology commercialized or at least transferred to projects with that purpose.
- A list of suggested questions to consider when reviewing posters would have been helpful, especially with regard to specific performance or cost targets that need to be met or testing protocols that should be satisfied.
- If DOE can offer some monetary compensation to reviewers, it could tap into a vast pool of retired technical experts from the industry and those from foreign countries as well. Also, DOE should look into the possibility of using web conferencing facilities for potential remote reviewing. This might save some money, too.

- Some presentations were missed because of scheduling conflicts with other presentations.
- The elimination of the first Plenary Session on Monday would have enabled elimination of the Friday project reviews.
- There are too many small projects being reviewed in oral sessions. A bar, such as a minimum level of funding, should be applied. In addition, really large, complex projects should be allotted additional time, even as much as two 30-minute slots.
- This meeting is very unpleasant because of the crowds and high noise level. It is very hard to hear at breaks and meals.
- It is very disturbing that there seems to be no “quality control” in terms of defining how well various additives or improvements perform. There are way too many presentations in which the PI states that something that he/she did improved durability from X to Y cycles, with no indication whether Y is actually any good. Standards need to be enforced.

#### 4. Responses from Presenters

- 4.1. The request to provide a presentation for the Annual Merit Review was provided sufficiently prior to the deadline for submission.

The top number is the count of respondents selecting the option. The bottom percentage is the percent of the total respondents selecting the option.

Highly Disagree	Disagree	Neutral	Agree	Highly Agree
0	2	2	28	31
0%	3%	3%	44%	49%

##### 10 Comments

- *From 3 respondents:* The deadline for submission was too early and it should be pushed back to one month before the presentation.
- *From 2 respondents:* It would be useful to be able to update the presentation with more current information closer to the review date.
- Timing is a little tight, but it can be managed because it is already known roughly when the request for the presentation will occur.
- An approval from a cooperative research and development agreement (CRADA) industrial partner can sometimes take a while to get.
- The timetable for the AMR presentation submission is typically at odds with project timelines in relation to the fiscal year.
- A mistake regarding the presentation date in the first version of the program led to a cost of changing travel plans.
- The requirement to submit materials approximately 8 weeks in advance necessitated “estimating” whether milestones scheduled for achievement in the 8-week run-up to the presentation would actually be achieved. This impacts comments on the accomplishments to date as well as on the future work sections. It is understood that having a large number of presentations previewed by a small number of reviewers requires a long lead time, but it would be appreciated if there could be a way to substitute one-for-one a few key slides to support presenting the most current information.

#### 4.2. Instructions for preparing the presentation were sufficient.

The top number is the count of respondents selecting the option. The bottom percentage is the percent of the total respondents selecting the option.

Highly Disagree	Disagree	Neutral	Agree	Highly Agree
0	0	3	26	34
0%	0%	5%	41%	54%

##### 2 Comments

- The step-by-step guide of what information goes on the slides was great. Apparently it is “not OK” during the actual presentation to invite attendees to offer suggestions in areas where the project is experiencing difficulty. The presenter missed those instructions. If that restriction is not in the instructions, it is recommended that it be added.
- The presenter tried to follow the format requested for the presentation but found that many other presenters largely ignored it. Some presenters did conventional “storytelling” presentations, where it was not clear what they did during this fiscal year, what they did previously, and what other people had done outside of their project. The “storytelling” presentations were well received by the general audience, but it is not clear what the reviewer feedback will be.

#### 4.3. The audio and visual equipment worked properly and were adequate.

The top number is the count of respondents selecting the option. The bottom percentage is the percent of the total respondents selecting the option.

Highly Disagree	Disagree	Neutral	Agree	Highly Agree
0	2	3	19	38
0%	3%	5%	31%	61%

##### 6 Comments

- A malfunctioning projector was quickly replaced.
- The “red box” to get to the next presentation was a source of confusion for many people, even though an email notification did describe how it would work. This presenter thought it was fine and that it worked well.
- The lapel microphone is preferred.
- There was no audio equipment in this presenter’s room, so it was difficult to hear the speakers and questions.
- The speaker’s time clock failed during the presentation—this was not noticed until the allotted time had been exceeded.
- It would be good to have a mouse with the computer for starting movies. It would be good to have the computer set up so that the mouse can also be used as a pointer. A pointer did not seem to be available at the beginning of the session.

4.4. The evaluation criteria upon which the Review was organized were clearly defined and used appropriately.

The top number is the count of respondents selecting the option. The bottom percentage is the percent of the total respondents selecting the option.

	Highly Disagree	Disagree	Neutral	Agree	Highly Agree
Relevance	0	1	7	29	22
	0%	2%	12%	49%	37%
Approach	0	0	4	34	21
	0%	0%	7%	58%	36%
Technical Accomplishments and Progress	0	0	5	30	24
	0%	0%	8%	51%	41%
Technology Transfer and Collaboration	0	0	8	32	19
	0%	0%	14%	54%	32%
Proposed Future Research	0	0	6	34	18
	0%	0%	10%	59%	31%

2 Comments

- The project relevance is crucial so the principal investigators can see how their work fits into the larger picture. However, this respondent is not as sure about technology transfer.
- Without seeing the review, it is hard to evaluate this. There is a concern that “storytelling” presentations may be evaluated based on background information, the results from other projects, and the results from prior years. “Storytelling” presentations were received well by the audience, but it is not known how the reviewers evaluated those presentations.

4.5. Explanation of the questions within the criteria was clear and sufficient.

The top number is the count of respondents selecting the option. The bottom percentage is the percent of the total respondents selecting the option.

	Highly Disagree	Disagree	Neutral	Agree	Highly Agree
Relevance	0	2	5	33	17
	0%	4%	9%	58%	30%
Approach	0	1	4	33	19
	0%	2%	7%	58%	33%
Technical Accomplishments and Progress	0	1	6	32	18
	0%	2%	11%	56%	32%
Technology Transfer and Collaboration	0	1	7	31	18
	0%	2%	12%	54%	32%
Proposed Future Research	0	1	6	34	15
	0%	2%	11%	61%	27%

3 Comments

- It seems like most projects are bunched around a score of 3.0. Using a 10.0 scale instead of a 4.0 scale may help differentiate projects that are close to the average. Using at least a 5.0 scale might help alleviate this problem.
- Two respondents did not understand this question.

#### 4.6. The right criteria and weightings were used to evaluate the project(s)/program(s).

The top number is the count of respondents selecting the option. The bottom percentage is the percent of the total respondents selecting the option.

	Highly Disagree	Disagree	Neutral	Agree	Highly Agree
Relevance	0	3	8	27	17
	0%	5%	15%	49%	31%
Approach	0	2	7	27	19
	0%	4%	13%	49%	35%
Technical Accomplishments and Progress	0	1	6	27	21
	0%	2%	11%	49%	38%
Technology Transfer and Collaboration	0	2	13	24	15
	0%	4%	24%	44%	28%
Proposed Future Research	0	1	8	29	16
	0%	2%	15%	54%	30%

#### 5 Comments

- This respondent did not recall being shown these weightings.
- It is hard to comment on this before the comments come back.
- It is not clear if it is appropriate to use the same weighting throughout the project timeline, but there are no recommendations to make on specific adjustments.
- Too much emphasis is placed on the relevance, approach, and collaboration criteria. More emphasis should be placed on the technical accomplishments and progress, which is the heart of the work.
- It is logical to use the same metrics to evaluate projects with clearly defined criteria and weightings. However, there are other factors that make a project successful, which might be difficult to judge by using the same framework. The current method of evaluation will also guide the research to come up with the results to satisfy the metrics; this is not necessarily in line with the intent of the project. Some soft weighting factors might be useful for the program administration to consider.

#### 4.7. Please provide additional comments:

#### 6 Response(s)

- Overall, it was a well organized and smoothly run review.
- The presentation room (Crystal Gateway Alexandria Room) was too small. The ceiling was quite low, so audience members in the back had a hard time seeing the slides presented.
- The presentation time should be increased to 30 minutes, plus 10 minutes for questions and answers.
- The indemnification clause requirement is controversial at best, and it is against the advice of our legal department. Hopefully next year this can be corrected.
- For all sessions, a 15-minute overview talk would be helpful with three key points: (1) the current state-of-the-art or “best practice” in industry and key metrics (two or three), (2) the key research challenges and directions (two or three), and (3) the performance gains/targets for the key research challenges and directions according to the two or three metrics.
- The speaker timer (with giant numbers indicating how much time is left) that points right at the speaker is distracting when giving a presentation. It would be better to have a clock that presenters can look at a couple of times, but that is not staring the presenter right in the face.