

Hydrogen Storage System Modeling: Public Access, Maintenance, and Enhancements



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DOE Hydrogen and Fuel Cells Program

2019 Annual Merit Review and Peer Evaluation Meeting

April 29, 2019

Project ID # ST008



This presentation does not contain any proprietary, confidential, or otherwise restricted information.

Overview

Timeline

- **Start: October 1, 2015**
- **End: September 30, 2021***
- **60% FY19 Complete (as of 5/1/19)**

Budget

- **Total Project Funding: \$1,375,000***
 - **FY16 Funding: \$336,000**
 - **FY17 Funding: \$389,000**
 - **FY18 Funding: \$375,000**
 - **FY19 Funding: \$275,000**

Barriers

- A. System Weight and Volume**
- B. System Cost**
- C. Efficiency**
- E. Charging/Discharging Rates**
- I. Dispensing Technology**
- K. System Life-Cycle Assessment**

Partners



***Project continuation and direction determined annually by DOE.**

Relevance

Collaborative effort to manage, update, and enhance hydrogen storage system models developed under the Hydrogen Storage Engineering Center of Excellence (HSECoE).

- Transfer engineering development **knowledge from HSECoE on to future materials research.**
- Manage the **HSECoE model dissemination** web page.
- Manage, update, enhance, and validate the **modeling framework and the specific storage system models** developed by the HSECoE.
- Develop models that will **accept direct materials property inputs** and can be measured by materials researchers.
- **Ultimate Goal: Provide validated modeling tools that will be used by researchers to evaluate the performance of their new materials in engineered systems relative to the DOE Technical Targets.**

Relevance – Barriers Addressed with Models

Barriers	Model Addressing Barrier
A. System Weight and Volume	System Estimator
B. System Cost	Tank Volume/Cost Model
C. Efficiency	Framework Model <ul style="list-style-type: none">- On-Board Efficiency- Fuel Economy
E. Charging/Discharging Rates	Framework Model <ul style="list-style-type: none">- Drive cycles
I. Dispensing Technology	Framework Model <ul style="list-style-type: none">- Initial and Final System Conditions
K. System Life-Cycle Assessment	All Models

Relevance – Focus: Improve Model Utilities for Materials

Researchers

Materials Research

H₂ Capacity
Thermodynamics
Kinetics
Adsorption Isotherms

Isotherm Fitting Tool

DA Parameters

Available at
www.hsecoc.org

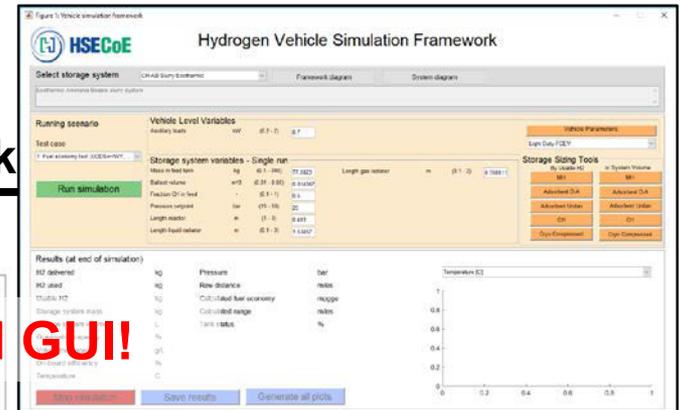
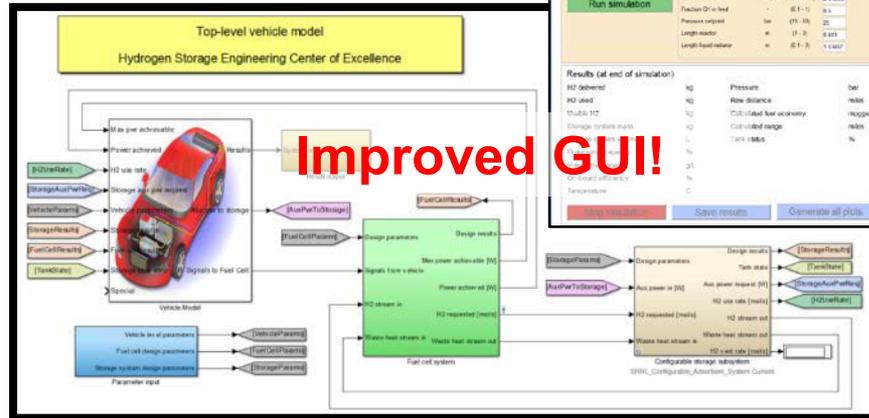
Stand Alone System Design Tools

Component and System Mass & Volume

Stand-Alone Values

Estimated Gravimetric & Volumetric Capacity

Modeling Framework



DOE Technical Targets

- Gravimetric & Volumetric Capacity
- Durability & Operability
- Operating Temperature and Pressure
- On-Board Efficiency
- Charging/Discharging Rates
- Startup
- Refueling

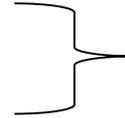
Approach – Modeling Tools Available / In Progress

Finite Element Models:

- Metal Hydride (MH)
- Adsorbent (AD) – HexCell and MATI

SRNL

SRNL



Tank Heat and Mass Transfer Models

Stand-alone System Design Tool:

- Adsorbent (AD)
- Chemical Hydrogen (CH)
- Metal Hydride (MH)
- Compressed/Cryo-Compressed H₂

SRNL

PNNL

PNNL

SRNL

New Mass or Volume-Based Tool

New D-A or UNILAN Isotherm-Based Tool

New Mass or Volume-Based Tool

New Mass or Volume-Based Tool

Framework Model with:

- Physical Storage
- Compressed/Cryo-Compressed H₂
- Chemical Hydrogen (CH)
- Adsorbent (AD)
- Metal Hydride (MH)

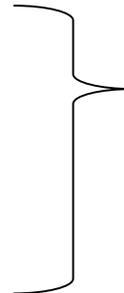
UTRC/NREL

SRNL/NREL

PNNL/NREL

SRNL/NREL

PNNL/NREL



Estimate performance of light-duty vehicles with four drive cycles for each storage system

Updating for UNILAN Isotherm Theory

Updated to allow user input

Additional Tool / Models:

- MH Acceptability Envelope
- Tank Volume/Cost Model
- AD Isotherm Fitting Tool

SRNL

PNNL

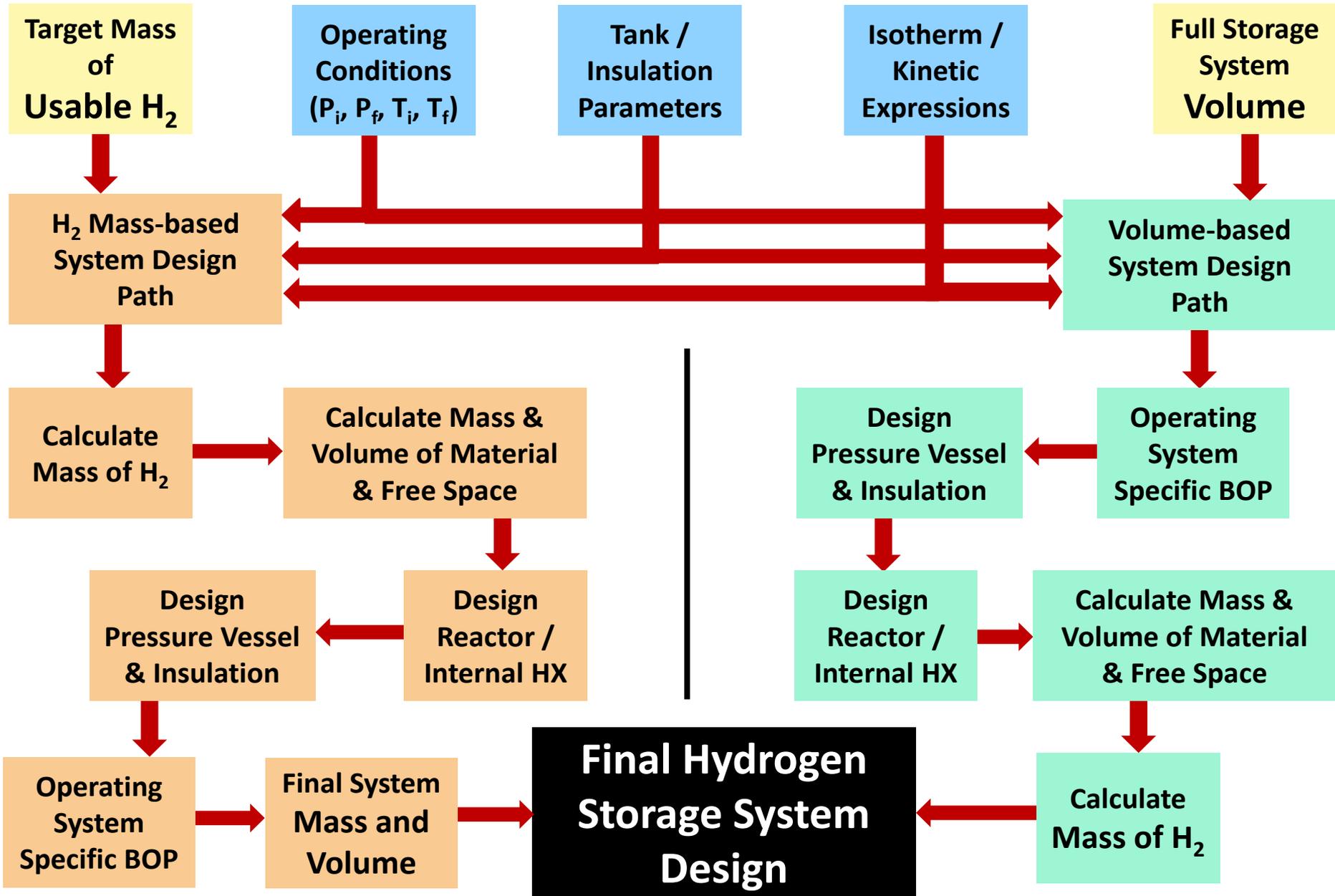
SRNL

Accomplishments and Progress – Design Tools Estimate All Input Parameters Needed to Design a Hydrogen Storage System

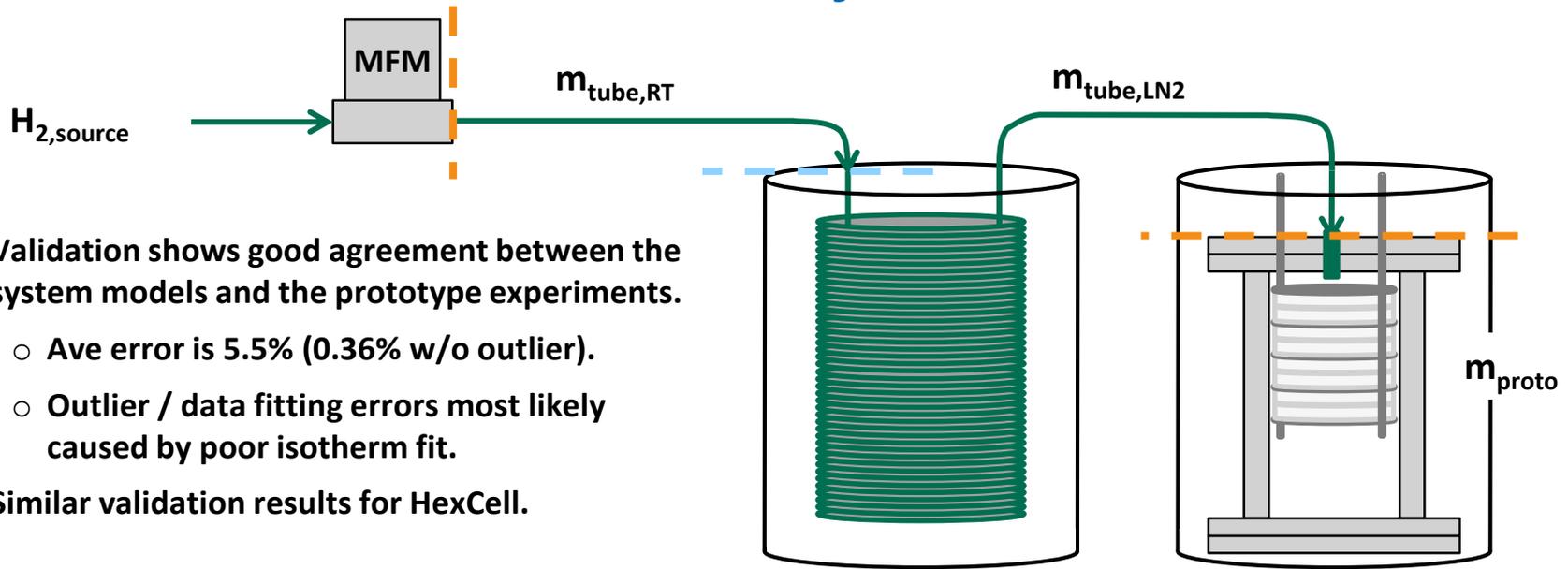
Capabilities:

- **All** hydrogen storage methods: adsorbents, metal hydrides, chemical hydrogen storage, and pure hydrogen storage
- Available as a **stand-alone** executable or as part of the **full vehicle** framework within MATLAB / Simulink
- **Material-specific** property inputs measured by materials researchers to design material-specific storage systems
- **Validated** design tools against known storage systems.
- Usable-H₂ **mass based** and full storage system **volume based** capabilities for each design tool
- **Multiple kinetics / isotherm expressions** available for each storage method.

Accomplishments and Progress – Design Tools Flowchart



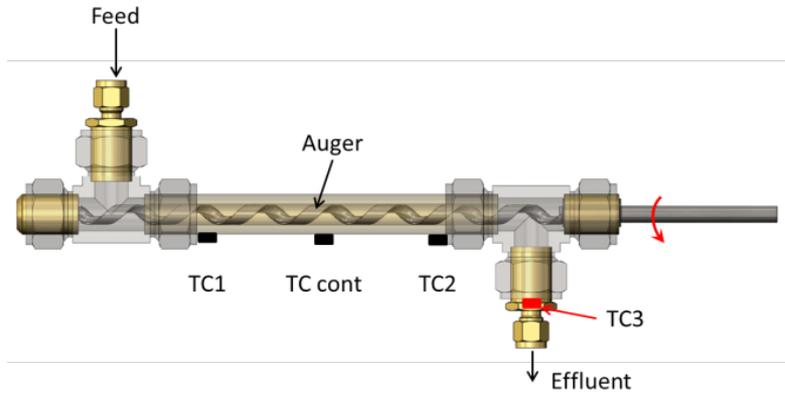
Accomplishments and Progress – MATI Adsorbent Storage System Validation



- Validation shows good agreement between the system models and the prototype experiments.
 - Ave error is 5.5% (0.36% w/o outlier).
 - Outlier / data fitting errors most likely caused by poor isotherm fit.
- Similar validation results for HexCell.

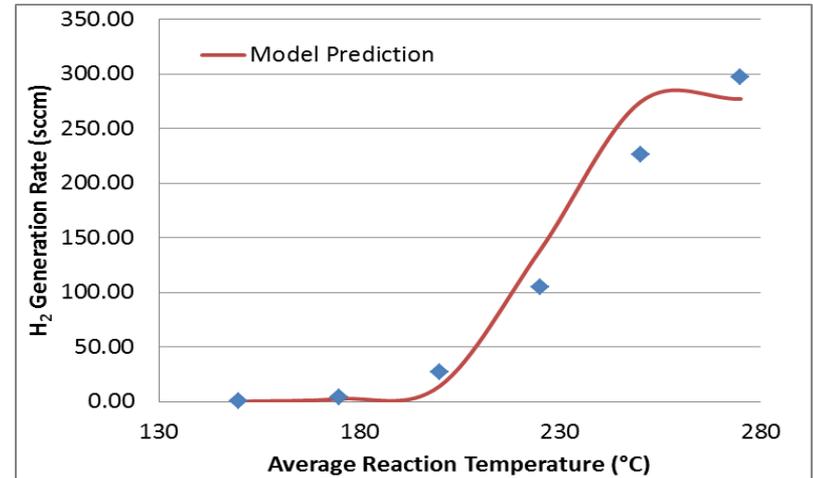
Op. Conditions	$H_{2,\text{in}}$	$m_{\text{tube,tot}}$	$m_{\text{proto,exp}}$	$m_{\text{proto,model}}$	%-Diff
(1.07 bar, 83.7 K) → (60.0 bar, 91.3 K)	86.85 g	41.69 g	45.16 g	45.45 g	0.639%
(1.09 bar, 83.7 K) → (100.0 bar, 84.5 K)	140.54 g	72.56 g	67.99 g	68.09 g	0.158%
(5.05 bar, 84.0 K) → (60.5 bar, 106.6 K)	59.55 g	28.51 g	31.04 g	24.57 g	-20.86%
(5.23 bar, 83.2 K) → (100.2 bar, 102.4 K)	107.24 g	58.10 g	49.14 g	49.00 g	-0.285%

Accomplishments and Progress – Chemical Hydrogen Storage Model Validation

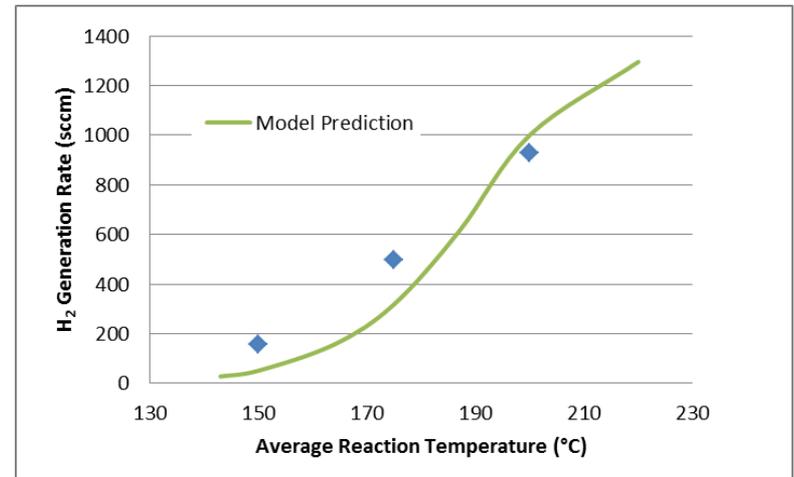


Flow-through reactor design used to validate the model

Solids Loading (wt%)	Reactor Residence Time (min)	Auger Speed (rpm)	Average Reaction Temperature (°C)	Measured Alane Conversion (mol/mol)	Model Conversion Values (mol/mol)
50%	7.6	12	185	16%	11%
50%	7.6	40	185	11%	4.6%
50%	4.2	12	187	7%	6.6%
50%	7.6	12	214	88%	80%
50%	7.6	40	214	74%	53%
50%	4.2	12	214	38%	49%
20%	6.8	40	188	10%	7.1%
20%	6.8	40	212	38%	50%
20%	6.8	40	235	84%	100%
60%	7.2	12	180	5%	6.5%
60%	7.2	12	194	20%	21%
60%	7.2	12	208	48%	55%



Comparison of model predicted hydrogen flow rate to that measured experimentally for 20 wt% alane slurry

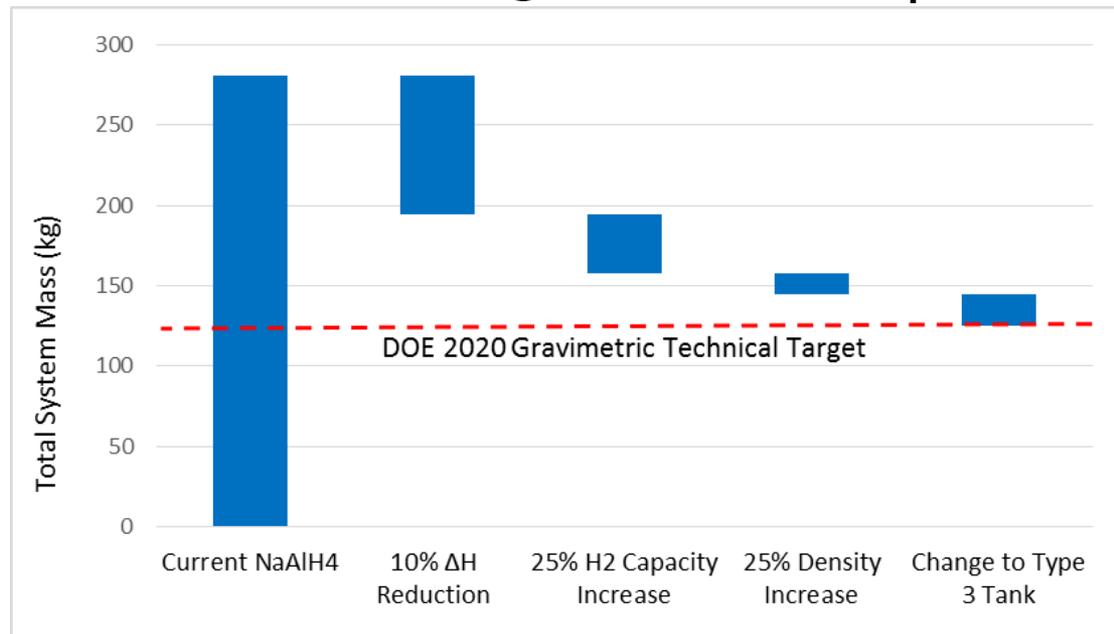


Comparison of model predicted hydrogen flow rate to that measured experimentally for 20 wt% AB slurry

Accomplishments and Progress – Model Improvements

Original Model	Updated Model
Adsorbent Model	
BOP for cryogenic operation only	BOP options for room temperature, cold, and cryogenic operations
Insulation thickness hard coded to 1-inch	Insulation thickness is user controlled
LN ₂ tank cooling channel always included	LN ₂ tank cooling channels user controlled
D-A Isotherm Model used only	D-A and UNILAN Isotherm Model options
MOF-5 Material Properties hard coded	User defined Adsorbent Material Properties (with MOF-5 default values)
Mass of usable H ₂ is the starting point of the calculation	Mass of usable H ₂ or Maximum total storage system volume starting point
Metal Hydride Model	
Single Step Irreversible Reaction	Single Step Irreversible or Two Step Reversible Models Selectable
Hard coded reaction rate and enthalpy (30 kJ/mol)	Reaction parameters and material properties as inputs
Mass of usable H ₂ is the starting point of the calculation	Mass of usable H ₂ or Maximum total storage system volume starting point

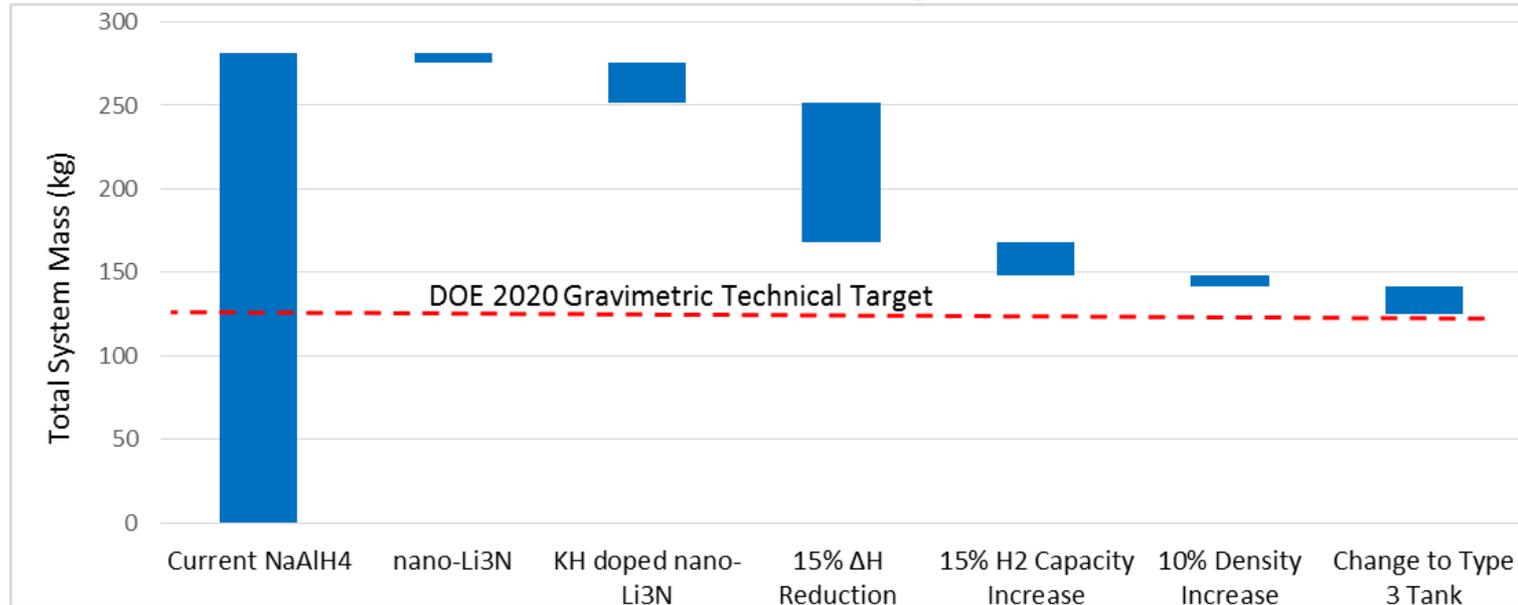
Accomplishments and Progress –One Possible Pathway to Meet DOE Gravimetric Target for NaAlH₄



Reaction Enthalpy (kJ/mol)	42	37.8	37.8	37.8	37.8
x _{H₂} (wt%)	5.6%	5.6%	7.0%	7.0%	7.0%
Bed Density (kg/m ³)	720	720	720	900	900
Tank Type	Type 1-Al	Type 1-Al	Type 1-Al	Type 1-Al	Type 3-Al liner
System Mass (kg)	281	194	158	145	125
Gravimetric Capacity (5.6 kg useable H ₂)	0.020	0.029	0.035	0.039	0.045

One possible set of material improvements to meet DOE gravimetric target: 1) reduce ΔH_{rxn} so that fuel cell heat can be used, 2) increase H₂ capacity and 3) density and 4) Type 3 tank

Accomplishments and Progress –Evaluate new materials relative to DOE Technical Targets



Reaction Enthalpy (kJ/mol)	42	42.1	41.7	35.4	35.4	35.4	35.4
x_{H_2} (wt%)	5.6%	6.1%	6.4%	6.4%	7.36%	7.36%	7.36%
Bed Density (kg/m ³)	720	740	760	760	760	836	836
Tank Type	Type 1-Al	Type 3-Al liner					
System Mass (kg)	281	276	252	168	148	142	125
Gravimetric Capacity (5.6 kg useable H ₂)	0.020	0.020	0.022	0.033	0.038	0.039	0.045

6 nm KH doped nano-Li₃N developed by Dr. Stavila: Requires larger ΔH_{rxn} reduction, but smaller increases in H₂ capacity and density than NaAlH₄ to meet the DOE Gravimetric target

Accomplishments and Progress – Vehicle Framework GUI

Figure 1: Vehicle simulation framework

Hydrogen Vehicle Simulation Framework

Select storage system: CHAD Slurry Exothermic

Running scenario: Vehicle Level Variables

Test case: 1 Fuel economy test (UDDS+HWY...)

Storage system variables - Single run

Mass in feed tank	kg (0.1 - 200)	77.5623	Length gas radiator	m (0.1 - 3)	0.708811
Dalast volume	m³ (0.01 - 0.05)	0.014067			
Fraction CH in feed	- (0.1 - 1)	0.5			
Pressure setpoint	bar (15 - 50)	25			
Length reactor	m (0 - 3)	0.403			
Length liquid radiator	m (0 - 3)	1.63467			

Storage Sizing Tools

By Usable H2 or System Volume

MH	MH
Adsorbent D-A	Adsorbent D-A
Adsorbent Unilan	Adsorbent Unilan
CH	CH
Cryo Compressed	Cryo Compressed

Results (at end of simulation)

H2 delivered	kg	Pressure
H2 used	kg	Raw dist
Usable H2	kg	Calculat
Storage system mass	kg	Calculat
Storage system volume	L	Tank stat
Gravimetric capacity	%	
Volumetric capacity	g/L	
On-board efficiency	%	
Temperature	C	

MH_System.mDes

Load Inputs ..inputs/vmh_testing_Default.mat **Save**

Name: MH-GH/3s v3

Description: Generic metal hydride model 30 kJ/mol enthalpy of dehydrogenation. Note that the er

Material Properties

f_H2	0.11
f_inert	0.1
kbed	9
rho_cry	851
f_void	0.3
rho_inert	2100
dH_rxn1	-42000
dS_rxn1	-124
dH_rxn2	-51134
dS_rxn2	-134.86
beta_rxn1	1
beta_rxn2	1.5

System Parameters

dmH2	5.6
r	0.01
th_tube	0.00089
dT	45
PH2hi	100
PH2lo	5
HemObl	1
Type	1
Loverd	0
Ltank_in	1.88
d_tank_in	0
dt	300
eff_comb	0.7

Design Parameters

msys	202.397
Vsys	0.190415
burn	2
dmburn	2.17697
D_tank	0.348685
L_tank	1.91238
ntubes	27
m_total_HM	77.7697
sysrhofrac	61.4852
volrhofrac	98.0316
flag	Percentage of DOE 2020 Gravimetri
d_pipe_OD	0.02
d_pipe_ID	0.01822
gap_cooltube	0.06
TH2hi	147.778

Run System Design **Create Model Files** **System Diagram**

Design Documentation **General Documentation** **Exit**

Storage Volume and Mass Outputs

Accomplishments and Progress – Adsorbent System Design Tool in the Framework

Storage Sizing Tools

By Usable H2 or System Volume

MH	MH
Adsorbent D-A	Adsorbent D-A
Adsorbent Unilan	Adsorbent Unilan
CH	CH
Cryo Compressed	Cryo Compressed

System Volume input and Mass Output

Ads_SystemDesignGUI

Load System

Inputs

Pi	1e+07
Pf	500000
Ti	80
Tf	160
System_Vol	267.678
type_Ads	2
Temp_Op	3
Add_Cool	0
Emax	5040.27
Emin	1061.55
nmax	67.75
Va	0.00140392
Vv	0.0073
rho_ads	130
k	0.3
Cp	780
Ads_Cost	11.8
Therm	0
HemObl	0
Vessel	1
TType	4

Name: Cryoadsorbent

Description: Cryoadsorbent system based on MOF-5. Cooling during refuel is done either with a microchannel heat exchanger (MATI) or with flow-through of cold gas.

Results:

Results:	Output values	
H2stored	5.7187 kg_H2	Total hydrogen stored
H2usable	5.6043 kg_H2	Usable hydrogen
System_mass	151.5204 kg	Total H2 Storage System Mass
System_Cost	3.3600e+03 \$	Total Projected H2 Storage System Cost
Grav_Cap	0.0370 g_H2/g_sys	System-based gravimetric capacity
Vol_Cap	20.9367 g_H2/L_sys	System-based volumetric capacity
Rank	6.5186	Overall system rank based on mass, volume, and cost (better s

Input values

Pi	100 bar	Initial/Full tank pressure
Ti	80 K	Initial/Full tank temperature
	5.5000 bar	Final/Empty tank pressure
Tf	160 K	Final/Empty tank temperature
System_Vol	267.6779 L	Target H2 Storage System Volume
type_Ads	2	Type of adsorbent/HX: 1) None? 2) Powder/HexCell, 3) Comp
Temp_Op	3	Operating Temperature: 1) Room Temperature Operation, 2) Col
Add_Cool	0	Additional coolant (1) present
Emax	5.0403e+03 J/mol_H2	D.A. Parameter -- Enthalpic contribution to the characeristic free
Emin	1.0616e+03 J/mol_H2/K	D.A. Parameter -- Entropic contribution to the characeristic free
nmax	67.7500 mol_H2/kg_ads	D.A. Parameter -- Maximum H2 loading of the entire adsorption
Va	0.0014 m^3/kg_ads	D.A. Parameter -- Adsorbed volume per mass of adsorbent
Vv	0.0073 m^3/kg_ads	D.A. Parameter -- Void volume per mass of adsorbent
rho_ads	130 kg_ads/m^3	D.A. Parameter -- Bulk Density of the MOF-5
k	0.3000 W/m/K	Thermal conductivity of the adsorbent
Cp	780 J/kg/K	Specific Heat of the adsorbent
Ads_Cost	11.8000 \$/kg_ads	Projected cost of the adsorbent per unit mass

Run System Design

Save Results to Excel

Create Model File

System Diagram

Exit

Design Documentation

General Documentation

Save

Accomplishments and Progress – Model Downloads and Web Analytics

MODEL Downloaded	Total	Totals AMR2018	Since AMR2018
H ₂ Storage Tank Mass and Cost Model	241	194	47
MHAE Model	66	60	6
MHFE Model	107	92	15
Vehicle Simulator Framework Model	165	138	27
CH System Design Standalone	31	18	13
Adsorbent System Design Standalone	30	18	12

Global Interest



4/1/18 - 3/1/19

Weekly Web Activity



Web Page Flow



Collaboration and Coordination

Organization	Relationship	Type	Responsibility
NREL	Team Member	Federal Lab	Update Website and Framework
SRNL	Team Member	Federal Lab	Adsorbent and Compressed Gas Modeling
PNNL	Team Member	Federal Lab	Chemical Hydrogen and Metal Hydride Modeling
Ford	Consultant	Industry	Beta Testing, Fuel Cell Model, Adsorption Data
RCB Hydrides LLC	Consultant	Industry	Beta Testing, H ₂ Storage Expertise
University of Michigan	Material Developer	Academia	Adsorption Data
University of California Berkeley	Material Developer	Academia	Adsorption Data
Purdue University	Material Developer	Academia	Chemical Hydrogen Storage Reaction Rate
HyMARC	Material Research	Federal Lab / Collaboration	Material development

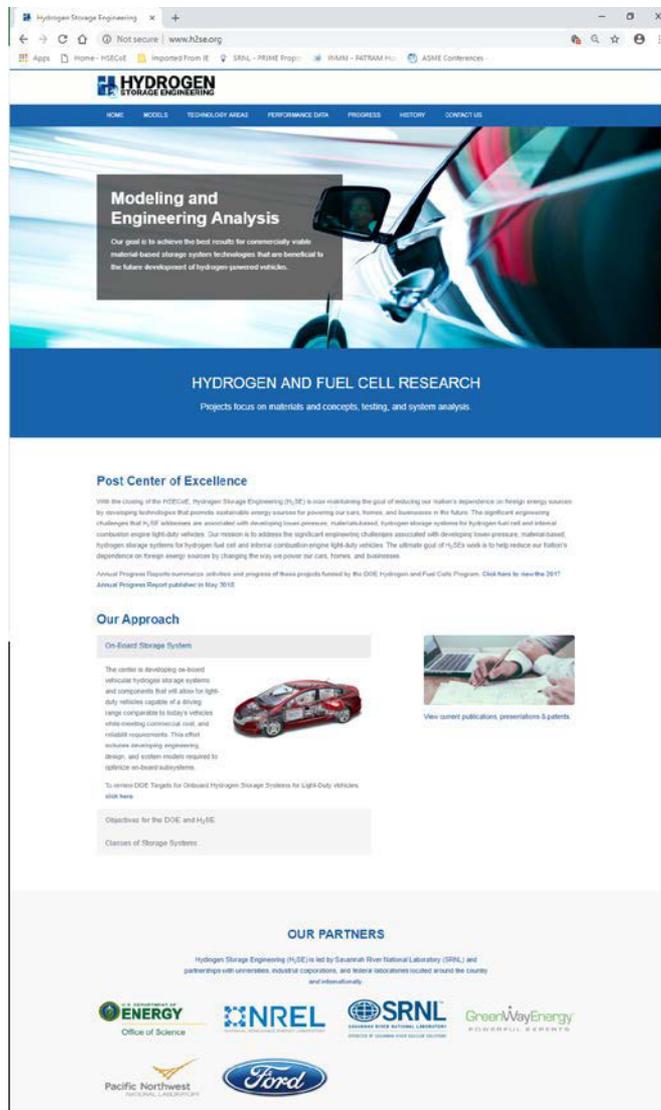
Proposed Future Work – FY19 Milestones and Next Steps

Deliverable		Due
FY19-Q1	Update storage system model documentation for all web available HSECoE models and post new Framework Model versions, including MH Stand-alone design tools and Adsorbent volume-based design tool.	Completed
FY19-Q2	Provide updates on web portal activity – web site hits and time on site, web site use locations, and model downloads	Completed
FY19-Q3	<u>SMART Milestone</u> : Standalone Fully-Excel Model. Convert all existing stand-alone executable models to fully MS Excel (FMSE) models using VBA. These FMSE models will include both mass- and volume-based formulations of the Adsorbent, MH, and CH Storage stand-alone models. The existing executable models will be used for validations with an error of less than 2% between versions.	In Progress
FY19-Q4	Two to three Journal Article Submissions: one related to the ideal adsorbent isotherm shape, one on the adsorbent stand-alone system design tool, and one on the metal hydride stand-alone model.	9/30/2019
Future	Update and modernize www.HSECoE.org to improve its value and usability.	In Progress
Future	Work with material-based H ₂ storage developers to apply models to their materials	In Progress
Future	Expand the usability of the analysis tools to reverse engineer optimum material properties to meet DOE technical targets.	Open
Future	Expand model to other vehicle platforms (medium and heavy duty trucks, forklifts, buses, etc.)	Open

Technology Transfer Activities – Updated HSECoE Model Website

(under development)

HSECoE website: <http://hsecoe.org/>



The screenshot shows the homepage of the Hydrogen Storage Engineering website. At the top, there is a navigation bar with links for HOME, MODELS, TECHNOLOGY AREAS, PERFORMANCE DATA, PROGRESS, HISTORY, and CONTACT US. The main header features the HSECoE logo and a large image of a car with a hydrogen storage tank. Below this, a section titled "Modeling and Engineering Analysis" states the goal of achieving the best results for commercially viable material-based storage systems. A blue banner below reads "HYDROGEN AND FUEL CELL RESEARCH" with the subtext "Projects focus on materials and concepts, testing, and system analysis."

Post Center of Excellence

With the closing of the HSECoE, Hydrogen Storage Engineering (HSE) is now maintaining the goal of reducing our nation's dependence on foreign energy sources by developing technologies that provide sustainable energy sources for powering our cars, homes, and businesses in the future. The significant engineering challenges that HSE addresses are associated with developing more powerful, material-based, hydrogen storage systems for hydrogen fuel cell and internal combustion engine light-duty vehicles. Our mission is to address the significant engineering challenges associated with developing more powerful, material-based, hydrogen storage systems for hydrogen fuel cell and internal combustion engine light-duty vehicles. The ultimate goal of HSE work is to help reduce our nation's dependence on foreign energy sources by changing the way we power our cars, homes, and businesses.

Annual Progress Reports summarize activities and progress of these projects funded by the DOE Hydrogen and Fuel Cells Program. Click here to view the 2017 Annual Progress Report published in May 2018.

Our Approach

On-Board Storage System

The center is developing on-board vehicular hydrogen storage systems and components that will allow for light-duty vehicles capable of a driving range comparable to today's vehicles while meeting commercial cost and reliability requirements. This effort includes developing engineering design and system models required to replicate on-board subsystems.

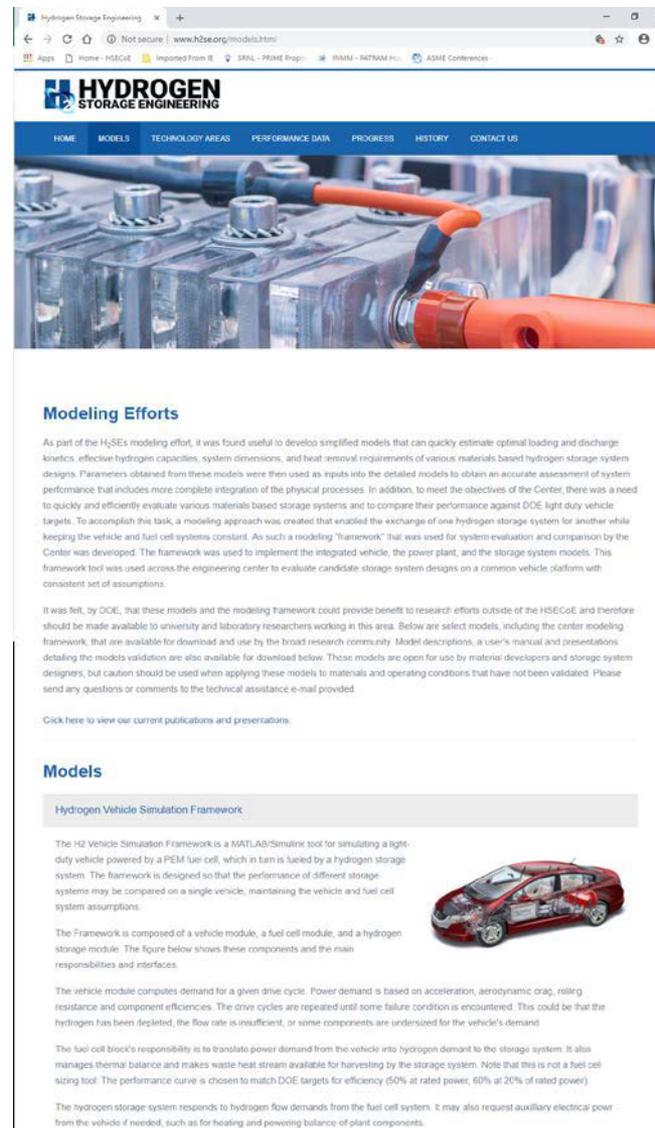
To review DOE Targets for Onboard Hydrogen Storage Systems for Light-Duty Vehicles, click here.

Objectives for the DOE and HSE

Classes of Storage Systems

OUR PARTNERS

Hydrogen Storage Engineering (HSE) is led by Savannah River National Laboratory (SRNL) and partnerships with universities, industrial corporations, and federal laboratories located around the country and internationally.



The screenshot shows the "Modeling Efforts" page of the HSECoE website. The page features a large image of a hydrogen storage system with orange and blue components. Below the image, the section "Modeling Efforts" is introduced. The text explains that as part of the HSE modeling effort, simplified models were developed to estimate optimal loading and discharge kinetics, effective hydrogen capacities, system dimensions, and heat removal requirements. Parameters from these models were used as inputs into detailed models to obtain an accurate assessment of system performance. A modeling framework was created to enable the exchange of one hydrogen storage system for another while keeping the vehicle and fuel cell systems constant. This framework was used to implement the integrated vehicle, the power plant, and the storage system models. The framework tool was used across the engineering center to evaluate candidate storage system designs on a common vehicle platform with consistent set of assumptions.

It was felt, by DOE, that these models and the modeling framework could provide benefit to research efforts outside of the HSECoE and therefore should be made available to university and laboratory researchers working in this area. Below are select models, including the center modeling framework, that are available for download and use by the broad research community. Model descriptions, a user's manual and presentations detailing the models validation are also available for download below. These models are open for use by material developers and storage system designers, but caution should be used when applying these models to materials and operating conditions that have not been validated. Please send any questions or comments to the technical assistance e-mail provided.

Click here to view our current publications and presentations.

Models

Hydrogen Vehicle Simulation Framework

The H2 Vehicle Simulation Framework is a MATLAB/Simulink tool for simulating a light-duty vehicle powered by a PEM fuel cell, which in turn is fueled by a hydrogen storage system. The framework is designed so that the performance of different storage systems may be compared on a single vehicle, maintaining the vehicle and fuel cell system assumptions.

The Framework is composed of a vehicle module, a fuel cell module, and a hydrogen storage module. The figure below shows these components and the main responsibilities and interfaces.



The vehicle module computes demand for a given drive cycle. Power demand is based on acceleration, aerodynamic drag, rolling resistance and component efficiencies. The drive cycles are repeated until some failure condition is encountered. This could be that the hydrogen has been depleted, the flow rate is insufficient, or some components are undersized for the vehicle's demand.

The fuel cell block's responsibility is to translate power demand from the vehicle into hydrogen demand to the storage system. It also manages thermal balance and makes waste heat stream available for harvesting by the storage system. Note that this is not a fuel cell sizing tool. The performance curve is chosen to match DOE targets for efficiency (50% at rated power, 60% at 20% of rated power).

The hydrogen storage system responds to hydrogen flow demands from the fuel cell system. It may also request auxiliary electrical power from the vehicle if needed, such as for heating and powering balance of plant components.

Summary

Relevance	<ul style="list-style-type: none">• Provide materials based hydrogen storage researchers with models and materials requirements to assess their material's performance in an automotive application.
Approach	<ul style="list-style-type: none">• Improve framework utility by bridging the gap between the information generated by the materials researcher and the parameters required for the framework model.
Technical Accomplishments and Progress	<ul style="list-style-type: none">• Developed system design tools for MH, CH, and Adsorbents that are both H₂ mass- or system volume-based.• System design tools used with framework GUI and as stand-alone executables.• Developed a system design tool based on multiple kinetics expressions / isotherm theories.• Improved website and model accessibility.
Collaborations	<ul style="list-style-type: none">• Project team includes NREL, SRNL, and PNNL.• Consultants from industry participate in team meetings and provide input.• Material developers from academia provide new material properties.
Proposed Future Research	<ul style="list-style-type: none">• Expand the use of models by demonstrating their utility with other storage materials and vehicle class options.

Responses to Previous Year Reviewers' Comments

2018 AMR Comment

1) This is a strong technical team with diverse expertise; hence, there are few weakness associated with the team's ability to develop and deploy the analytical tools. The primary limitation is the absence of validation results and feedback from outside users.

2) Validation of the models continues to remain a dominant issue. Greater emphasis is needed on a more detailed description of the approach for validating the models and design tools.

3) Correlation data between models and real life are desired to validate the models. Having more data on the website showing this correlation would be desirable.

The main project weakness is that the models are being developed but are not being utilized to make projections or develop strategies for closing the gap to the DOE hydrogen storage system targets. Also, the validation of the models should be further explained to allow researchers to gain confidence in the results.

2019 Response/Approach

The models have been validated against fundamental material data measurements and prototype system data where available. In addition, several hydrogen model system design components have been validated against natural gas or similar system components. As no full-scale MH, CH, or Adsorbent hydrogen storage systems have been built, it is difficult to find full-scale data to use. Citations for papers outlining the validations efforts are available on www.hsecoe.org.

The primary purpose of this project is to assist DOE and the research community in closing the Technology Target Gaps. The intent moving forward is to work more closely with the materials development community to more efficiently meet this objective.

As for the comment on validation, please see the response above.

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