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

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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)

Barriers

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

Budget

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

Partners

NREL NATIONAL RENEWABLE ENERGY LABORATORY

SRNL SAVANNAH RIVER NATIONAL LABORATORY

Pacific Northwest NATIONAL LABORATORY

*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 - On-Board Efficiency - Fuel Economy
E. Charging/Discharging Rates	Framework Model - Drive cycles
I. Dispensing Technology	Framework Model - Initial and Final System Conditions
K. System Life-Cycle Assessment	All Models

Relevance – Focus: Improve Model Utilities for Materials Researchers

Materials Research

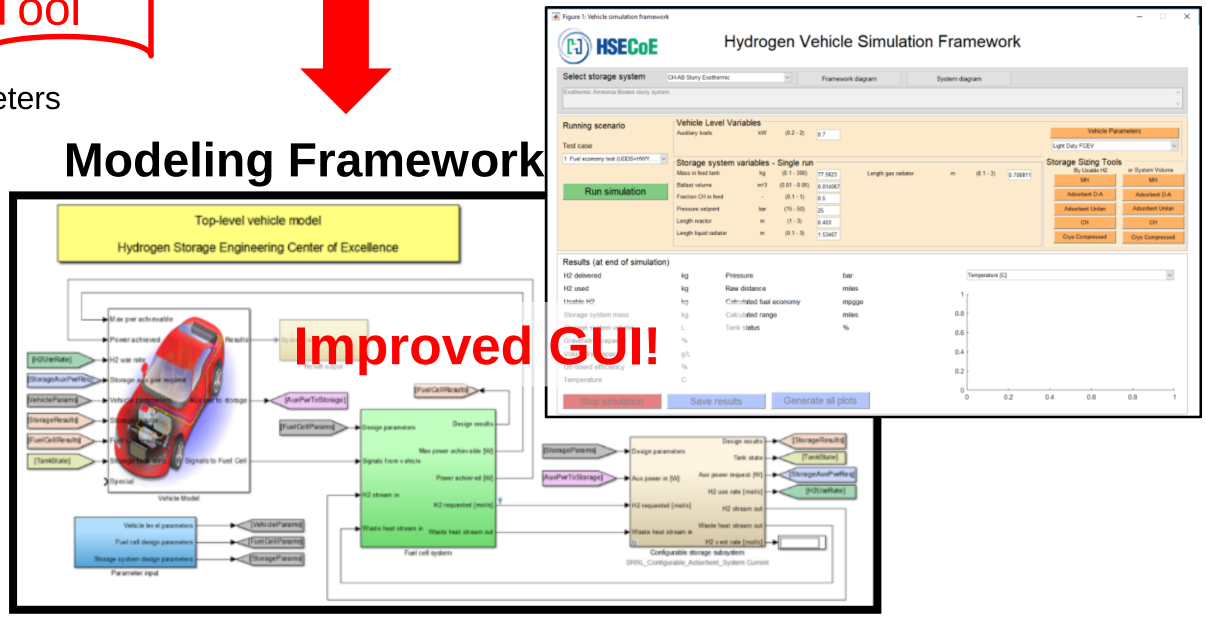
H_2 Capacity
Thermodynamics
Kinetics
Adsorption Isotherms

Isotherm Fitting Tool

DA Parameters

Available at www.hsecoe.org

Modeling Framework



Stand Alone System Design Tools

Component and System Mass & Volume

Stand-Alone Values

Estimated Gravimetric & Volumetric Capacity

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) — SRNL
- Adsorbent (AD) – HexCell and MATI — SRNL

Tank Heat and Mass Transfer Models

Stand-alone System Design Tool:

- Adsorbent (AD) — SRNL — New Mass or Volume-Based Tool; New D-A or UNILAN Isotherm-Based Tool
- Chemical Hydrogen (CH) — PNNL — New Mass or Volume-Based Tool
- Metal Hydride (MH) — PNNL — New Mass or Volume-Based Tool
- Compressed/Cryo-Compressed H_2 — SRNL

Framework Model with:

- Physical Storage — UTRC/NREL
- Compressed/Cryo-Compressed H_2 — SRNL/NREL
- Chemical Hydrogen (CH) — PNNL/NREL
- Adsorbent (AD) — SRNL/NREL — Updating for UNILAN Isotherm Theory
- Metal Hydride (MH) — PNNL/NREL — Updated to allow user input

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

Additional Tool / Models:

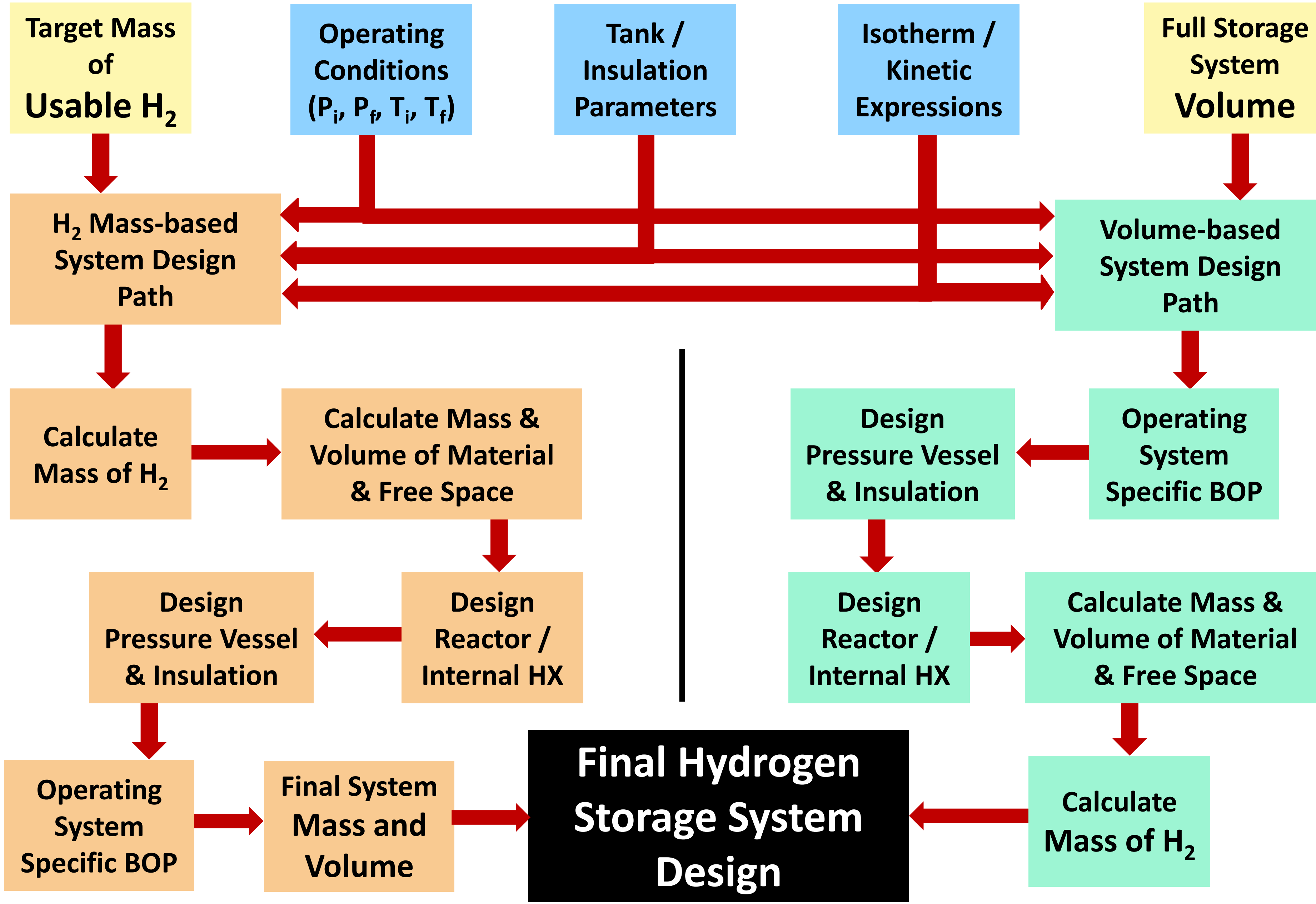
- MH Acceptability Envelope — SRNL
- Tank Volume/Cost Model — PNNL
- AD Isotherm Fitting Tool — SRNL

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

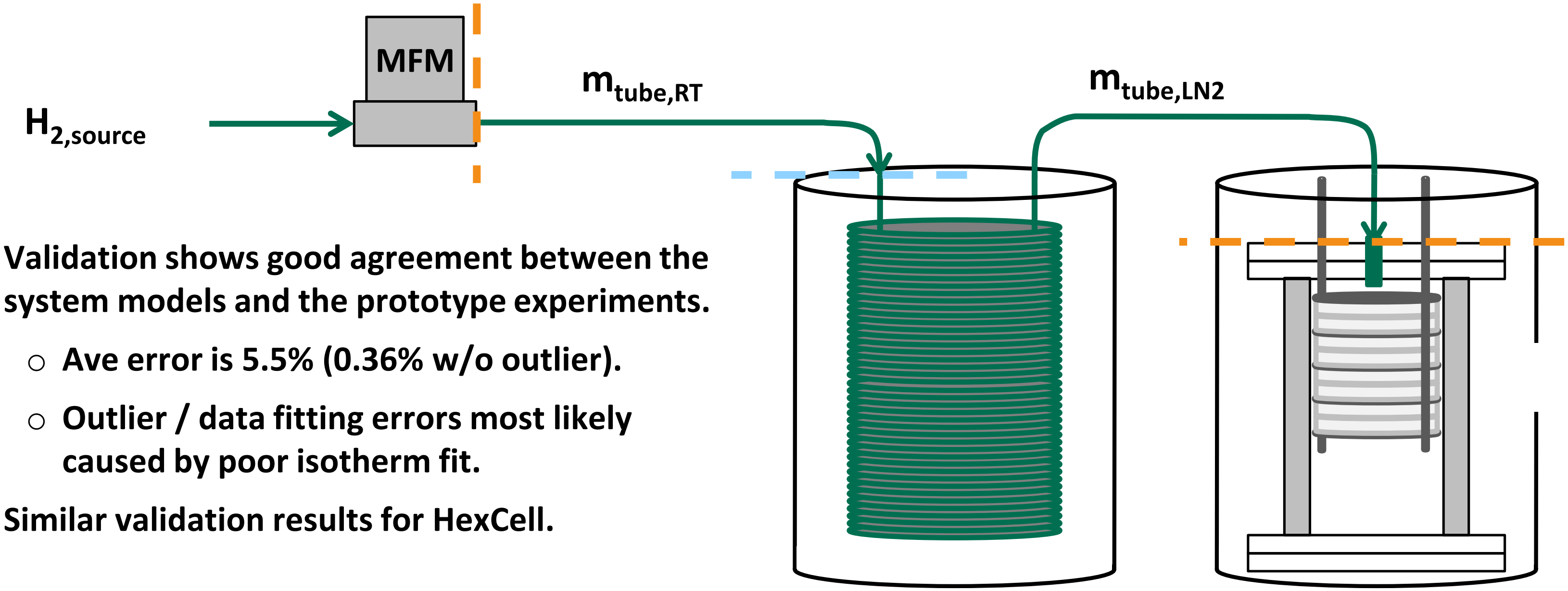
Capabilities:

- 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-H_2 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



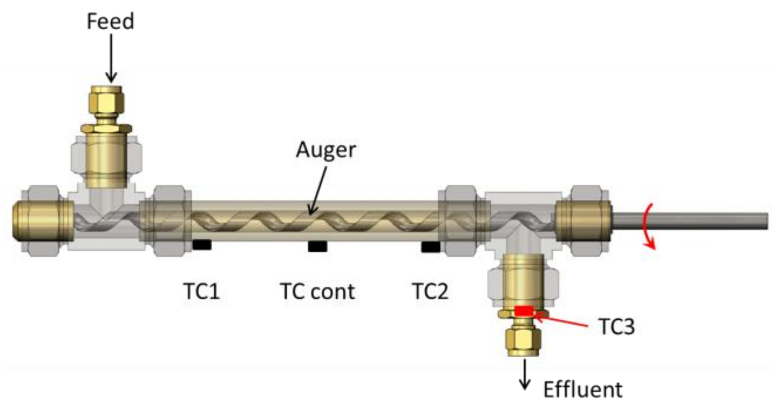
Accomplishments and Progress – MATI Adsorbent Storage System Validation



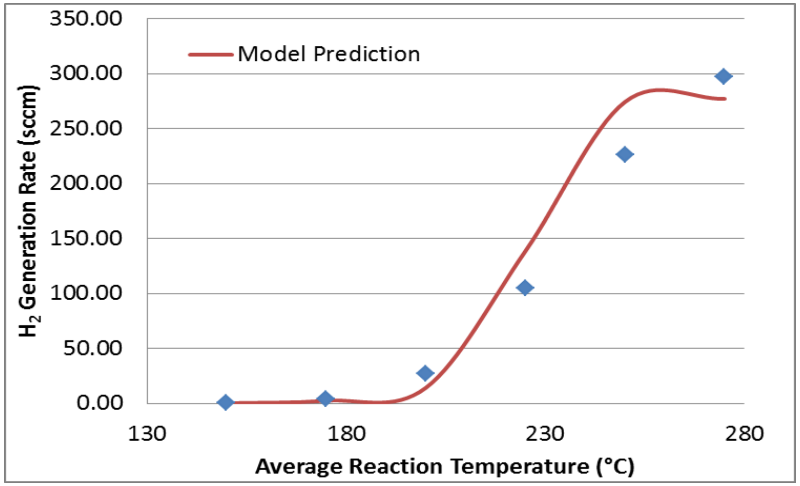
- Validation shows good agreement between the system models and the prototype experiments.
  - Ave error is 5.5% (0.36% w/o outlier).
  - Outlier / data fitting errors most likely caused by poor isotherm fit.
- Similar validation results for HexCell.

Op. Conditions	$H_{2,in}$	$m_{tube,tot}$	$m_{proto,exp}$	$m_{proto,model}$	% 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

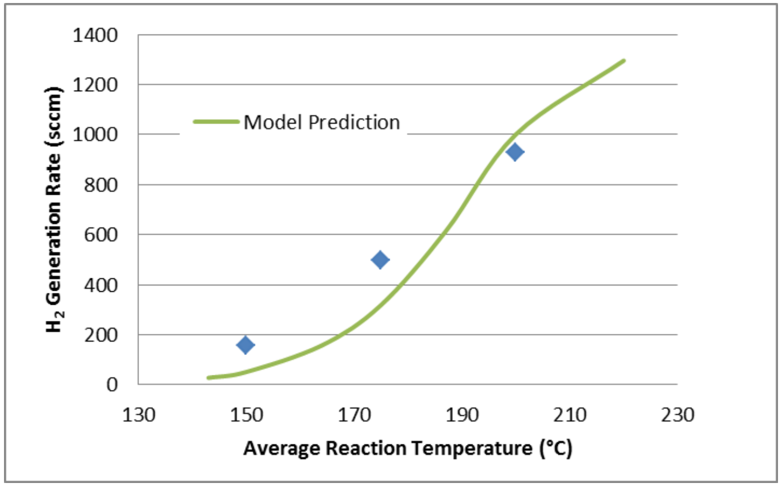


Flow-through reactor design used to validate the model



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

Solids Loading	Reactor Residence Time	Auger Speed	Average Reaction Temperature	Measured Alane Conversion	Model Conversion Values
(wt%)	(min)	(rpm)	(°C)	(mol/mol)	(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%

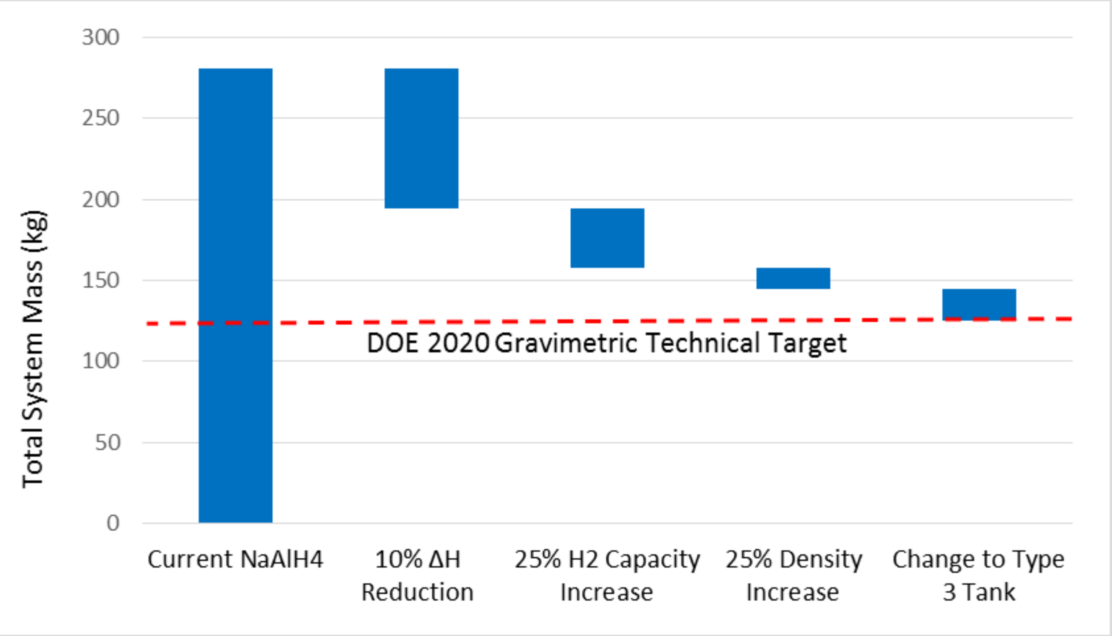


Comparison of model predicted hydrogen flow rate to that measured experimentally for 20 wt% AB slurry

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

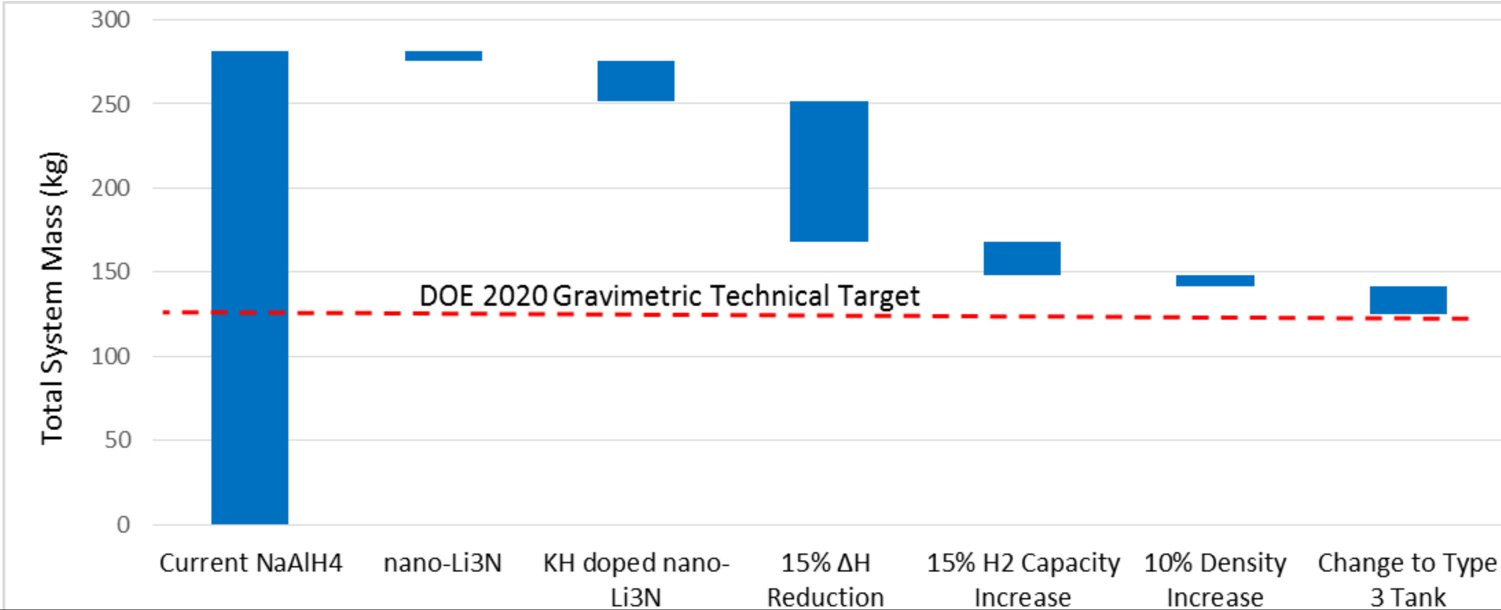
Accomplishments and Progress –One Possible Pathway to Meet DOE Gravimetric Target for $NaAlH_4$



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 H_2 capacity and 3) density and 4) Type 3 tank

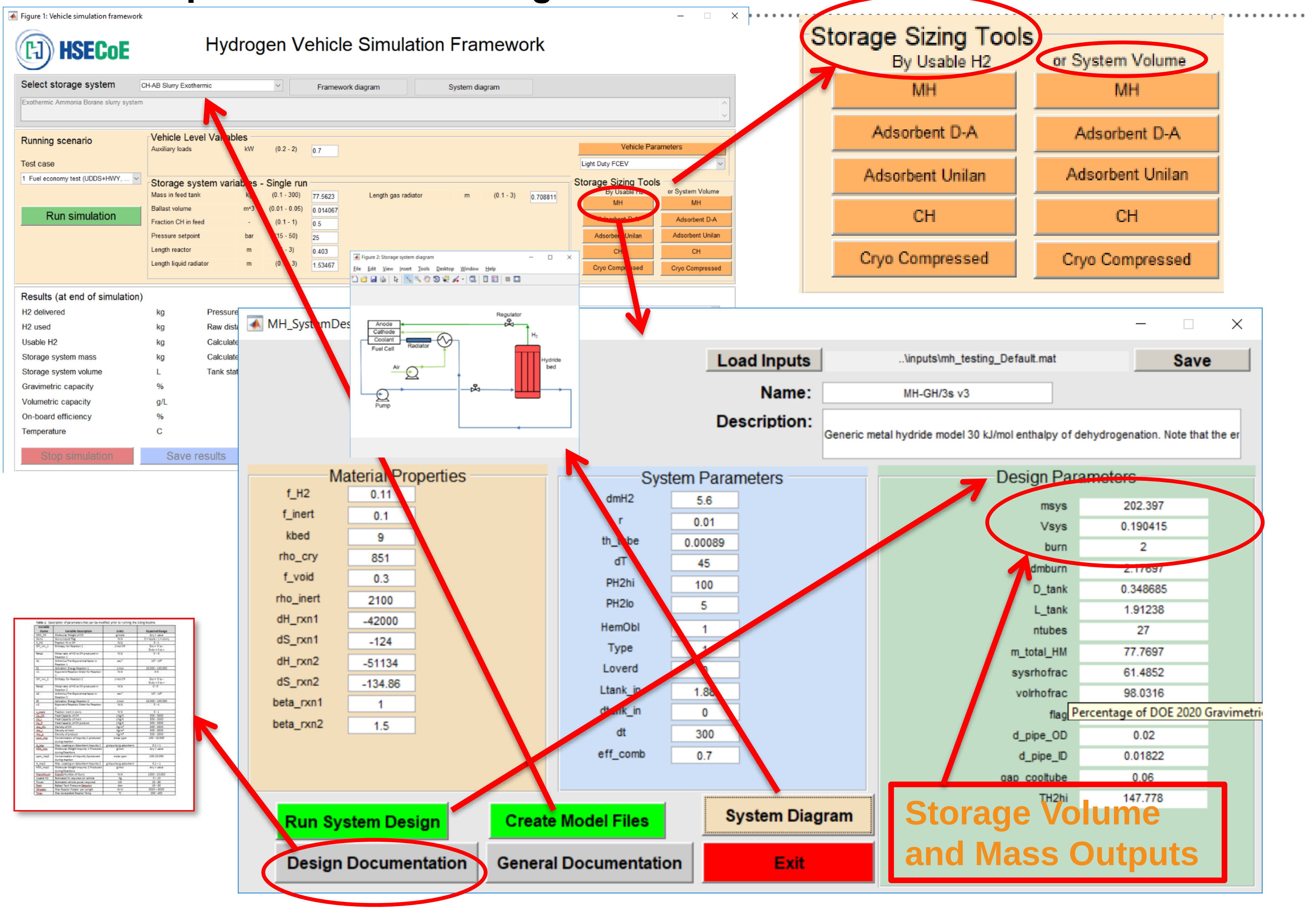
Accomplishments and Progress –Evaluate new materials relative to DOE Technical Targets



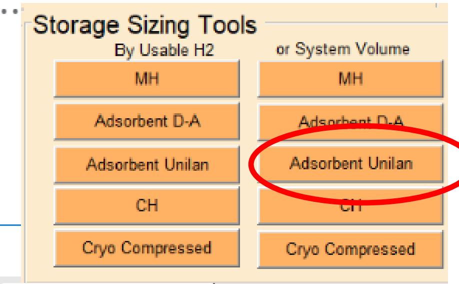
Reaction Enthalpy (kJ/mol)	42	42.1	41.7	35.4	35.4	35.4	35.4
x_{H2} (wt%)	5.6%	6.1%	6.4%	6.4%	7.36%	7.36%	7.36%
Bed Density (kg/m^3)	720	740	760	760	760	836	836
Tank Type	Type 1-Al	Type 1-Al	Type 1-Al	Type 1-Al	Type 1-Al	Type 1-Al	Type 3-Al liner
System Mass (kg)	281	276	252	168	148	142	125
Gravimetric Capacity (5.6 kg useable H_2)	0.020	0.020	0.022	0.033	0.038	0.039	0.045

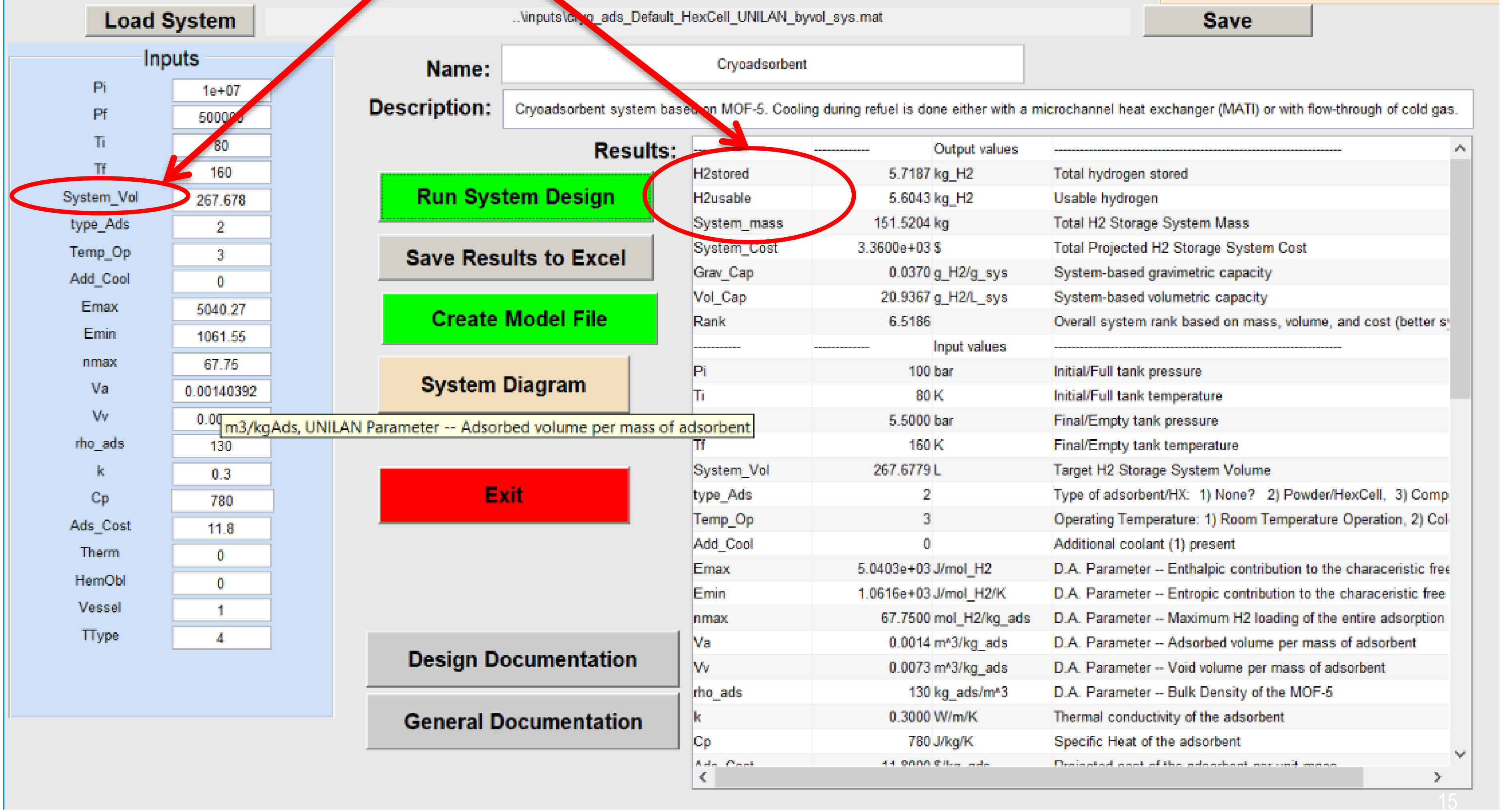
6 nm KH doped nano-Li_3N developed by Dr. Stavila: Requires larger ΔH_{rxn} reduction, but smaller increases in H_2 capacity and density than $NaAlH_4$ to meet the DOE Gravimetric target

Accomplishments and Progress – Vehicle Framework GUI



Accomplishments and Progress – Adsorbent System Design Tool in the Framework

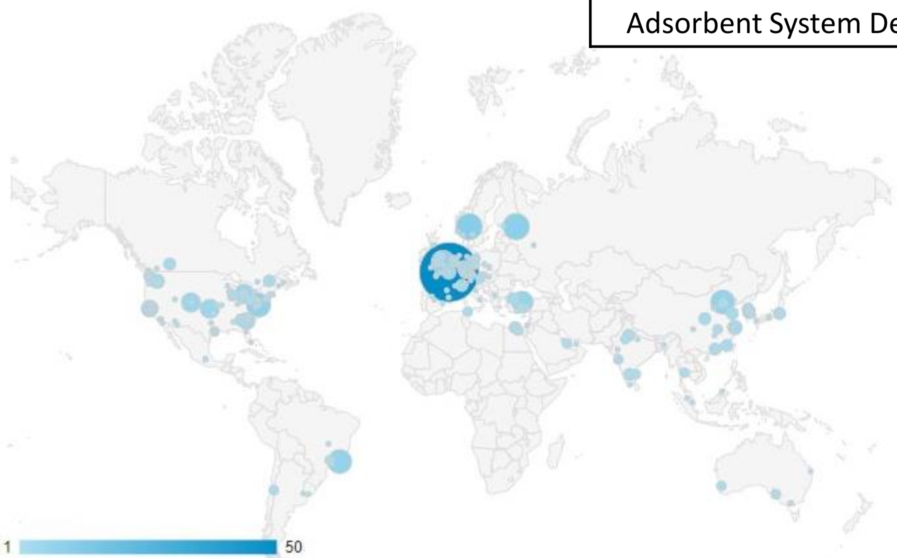




Accomplishments and Progress – Model Downloads and Web Analytics

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

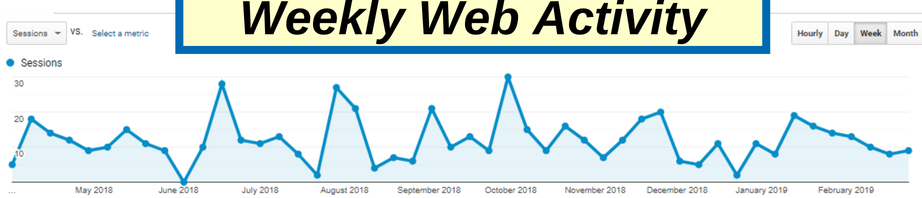
Global Interest



4/1/18 - 3/1/19

Web Page Flow

Weekly Web Activity



Collaboration and Coordination

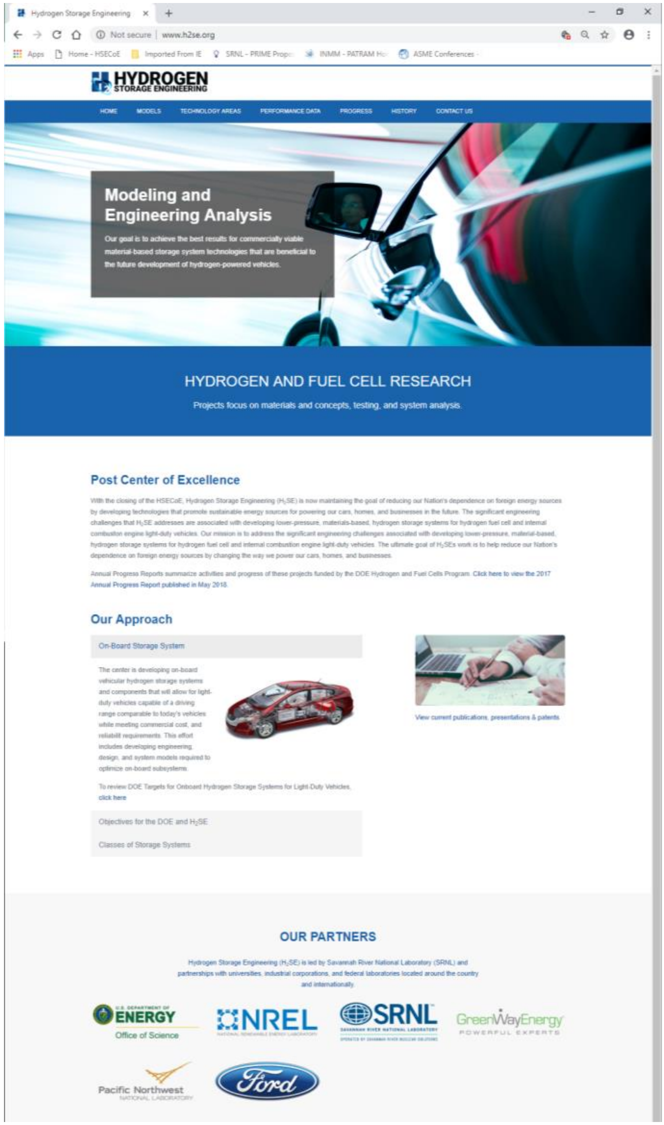
Organization	Relationship	Type	Responsibility
NREL	Team Member	Federal Lab	Update Website and Framework
SRNL	Team Member	Federal Lab	Adsorbent and Compressed Gas Modeling
PNNL	Team Member	Federal Lab	Chemical Hydrogen and Metal Hydride Modeling
Ford	Consultant	Industry	Beta Testing, Fuel Cell Model, 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	SMART Milestone: 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/



Summary

Relevance	• Provide materials based hydrogen storage researchers with models and materials requirements to assess their material's performance in an automotive application.
Approach	• 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	• Developed system design tools for MH, CH, and Adsorbents that are both H_2 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	• 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	• 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	2019 Response/Approach
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 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 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.	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.