IV.B.2 Hydrogen Storage System Modeling: Public Access, Maintenance, and Enhancements

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Project Start Date: October 1, 2015
Project End Date: September 30, 2018

Overall Objectives

- Coordinate the public access of select models developed under the Hydrogen Storage Engineering Center of Excellence (HSECoE) activity, including web posting documentation and tracking downloads and web activity.
- Maintain performance of existing storage system models and update and validate as new experimental data becomes available.
- Enhance and expand existing models to improve simulation speed and application to other uses. This will focus on expanding the parameterization of the models and their flexibility in evaluating new hydrogen storage material candidates. This will also include the development of pre-processor sizing routines for both the adsorbent and chemical hydrogen storage systems.

Fiscal Year (FY) 2016 Objectives

- Coordinate the public access of selected HSECoE models, including web posting documentation and tracking downloads and web activity.
- Update storage system model documentation.
- Update all adsorbent and chemical hydrogen (CH) storage HSECoE models based on experimental results.
- Develop storage system sizing pre-processor (CH storage system).
- Develop a stand-alone isotherm data fitting routine to convert raw excess adsorption H_2 data into its Dubinin-Astakhov parameters.

Technical Barriers

This project addresses the following technical barriers from the Hydrogen Storage section of the Fuel Cell Technologies Program's Multi-Year Research, Development, and Demonstration Plan.

(A) System Weight and Volume

(B) System Cost

(C) Efficiency

(E) Charging/Discharging Rates

(I) Dispensing Technology

(K) Systems Life-Cycle Assessments

Technical Targets

This project is conducting simulation and modeling studies of advanced onboard materials-based hydrogen storage technologies. Insights gleaned from these studies are being applied toward the design and synthesis of hydrogen storage vessels that meet the following DOE 2020 hydrogen storage for light-duty vehicle targets.

- Cost: to be determined
- Specific energy: 0.055 kg H_2/kg system
- Energy density: 0.040 kg H_2/L system
- Charging/discharging rates: 3–5 min
- Well to power plant efficiency: 60%

FY 2016 Accomplishments

- Updated and integrated several HSECoE storage system models within the vehicle modeling framework and posted them on the website portal. These included a 700 bar physical storage model, a metal hydride model, two CH models, and two adsorbent system models.

- Update all adsorbent and CH HSECoE models based on experimental results. Validated adsorbent models based on 2-L prototype experimental results.
- Develop storage system sizing pre-processor (CH storage system).
- Completed documentation updates for the posted models (including website text and downloadable user manual).
- Adjusted CH tank size to ensure 5.6 kg of usable hydrogen.
- Troubleshooting of compiler and software versions.
- Tracking and monitoring web activity and downloads.

INTRODUCTION

Overcoming challenges associated with onboard hydrogen storage is critical to the widespread adoption of fuel cell electric vehicles. The overarching challenge is identifying a means to store enough hydrogen onboard to enable a driving range greater than 300 miles within vehicle-related packaging, cost, safety, and performance constraints. As new hydrogen storage materials are discovered and created, material developers must predict their full-scale vehicle performance and compare their performance with pure hydrogen storage (700 bar, cryo-compressed, and liquid H_2 storage). The goal of this work is to provide material developers with the modeling tools necessary to make these predictions based on the work done by the HSECoE.

APPROACH

The approach for FY 2016 is to update, document, and perform validation, enhancement, troubleshooting, and debugging of these framework and other models developed by HSECoE so that they can be made accessible to and useful for other research within the hydrogen storage community. During subsequent years, these models will be updated with alternative storage system formulations, such as different isotherm models for adsorbents and alternative chemical reaction kinetic expressions for CHs. In addition, stand-alone system estimators that do not require special software will be developed to serve as a scoping tool for the new hydrogen storage materials.

RESULTS

The following will provide results from work completed this year with a focus on the coordination of the public access of select HSECoE models, including web posting documentation and tracking downloads and web activity. The multi-lab team worked on the validation, refinement, graphical user interface (GUI) improvements, troubleshooting, improving simulation run time, updating model documentation for selected web postings, and monitoring or tracking web activity and model downloads. To date, there have been 120 downloads of the tank volume and cost model, 85 down loads of the framework model, 53 down loads of the metal hydride (MH) finite element model, and 36 down loads of the MH acceptability envelop.

Model validation work on the HSECoE adsorbent and CH framework models, based on experimental data from the center, have been compete. Documentation and users guides for all of these HSECoE models have also been updated this year and all are currently available via the HSECoE web site (www.hsecoe.org). Figure 1 shows a screen caption of the current HSECoE home page as well as the models page, which has direct links to the documentation, user guides, and download area for all available models. All of the select HSECoE models that are available on the website are listed in Table 1.

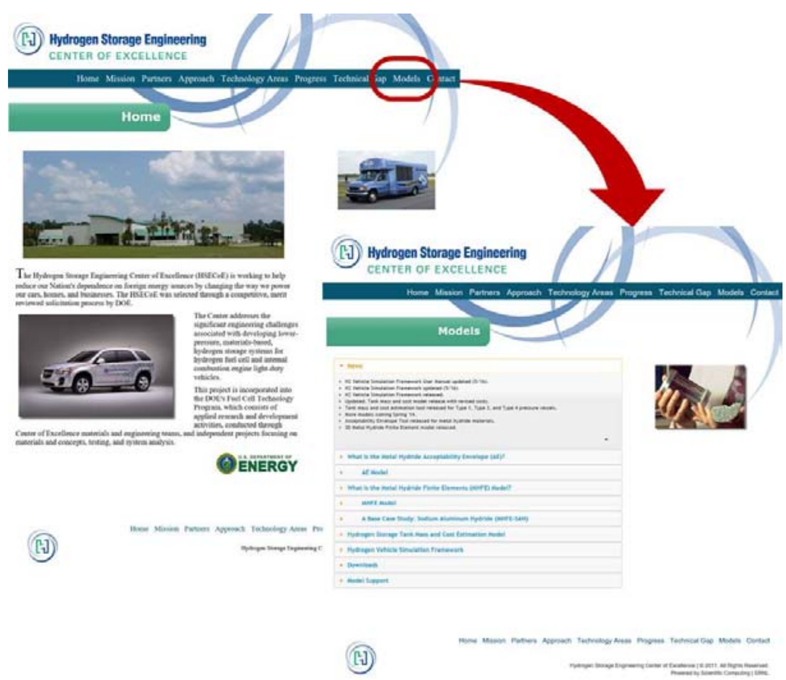


FIGURE 1. HSECoE web home page and web models documentation and download page

TABLE 1. HSECoE Models Available on Web Portal and Model Posting Status

Model Name	HSECoE Lead	Status
MH Acceptability Envelop	SRNL	Complete
MH Finite Element Model	SRNL	Complete
AD Finite Element Model	SRNL	Complete
Tank Volume/Cost Model	PNNL	Complete
MH Framework Model	UTRC/NREL	Complete
CH Framework Model	PNNL/UTRC/NREL	Complete
AD Framework Model	SRNL/UTRC/NREL	Complete

AD – Adsorption; UTRC – United Technologies Research Center

One purpose of the framework is to provide a model that can be used by material developers to evaluate newly identified materials in terms of system sizing and drive cycle performance. The current chemical hydrogen storage module within the framework requires that these material developers not only determine kinetic and thermodynamic properties of the material, but also estimate the dimensions of the system components and the control parameters. Estimating system sizing and control parameters would be challenging to those not familiar with the model. To allow greater use of the framework by the hydrogen storage community, PNNL developed a pre-processor that uses the kinetic and thermodynamic information for a new material that would normally be measured experimentally (i.e., fraction of hydrogen, reaction enthalpy, activation energy) to estimate the system sizing and control parameters. Such design parameters as the mass of chemical hydrogen storage material required, the length of the radiators and reactors, and the volume of the ballast tank are estimated and can then be used in the model. Additionally, control parameters such as the initial reaction and maximum temperatures are estimated. Currently the pre-processor is a stand-alone model, but it will be implemented into the framework next fiscal year to allow seamless operations between the initial size estimation and the framework.

The preliminary pre-processor was tested using material properties for ammonia borane (AB) and alane. While the values produced by the pre-processor are different than those assumed during the system storage model development, the framework models using the predicted system sizing both AB and alane run successfully. The model result with the US06 aggressive cycle run are compared for the two inputs shown in Table 2. The pre-processor estimates for reactor length and ballast tank volume are less than the values originally included in the model resulting in a reduced storage system mass and volume. The onboard efficiency and raw distance traveled are similar between the original and preprocessor values.

TABLE 2. Framework Results for Chemical Hydrogen Storage Materials with US06 Drive Cycle Comparing Originally Estimated Model Inputs and the Pre-processor Inputs

Framework Input Parameter	Ammonia Borane		Alane	
	Original Values	Pre-processor	Original Values	Pre-processor
Reactor Length (m)	1.2	0.96	2.0	1.45
Ballast Tank Volume (m^3)	0.02	0.007	0.03	0.017
Mass CH (kg)	86	82	140	155
Length Gas HX (m)	1.25	1.39	1	1.45
Length Liquid HX (m)	1.33	0.9	1	1.08
Framework Output Parameters				
Useable H_2 (kg)	5.7	5.5	5.41	5.48
Storage System Mass (kg)	138	131	186	199
Storage System Volume (L)	146	128	164	162
On-Board Efficiency	97.8%	97.8%	84.2%	85.1%
Maximum Temperature (°C)	301	333	329	315
Raw Distance (miles)	333	320	314	317

HX – Heat exchanger

Using experimental data (and finite element model results in the case of the HexCell storage system), the adsorbent storage system model was validated prior to being updated within the vehicle framework. Table 3 shows the experimental measurements and the projected resulting full-scale vehicle models based on the validated models. Note that the adsorbent and heat exchanger portions of the model were validated using the 2-L prototypes, while the tank sizing tool (based on the Tank Volume/Cost Model) and the balance of plant estimates were validated and updated based on the latest information from other HSECoE sources.

The adsorbent storage system validation (as listed in Table 3) includes columns for the powder metal organic framework (MOF)-5 HexCell heat exchanger storage system design, 0.4 g/cc compacted metal organic framework MOF-5 modular adsorbent tank insert (MATI) heat exchanger storage system design, and images corresponding to the validation and projection rows. The rows shown in Table 1 correspond to the experimental measurements of 2-L prototype-level adsorbent + heat exchanger values; the projected full-scale adsorbent + heat exchanger values; and the projected full-scale full storage system estimates. The adsorbent storage system models were able to estimate the 2-L prototype experiments within 10% of the recorded values.

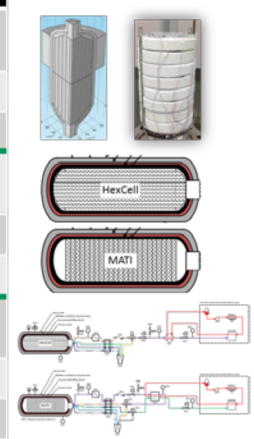
The current version of the adsorbent storage system model has the capability of sizing the adsorbent system for a wide range of operating conditions and target usable hydrogen. However, as of the writing of this document, the user is limited to analyzing only powder and compacted MOF-5. No other adsorbents, nor the capability to add another adsorbent, are currently available. During the next set of GUI updates, this will change and the capability to add new adsorbents (via their physical and adsorptions properties) will be included. In addition, a stand-alone fitting routine is being developed (estimated availability is 9/30/2016) to allow material developers to fit their raw excess adsorption hydrogen storage data into its Dubinin-Astakhov isotherm parameters so that it can be directly implemented within the adsorbent storage models.

In FY 2015 UTRC, NREL, and other HSECoE partners teamed on the GUI improvement effort. The updated version of the GUI framework is shown in Figure 2, which highlights the model selection pulldown menu showing the hydrogen storage models available to the user at this time. Specific storage system diagrams for each of the storage models have also been added to the GUI (not shown). In the coming months, the GUI updates will continue and include increased user controls as well as additional results options for the storage systems. Some of the planned updates include the ability to run sizing pre-processors and modify material properties for each of the storage systems.

Now that several HSECoE models are available to a wider research audience via the HSECoE web page, the final task for this year has been to continue tracking and documenting website activity and model down loads. Figure 3 shows the latest web site activity over the last three months. The site has received over 1,100 visitors during this

TABLE 3. Adsorbent Storage System Validation Information

	Powder MOF-5 HexCell HX	Compact MOF-5 MATI HX
Measured 2-liter Prototype (material + $HX_{internal}$)	(90 K, 80 bar) → (85 K, 1.7 bar)	(84.5 K, 100 bar) → (83.7 K, 1.1 bar)
Gravimetric Capacity	0.112 g/g	0.092 g/g
Volumetric Capacity	23.6 g/l	37.2 g/l
Full-scale 5.6 kg System model (material + $HX_{internal}$)	(80 K, 100 bar) → (160 K, 5.0 bar)	(80 K, 100 bar) → (160 K, 5.0 bar)
Gravimetric Capacity	0.125 g/g	0.100 g/g
Volumetric Capacity	32.9 g/l	44.4 g/l
Full-scale 5.6 kg System model (full system)	(80 K, 100 bar) → (160 K, 5.0 bar)	(80 K, 100 bar) → (160 K, 5.0 bar)
Gravimetric Capacity	0.0321 g/g	0.0315 g/g
Volumetric Capacity	18.9 g/l	21.0 g/l



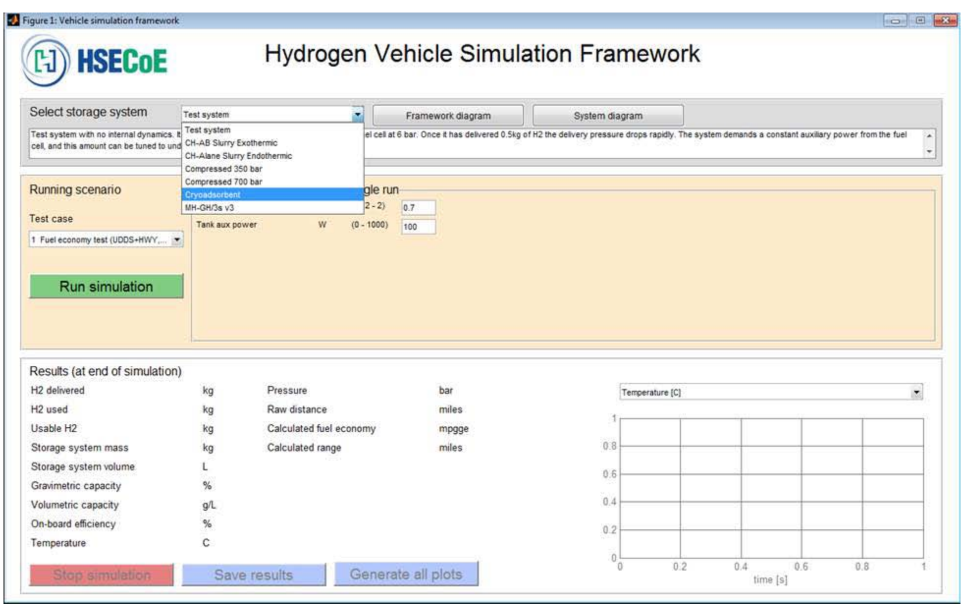


FIGURE 2. HSECoE framework model GUI

time, with roughly 83% of those being new visitors. The bounce rate, which indicates sessions under 10 s, is 85%, indicating that 15% of the visitors stay longer than 10 s and have an average stay of approximately 48 s. Figures 4 and 5 provide the user flows for the site and user origin countries, respectively.

FUTURE DIRECTION

- Work with center partners to continue to update and improve center developed models available and accessible to the broader research and academic community through a controlled web-based access portal and track downloads and website activity.
- Create stand-alone executable versions of the center developed material storage models to provide first-order storage system estimates based on material property information.
- Update the hydrogen storage equations with additional, alternative theoretical storage system formulations to allow users to choose the most appropriate system for their material.

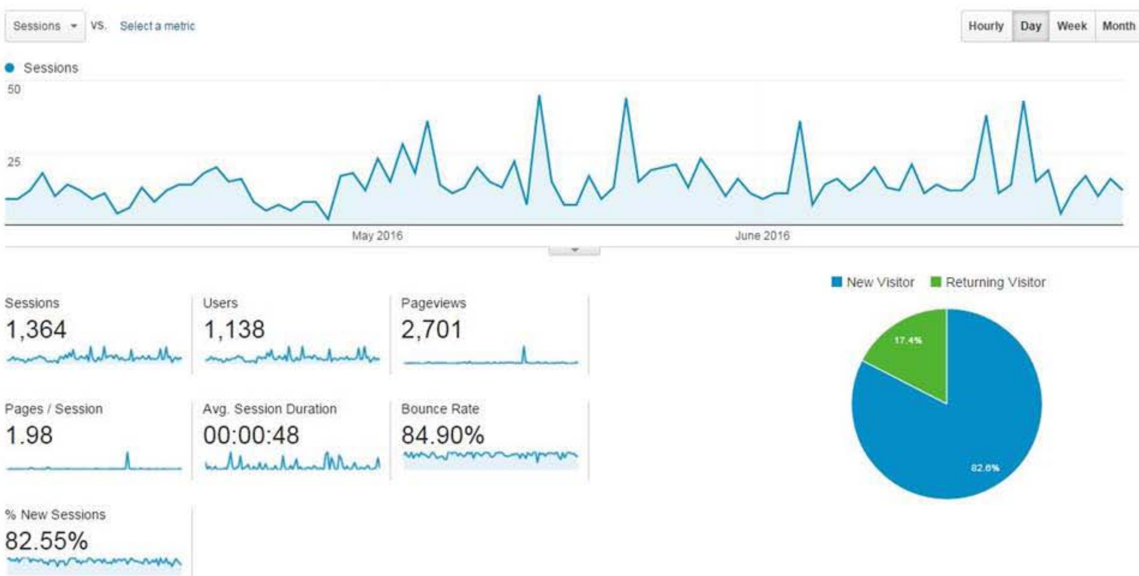


FIGURE 3. HSECoE web analytics: three-month site activity metrics

FIGURE 4. HSECoE web analytics: user flows

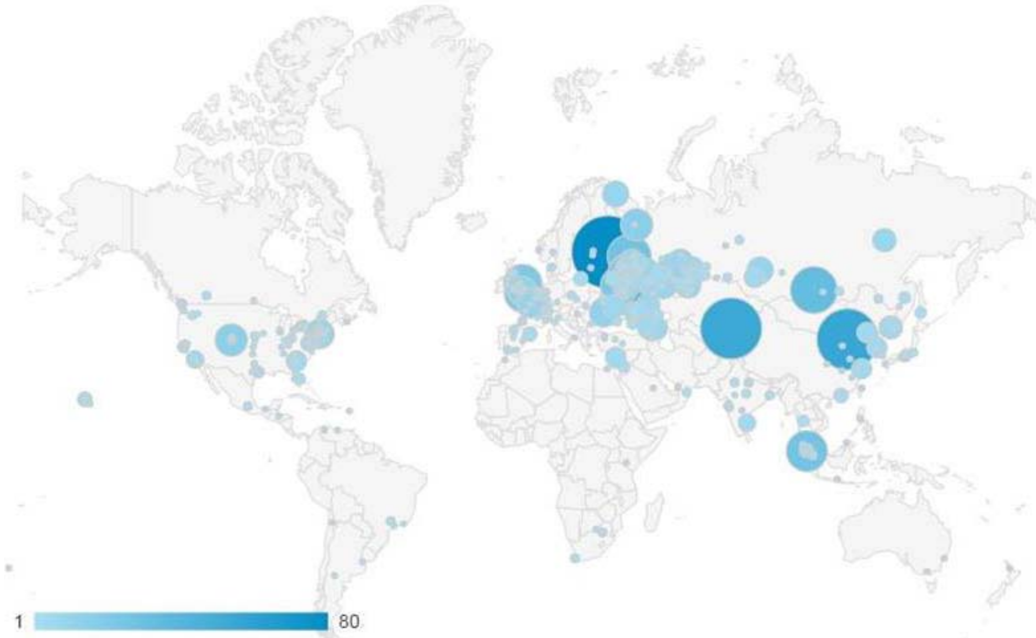


FIGURE 5. HSECoE web analytics: user origin countries

FY 2016 PUBLICATIONS/PRESENTATIONS

1. Thornton, M., D. Tamburello, K. Brooks, J. Gonder, S. Sprik, "Hydrogen Storage System Modeling: Public Access, Maintenance, and Enhancements," U.S. Department of Energy Hydrogen and Fuel Cells Program Annual Merit Review and Peer Evaluation Meeting, June 9, 2016.

2. Thornton, M., D. Tamburello, K. Brooks, J. Gonder, S. Sprik, "HSECoE Models on the WEB," Hydrogen Storage Technical Team Review, February 18, 2016.