IV.D.2 System Design, Analysis, Modeling, and Media Engineering Properties for Hydrogen Energy Storage

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Fiscal Year (FY) 2011 Objectives

- Perform vehicle-level modeling and simulations of various storage systems configurations.
- Lead the storage system energy analysis and provide results.
- Compile and obtain media engineering properties for adsorbent materials.

Technical Barriers

This project addresses the following technical barriers from the Hydrogen Storage section of the Fuel Cell Technologies Program 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 solid-state 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 2015 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: 3.3 min
- Well-to-power-plant (WTPP) efficiency: 60%

FY 2011 Accomplishments

- Developed a vehicle model framework and test cycle matrix to aid in the analysis and understanding of hydrogen storage system requirements for light-duty vehicles.
- Integrated the hydrogen storage simulator (HSSIM vehicle model) with the center fuel cell and hydrogen storage models to create a model framework that could be used across the center to evaluate all storage system designs on a common basis and with consistent assumptions.
- Used the vehicle model and the center modeling framework to evaluate the performance of specific storage system designs across all material classes and assess the impact on vehicle performance.
- Performed vehicle-level tradeoff analyses to better understand the impact of key engineering designs, for example, the tradeoff between mass, onboard hydrogen storage capacity, and vehicle range.
- Used the Hydrogen Delivery Scenario Analysis Model (HDSAM) to calculate preliminary greenhouse gas (GHG) emissions and WTPP efficiency figures for baseline physical storage systems and candidate solid-state storage systems for each material class.
- Identified potential materials for analysis and provided storage system design guidance to help meet DOE storage targets with adsorbent materials.

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Introduction

Overcoming challenges associated with onboard hydrogen storage is critical to the widespread adoption of hydrogen-fueled 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. By means of systems analysis and modeling, hydrogen storage system requirements for light-duty vehicles can be assessed. With these findings and through collaboration with our Hydrogen Storage Engineering Center of Excellence (HSECoE) partners, optimal pathways for successful hydrogen storage system technology can be identified to enable future commercialization of hydrogen-fueled vehicles.

Approach

An array of tools and experience at NREL are being used to meet the objectives of the HSECoE. Specifically, extensive knowledge of multiple vehicle simulations, well-to-wheels (WTW) analysis, and optimization are being employed and integrated with fuel cell and material-based hydrogen storage system models developed by other HSECoE partners. This integrated model framework allows for the evaluation of various hydrogen storage options on a common basis. Engineering requirements are defined from these studies thus enabling the design of hydrogen storage vessels that could meet DOE performance and cost targets in a vehicle system context.

In the area of media engineering, attaining the objectives of the HSECoE relies on NREL's leadership in developing custom analytical instrumentation for hydrogen adsorbent analysis. These tools are used to thoroughly characterize hydrogen storage adsorbents so that an optimized storage vessel specific to the adsorbent material may be efficiently engineered. NREL will use these methods to analyze adsorbent materials identified by the HSECoE as holding promise for application in commercial on-vehicle refuelable hydrogen storage systems capable of meeting DOE targets.

Results

The following will provide results from work completed this year to support the HSECoE with a focus on five main tasks. In collaboration with our original equipment manufacturer (OEM) partners, NREL (1) worked on the development of a vehicle model (hydrogen storage simulator, HSSIM) and final structure of a test cycle matrix used to support the overall modeling effort; (2) worked on the integration of the vehicle model with the center fuel cell and hydrogen storage models to create a model framework; (3) worked with the systems architects to perform simulations and tradeoff studies to help with the high-level storage system design and engineering, including system sizing; (4) performed energy analysis on specific systems design being considered by the HSECoE; and (5) continued work in the area of adsorbent materials characterization and analysis.

A key result was working with the center OEMs on finalizing the test matrix that will be used to evaluate all the storage systems being considered across the center on a common basis. The test matrix was structured to evaluate the performance of the storage systems against the technical targets under standard and realistic transient driving condition. The matrix was also designed to exercise a given systems from full to empty to provide an understanding of its performance over the entire range of fill conditions. Therefore, the test cases were designed to repeat a drive cycle or set of drive cycles until the storage system being evaluated was empty. Standard drive cycles are typically not long enough to achieve this and would not even deplete a buffer tank in some systems. The important point here is that when evaluating the complex dynamics of hydrogen storage systems, this approach of repeating drive cycles to create test cases is critical to gaining the feedback necessary to refine and improve the systems.

As shown in Table 1, the center test matrix includes five test cases:

The first case combines repeats of the urban dynamometer driving schedule (UDDS) and the highway fuel economy test (HWFET) until the storage systems is depleted. This is used to determine the vehicle-level fuel economy and from that figure the vehicle range. The fuel economy is calculated using the current Environmental Protection Agency (EPA) five-cycle procedure of adjusting and weighting the UDDS and HWFET to provide one fuel economy figure that represents real-world use–it is not the raw figures that come directly from running the cycles. Similarly, the range is then calculated from the adjusted and weighted UDDS and HWFET figure and not simply the cycles miles achieved until the storage systems is empty. Again, this test matrix is key to providing a means to evaluate the fuel economy, range, and other vehicle level performance feature of the storage systems on a common and comparable basis.

Secondly, NREL worked with other center partners on the integration of the vehicle model with the fuel cell and storage systems models within a single modeling framework. Figure 1 shows a representation of the modeling framework that allows for a common and consistent evaluation of given storage systems. The key is the integration of the various storage system models with a common vehicle and fuel cell model in Simulink®. NREL played a critical role in the development and structure of this framework and helped with the coding in Simulink® to ensure reliable, accurate, and validated results.

A third activity was working the center system architects to provide high-level feedback on the performance and design of their given material systems. Figure 2 shows an example of a tradeoff study quantifying the relative range impacts resulting from changes to the storage system capacity and reductions to the vehicle glider mass. Table 2 shows the example results from the application of this type of study to a $NaAlH_4$ system.

Fourth, NREL continued to support the HSECoE by performing energy analyses on various storage system designs that have become available. These analyses provide the center system architects and other partners with high-level estimates about the overall energy inputs required by a given system, including WTPP efficiency (%), hydrogen cost ($/kg) and GHG emissions (carbon dioxide equivalent) on a gram per mile basis.

Fifth, the HDSAM I was used to estimate the above parameters for each system. To date the HDSAM model has been run for $NaAlH_2$ metal hydride system and the AX-21

TABLE 1. Test Matrix used Across the Center to Evaluate the Performance of all the Storage Systems

Case	Test Schedule	Cycles	Description	Test Temp (°F)	Distance per cycle (miles)	Duration per cycle (minutes)	Top Speed (mph)	Average Speed (mph)	Max. Acc. (mph /sec)	Stops	Idle	Avg. H2 Flow (g/s)*	Peak H2 Flow (g/s)*	Expected Usage
1	Ambient Drive Cycle - Repeat the EPA FE cycles from full to empty and adjust for 5 cycle post-2008	UDDS	Low speeds in stop-and-go urban traffic	75 (24 C)	7.5	22.8	56.7	19.6	3.3	17	19%	0.09	0.69	1. Establish baseline fuel economy (adjust for the 5 cycle based on the average from the cycles) 2. Establish vehicle attributes 3. Utilize for storage sizing
		HWFET	Free-flow traffic at highway speeds	75 (24 C)	10.26	12.75	60	48.3	3.2	0	0%	0.15	0.56	
2	Aggressive Drive Cycle - Repeat from full to empty	US06	Higher speeds; harder acceleration & braking	75 (24 C)	8	9.9	80	48.4	8.46	4	7%	0.20	1.60	Confirm fast transient response capability – adjust if system does not perform function
3	Cold Drive Cycle - Repeat from full to empty	FTP-75 (cold)	FTP-75 at colder ambient temperature	-4 (-20 C)	11.04	31.2	56	21.1	3.3	23	18%	0.07	0.66	1. Cold start criteria 2. Confirm cold ambient capability – adjust if system does not perform function
4	Hot Drive Cycle - Repeat from full to empty	SC03	AC use under hot ambient conditions	95 (35 C)	3.6	9.9	54.8	21.2	5.1	5	19%	0.09	0.97	Confirm hot ambient capability - adjust if system does not perform function
5	Dormancy Test	n/a	Static test to evaluate the stability of the storage system	95 (35 C)	0	31 days	0	0	0	100%	100%			Confirm loss of useable H2 target

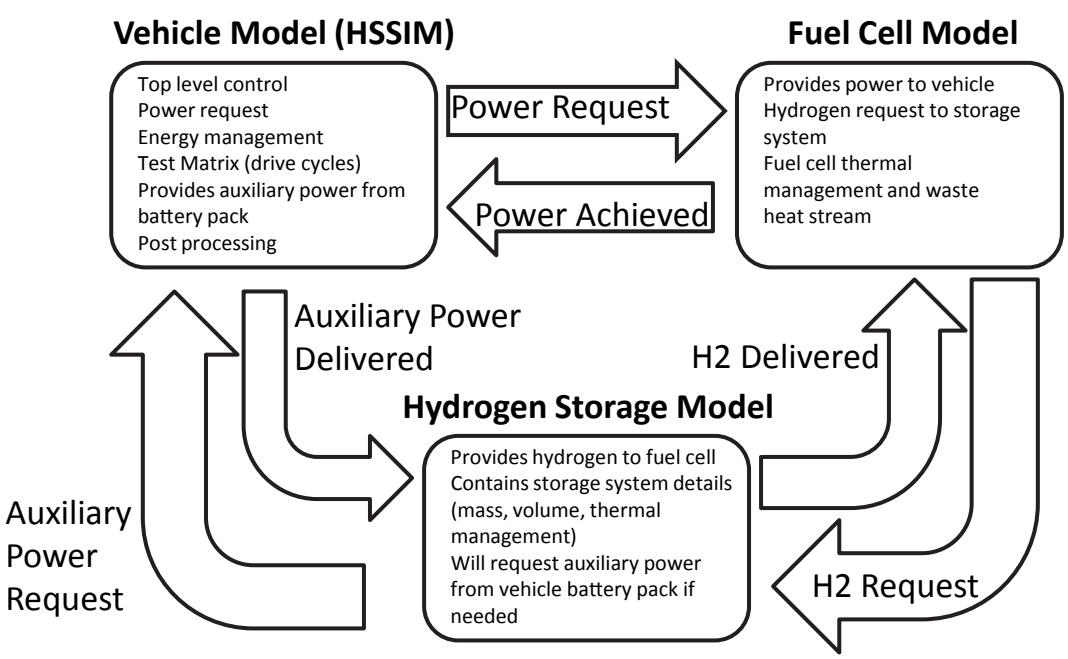

FIGURE 1. HSECoE Integrated Modeling Framework

and MOF-5 adsorbent systems to produce preliminary WTPP efficiency, GHG emissions, and hydrogen cost figures. NREL is currently working with the center adsorbent, metal hydride, and chemical hydride system architects to obtain these data and perform HDSAM runs for a liquid ammonia-borane and TiCr(Mn)H_2 systems.

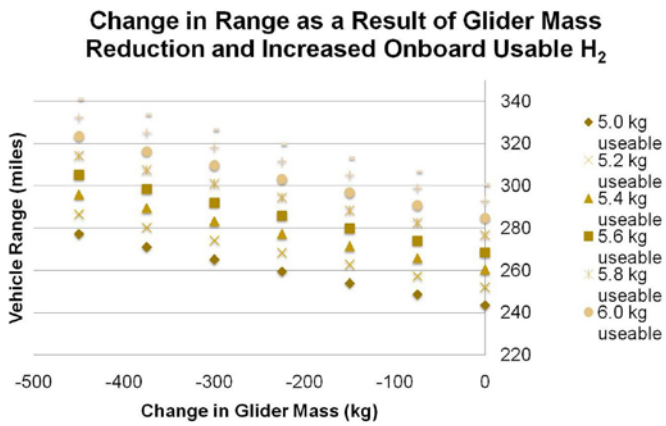

FIGURE 2. Example Storage System Design Tradeoff Study Results

TABLE 2. Example Storage System Design Trade-Off Study Results for a $NaAlH_4$ System

Vehicle Results	Units	$NaAlH_4$	$NaAlH_4$	$NaAlH_4$
Usable H_2	kg	5	6.4	5.6
Glider Mass	Kg	900	900	450
Vehicle Mass	kg	1791	1924	1398
UDDS Fuel Economy	mi/kg-H_2	46.6	44.9	52.6
HWFET Fuel Economy	mi/kg-H_2	51.5	49.8	57.0
Combined Fuel Economy	mi/kg-H_2	48.7	47.0	54.5
Range	miles	244	301	305
0 – 60 mph time	sec	10.8	11.3	9.3

For media engineering, NREL provided the HSECoE with specific engineering properties on adsorbent materials that were recommended as potential candidates for which to perform additional engineering analyses. These included high specific surface area (SSA) materials with high bulk densities, and searching for materials with higher than 10 kJ/mol hydrogen binding energies. Initially, this involved investigating representative materials that have more idealized and controlled pore sizes (in the range of 0.7 to 1.5 nm) such as pyrolized polyether-ether-ketone (PEEK) materials. As shown in Figures 3 and 4, these types of materials can be pressed to very high pressures (100,000 psi) with no significant loss of specific surface area or hydrogen storage capacities. At these pressures, bulk densities ranging from 0.7 to 1.5 g/mL can be achieved (Figure 3), resulting in substantial increases in Gibbs excess volumetric capacities (i.e., 40 to 80 g-H_2/L, see Figure 4). Thus, even though these materials may not have as high of Gibbs excess gravimetric capacities as metal-organic frameworks (Figure 3), due to their bulk densities being 2 to 5 times higher, their Gibbs excess volumetric capacities can be 2 to 4 times higher.

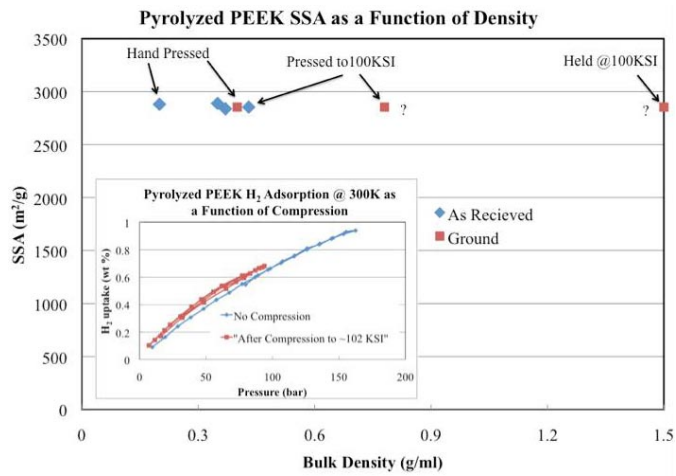

FIGURE 3. Engineering data of pyrolyzed PEEK materials demonstrating that very high bulk densities can be achieved with virtually no loss of SSA or hydrogen storage capacity.

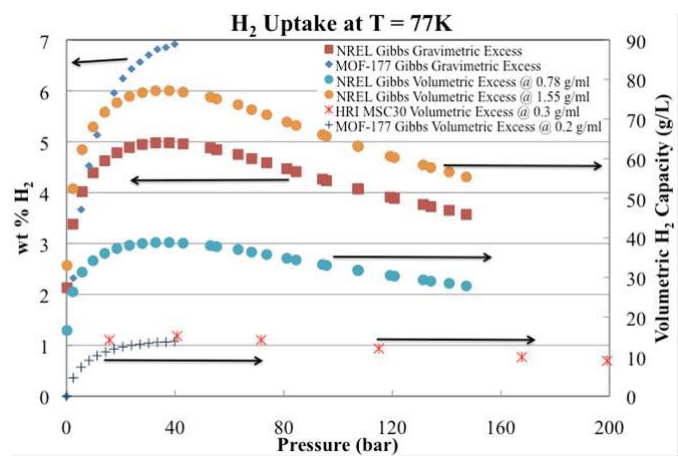

FIGURE 4. Engineering data for pyrolyzed PEEK that shows that volumetric capacity goals can be met with optimized pore size materials, much more easily than with lower bulk density materials such as MOFs.

Future Direction

- Continue to run vehicle simulations to support engineering design and support the center modeling framework refinements and enhancements:
  - Run vehicle simulations to support high-level storage system design and engineering tradeoffs.
  - Run vehicle simulations to support storage systems sizing analyses.
- Evaluate storage system impacts on vehicle performance (e.g., fuel economy, range).
- Evaluate storage system progress toward tech targets Run HDSAM to evaluate (liquid ammonia-borane and TiCr(Mn)H_2 systems:

  - WTPP efficiency
  - GHG emissions
  - H_2 cost
- Investigate adsorbent materials that enable high near-ambient temperature storage capacities including Pt/AC-IRMOF 8.

FY 2011 Publications/Presentations

1. Development of Heterogeneous Sorbents/ Sorbent Isotherm Measurement Materials Exchange, L.J. Simpson (invited talk), DOE LANL-AIST Hydrogen Workshop, September 17–20, 2010, San Francisco, CA.

2. Update of Sorbent Engineering Property Development Activities, L.J. Simpson (invited talk) DOE HSECoE Face-to-Face Architects Meeting, USCAR, September 17, 2010. Southfield MI.

3. Evaluation of Hydrogen Storage System Characteristics for Light-Duty Vehicle Applications (poster), M. Thornton, K. Day, and A. Brooker, National Hydrogen Association Conference & Expo, May 6, 2010, Long Beach, CA.

4. Evaluation of Hydrogen Storage System Characteristics for Light-Duty Vehicle Applications (poster), M. Thornton, K. Day and A. Brooker, World Hydrogen Energy Conference 2010, May 16, 2010, Essen, Germany.

5. Update of Sorbent Engineering Property Development Activities, L. J. Simpson (invited talk) DOE HSECoE Face-to-Face Meeting, PNNL, WA, October, 4–5, 2010.

6. A System Modeling Approach for Light-Duty Vehicle and On-Board Hydrogen Storage System, M. Thornton, K. Day, and A. Brooker, 2010 AIChE Annual Meeting, November 8, 2010, Salt Lake City, UT.

7. System Design, Analysis, Modeling, and Media Engineering Properties for Hydrogen Energy Storage, M. Thornton, DOE Annual Merit Review Meeting, May 11, 2011, Washington, D.C.