IV.B.5 System Design, Analysis, Modeling, and Media Engineering Properties for Hydrogen Energy Storage

Matthew Thornton (Primary Contact), Lin Simpson, Aaron Brooker, and Jonathon Cosgrove
National Renewable Energy Laboratory (NREL)
1617 Cole Boulevard
Golden, CO 80401
Phone: (303) 275-4273
Email: Matthew.Thornton@nrel.gov

DOE Managers
Ned Stetson
Phone: (202) 586-9995
Email: Ned.Stetson@ee.doe.gov
Jesse Adams
Phone: (720) 356-1421
Email: Jesse.Adams@go.doe.gov

Subcontractors:
- Strategic Analysis Inc., Arlington, VA
- Mark Paster, Annapolis, MD

Project Start Date: February 2, 2009
Project End Date: June 30, 2015

Overall and Fiscal Year (FY) 2013 Objectives

- Perform vehicle-level modeling and simulations of various storage system 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 Office 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) System 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 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 efficiency: 60%

FY 2013 Accomplishments

- Used the vehicle model and the center modeling framework, developed in previous years, to evaluate the performance of specific storage system designs across all material classes and assess the design impacts on vehicle performance to help guide specific system designs and focus engineering solutions that will overcome barriers to meeting technical targets.
- 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 Hydrogen Delivery Scenario Analysis Model (HDSAM) to calculate preliminary greenhouse gas (GHG) emissions and well-to-power plant (WTPP) efficiency figures for baseline physical storage systems and candidate materials-based storage systems for each material class.
- Applied an array of measurement techniques to provide engineering properties of sorbent materials.

✧ ✧ ✧ ✧ ✧

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 adsorption analysis. These tools are used to thoroughly characterize hydrogen storage adsorbents so that an optimized storage vessel specific to the adsorption material may be efficiently engineered. NREL uses these methods to analyze adsorption 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 three main tasks. In collaboration with our original equipment manufacturer (OEM) partners, NREL (1) worked with the system architects to perform simulations and tradeoff studies to help with the high-level storage system designs and engineering, including mass and volume trade-offs; (2) performed energy analysis on specific system designs being considered by the HSECoE; and (3) continued work in the area of adsorbent materials characterization and analysis.

To gain a better understanding of the interactions that exist between various materials-based hydrogen storage systems and the vehicle system as well as the engineering challenges that exist when integrating one of these systems with a vehicle, NREL developed a vehicle-level model designed to be sensitive to these issues. In previous work under the HSECoE, the Hydrogen Storage SIMulator (HSSIM) was developed as a specialized tool that could be used to assist in the design and engineering of materials-based hydrogen storage systems being considered by the HSECoE. This tool was designed to not only allow for understanding key trade-offs, but also to have a seamless integration with the HSECoE fuel cell and detailed hydrogen storage system models and to evaluate progress towards the U.S. Department of Energy's hydrogen storage technical targets. This model has been integrated with a fuel cell model developed by Ford Motor Company in a HSECoE common modeling framework developed by United Technologies Research Center and other HSECoE partners (Figure 1).

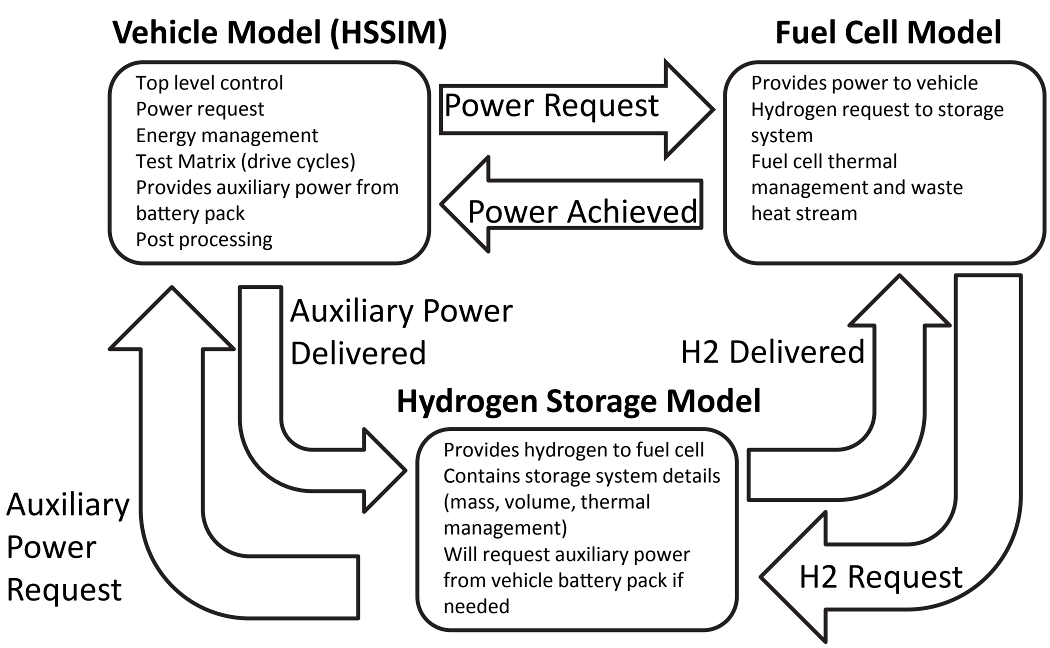

FIGURE 1. HSECoE Integrated Modeling Framework

The HSSIM vehicle model is designed to evaluate high-level attribute improvements. To accomplish this, the inputs, such as the glider and powertrain components, are also defined at a high level. The vehicle glider is defined with a specific frontal area, drag coefficient, mass, center of gravity, front axle weight fraction, and wheelbase. The wheels are defined by inertia, a rolling resistance coefficient, coefficient of friction, and radius. The inputs for the motor are power, peak efficiency, mass per unit of power, cost per unit of power, and time to full power. The battery inputs include power, energy, mass per unit of energy, and round trip efficiency. Auxiliary loads are assumed to be a specified constant plus an amount required for the fuel cell and hydrogen storage systems. These inputs match the DOE's technical target units, such as battery kilograms per kilowatt hour, so that the impact of improvements can be evaluated over time as the targets change.

A key part of developing the vehicle model was working with the center OEMs on developing a 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 conditions. The matrix was also designed to exercise a given system 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 system is depleted. This is used to determine the vehicle-level fuel economy (FE) 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 figures and not simply the cycles' miles traveled until the storage system is empty. Again, this test matrix is key to providing a means to evaluate the fuel economy, range, and other vehicle-level

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

performance features of the storage systems on a common and comparable basis.

NREL used these model outputs from the framework to evaluate the current status of various adsorbent and chemical hydrogen storage material-based systems being evaluated by the HSECoE. Because this work is in progress, the results presented here are preliminary and may change over time as the storage systems are refined and the models are adjusted accordingly. That is, the intent is to show how the model outputs can be used to evaluate and compare different storage systems and support engineering solutions to particular barriers. The intent, at least at this time, is not to develop an argument for which system or materials class has the most promise for actual vehicle application. Vehicle-level results will be presented for a select group of these systems (i.e., this is not a comprehensive set of systems being evaluated under the HSECoE, nor is it a complete set of storage models included in the framework). For the model application, example results discussed in this section's simulations were run with several adsorbent and chemical hydrogen storage material systems being evaluated for phase III of the project and include HexCell powder MOF-5 and MATI Puck MOF-5 (0.32 g/cc) adsorbent systems and the ammonia-borane slurry and alane slurry chemical hydrogen storage material systems. In addition, a 700-bar compressed gas system was included for comparison to the materials-based systems.

For the following discussion, model applications and results reported are based on Test Case 1 of the framework exclusively (i.e., UDDS and HWFET combined test cycles). In addition, a midsize car class was selected for the initial baseline simulations within the framework. The intent was to be representative of a high-sales-volume midsize car, such as the Ford Fusion, Chevrolet Malibu, or Toyota Camry. The attributes associated with this size vehicle are a frontal area of 2.2 m^2, drag coefficient of 0.29, and tire size of P195/65R15. The electric motor was sized to 100 kW with 85% efficiency from the motor to the road. Consistent with most fuel cell vehicles, the vehicle includes a 20-kW/1-kWh battery pack for hybridization for capturing regenerative braking and assistance with propulsion. The state of charge of the battery is maintained between 40% and 80%, with the target state of charge varying throughout the cycle depending on driving conditions. The vehicle glider weight (excluding the hydrogen storage system and other drive components) is 1,104 kg. The motor and power electronics combined weight is 105 kg, the battery system weight is 51 kg, the fuel cell system with cooling weight is 214 kg, and the hydrogen storage system weight varied. All of the following results are based on the vehicle configuration above, but the model is capable of simulating both larger and smaller vehicle classes and configurations.

For the example systems included in Table 2, the fuel economy for materials-based systems ranged from 49/48 miles per gasoline gallon equivalent (mpgge) for the MOF-5 systems to 44 mpgge for the alane slurry system. The alane slurry system performed the worst in terms of fuel economy due to its onboard endothermic nature. The system burns hydrogen to create the needed temperatures for the storage system hydrogen release and storage system thermal management. The use of hydrogen for system thermal management results in poor onboard efficiency and, subsequently, poor fuel economy. The ammonia-borane slurry and MOF-5 systems performed better in this example due to their high gravimetric efficiency, resulting in lower overall system and vehicle mass and therefore better fuel economy. As a result, the MOF-5 systems also offer the best range results of 274/269 miles based on the above vehicle configuration and 5.6 kg nominal usable hydrogen storage capacity. The compressed gas systems demonstrated slightly better, but comparable fuel economy and range relative to these example material-based systems.

The ammonia-borane slurry chemical hydrogen storage material system had a gravimetric density of 4.2 weight percent (i.e., the percent of hydrogen mass to the overall storage system mass; the DOE 2017 technical target for gravimetric density is 5.5 weight percent). This was the best-performing materials-based system and was comparable to the compressed gas system, which had a gravimetric density of 4.7 weight percent. That said, the ammonia-borane slurry system outperformed the compressed gas systems and all of the other materials-based systems in terms of volumetric density with nearly 37 g of hydrogen per system liter. The

TABLE 2. Vehicle-Level Performance Summary

Hydrogen Storage System	Adjusted Fuel Economy (mpgge)	Range (mi)	Onboard Efficiency (%) UDDS/HFET	Gravimetric Density (wt%)	Volumetric Density (g/l)	System Mass (kg)
Exothermic Ammonia-Borane Slurry	47	264	97	4.2	36.8	137.1
Endothermic Alane Slurry	44	244	93	3.4	34.3	185.1
HexCell Powder MOF-5	49*	274*	92**	3.5	17.5	137.6
MATI Puck MOF-5 (0.32 g/cc)	48*	269*	97**	3.4	20.7	149.3
700-bar Compressed Gas	50	279	100	4.7	25.0	119.0

*Preliminary Model Results **Off Model Calculations

DOE's 2017 technical target for volumetric density is 40 g/L. For all the example materials-based systems included here, the HexCell powder MOF-5 system performed the best in terms of fuel economy, range, and gravimetric density and was comparable to the compressed gas systems. As noted, the ammonia-borane slurry system performed best in terms of volumetric density, but it is important to remember that the ammonia-borane slurry system is an off-board regenerable system that is accompanied by unique refilling challenges, logistics, and costs that are not captured in the above analysis.

NREL also continued to support the HSECoE by performing energy analyses on various storage system designs being evaluated for phase III of the project. 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 for future 2020 scenarios.

HDSAM was used to estimate the above parameters for each system. To date, the HDSAM model has been run for the HexCell powder MOF-5, MATI Puck MOF-5 (0.32 g/cc) and 60-bar 80 K gas adsorbent systems, and the ammonia-borane slurry and alane slurry chemical hydrogen storage material systems to produce preliminary WTPP efficiency, GHG emissions, and hydrogen cost figures. In addition, model runs were performed on a 700-bar compressed gas system and a cryogenic-compressed liquid hydrogen system (CcH_2, <200 K) for comparison to the materials-based systems.

Table 3 shows the storage system results (i.e., WTW cost breakdown, WTW energy breakdown, WTW GHG breakdown, and volumetric efficiency) for the two chemical hydrogen storage systems and the three adsorbent system, as well as the 700-bar compressed gas and cold gas cryogenic-compressed liquid hydrogen systems. The ammonia-borane system, which offers several onboard advantages over the alane system—an exothermic onboard reaction leads to higher onboard efficiency (96% vs. 88%)—has higher regeneration cycle costs and energy inputs. Both materials showed a higher cost and lower efficiency than the adsorbent systems and the two physical storage systems. This indicates a need for advancements and cost reductions for chemical hydrogen storage material systems in general. This analysis supports the need for additional research focused on reducing the cost of chemical hydrogen storage material off-board regeneration cycles in order for these systems to be viable. The adsorbent systems performed better than the chemical hydrogen storage material systems in terms of cost, energy, and GHG emissions, but were still higher in all of these areas then the physical storage systems and also require additional advancements in order to compete with the incumbent systems.

NREL wrapped up the media engineering support component of the work early in the year. This work primarily involved completing an initial analysis of MOF-5 at temperatures below 77 K. The initial results suggest that the present model predictions for the hydrogen storage properties as a function of pressure of MOF-5 at these temperatures are reasonable. Based on this initial assessment, the effort was stopped to enable more focus on model transfer for public access. A set of plans for improving the cryostat-based low-temperature measurements and improving overall accuracy was developed and can be implemented in the future should measurements with temperatures below 77 K be needed in the future for advanced sorbent materials.

FUTURE DIRECTIONS

- 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 system sizing analyses.

TABLE 3. WTW Results Summary

	WTW H_2 Cost ($/kg-$H_2$)	WTW Energy Efficiency (%)	WTW GHG Emissions (g/mile)	Volumetric Efficiency (gms-H_2/L)
2020 700-bar Gas - T520*	3.91	56.4	230	25.6
2020 CcH_2 - Liquid H_2 Truck	4.49	46.5	289	41.8
2020 Liquid Ammonia-Borane	13.96	16.5	915	41.4
2020 Liquid Alane	7.89	24.7	642	32.2
2020 Absorbent 1 60-bar 80 K Gas-T340	5.92	40.4	401	24.1
2020 Absorbent HexCell 100-bar 80 K Gas-T340**	6.16	39.2	412	17.5
2020 Absorbent MATI 100-bar 80 K Gas-T340**	5.69	42.1	391	20.7

*T520, 520 Bar Insulated Tube Truck; **T340, 340 Bar Insulated Tube Truck

- Evaluate storage system impacts on vehicle performance (e.g., fuel economy, range).
- Work with HSECoE partners to make center-developed models available and accessible to the broader research and academic community through a controlled web-based access portal.

FY 2013 PUBLICATIONS/PRESENTATIONS

1. System Design, Analysis, Modeling, and Media Engineering Properties for Hydrogen Energy Storage, Matthew Thornton, DOE Annual Merit Review Meeting, May 14, 2013, Washington, D.C.