IV.B.1 Hydrogen Storage Engineering Center of Excellence

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- United Technologies Research Center, East Hartford, CT
- General Motors, Warren, MI
- Ford Motor Company, Dearborn, MI
- National Renewable Energy Laboratory, Golden, CO
- Los Alamos National Laboratory, Los Almaos, NM
- Jet Propulsion Laboratory, Pasadena, CA
- University of Michigan, Ann Arbor, MI
- California Institute of Technology, Pasadena, CA
- Oregon State University, Corvallis, OR
- Hexagon Lincoln LLC, Lincoln, NE
- Université du Québec a Trios-Rivieres, Trois-Rivieres, QC, Canada

Project Start Date: February 1, 2009
Project End Date: December 31, 2016

Overall Objectives

- Develop system models that will lend insight into overall fuel cycle efficiency.
- Compile all relevant materials data for candidate storage media and define future data requirements.
- Develop engineering and design models to further the understanding of onboard storage energy management requirements.
- Develop innovative onboard system concepts for metal hydride, chemical hydrogen storage materials, and adsorbent materials-based storage technologies.
- Design components and experimental test fixtures to evaluate the innovative storage devices and subsystem design concepts, validate model predictions, and improve both component design and predictive capability.
- Design, fabricate, test, and decommission the subscale prototype components and systems of each materials-based technology (adsorbents, metal hydrides, and chemical hydrogen storage materials).

Fiscal Year (FY) 2016 Objectives

- Coordination and facilitation of partner's activities.
- Complete evaluation of a 2-L adsorbent subscale prototype utilizing a HexCell heat exchange system.
- Complete evaluation a 2-L adsorbent subscale prototype utilizing a Modular Adsorbent Tank Insert (MATI) heat exchange system.
- Validated thermo-physical models of the mass and heat flow for a flow through adsorbent subscale prototype system.

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

(D) Durability/Operability

(E) Charging/Discharging Rates

(G) Materials of Construction

(H) Balance of Plant Components

(J) Thermal Management

(K) System Life Cycle Assessments

(L) High Pressure Conformality

(P) Lack of Understanding of Hydrogen Physisorption and Chemisorption

(S) By-Product/Spent Material Removal

Technical Targets

The projected scaled performance of the two adsorption systems, HexCell and MATI, being evaluated are given in Table 1 in comparison to the technical targets.

FY 2016 Accomplishments

- Completed characterization experiments of metal organic framework (MOF)-5 on the flow through subscale prototype system and model validation.

TABLE 1. System Status vs. Technical Targets for the Cryo-Adsorbent System

Target	Units	2020 DOE Goal (System)	Ultimate DOE Goal (System)	Projected Scaled HexCell (System)	Projected Scaled MATI (System)
Gravametric Capacity	kg H_2/kg system	0.055	0.075	0.0321	0.315
Volumetric Capacity	kg H_2/L system	0.04	0.07	0.019	0.021
System Cost	\$/kg H_2 stored	333	266	486	516
Fuel Cost	\$/gge at pump	2-4	2-4	6	6
Min. Operating Temp	°C	-40	-40	-40	-40
Max. Operating Temp	°C	60	60	60	60
Min. Delivery Temp	°C	-40	-40	-40	-40
Max. Delivery Temp	°C	85	85	85	85
Cycle Life	Cycles	1500	1500	1500	1500
Min. Delivery Pressure	bar	5	3	5	5
Max. Delivery Pressure	bar	12	12	12	12
Onboard Efficiency	%	90%	90%	90%	97%
Well to Power Plant Efficiency	%	60%	60%	40%	40%
System Fill Time	min.	3.3	2.5	3.3	3.3
Min. Full Flow Rate	(g/s/kW)	0.02	0.02	0.02	0.02
Start Time to Full Flow (20°C)	sec.	5	5	5	5
Start Time to Full Flow (-20°C)	sec.	15	15	15	15
Transient Response	sec.	0.75	0.75	0.75	0.75
Fuel Purity	%H_2	99.97	99.97	99.99	99.99
Permeation, Toxicity, Safety	-	Meets or Exceeds Standards	Meets or Exceeds Standards	Meets or Exceeds Standards	Meets or Exceeds Standards
Loss of Useable Hydrogen	(g/h)/kg H2 stored	0.05	0.05	0.81	0.69

gge – Gasoline gallon equivalent

- Completed characterization experiments of MOF-5 on the MATI subscale prototype system.
- Completed validation of the HexCell and MATI vehicle-level system models.

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INTRODUCTION

The Hydrogen Storage Engineering Center of Excellence brought together all of the materials and hydrogen storage technology efforts to address onboard hydrogen storage in light-duty vehicle applications. The effort began with a heavy emphasis on modeling and data gathering to determine the state-of-the-art in hydrogen storage systems. This effort spanned the design space of vehicle requirements, power plant and balance of plant requirements, storage system components, and materials engineering efforts. These data and models were then used to design components and subscale prototypes of hydrogen storage systems which were evaluated and tested to determine the status of potential system against the DOE 2020 and ultimate technical targets for hydrogen storage systems for light-duty vehicles.

APPROACH

A team of leading North American national laboratories, universities, and industrial laboratories, each with a high degree of hydrogen storage engineering expertise cultivated through prior DOE, international, and/or privately sponsored programs was assembled to study and analyze the engineering aspects of condensed phase hydrogen storage as applied to automotive applications. The technical activities of the center were divided into three system architectures: adsorbent, chemical hydrogen storage, and metal hydride matrixed with six technologies areas: Performance Analysis, Integrated Power Plant/Storage System Analysis, Materials Operating Requirements, Transport Phenomena, Enabling Technologies and Subscale Prototype Construction, and Testing and Evaluation. The program was divided into three phases: Phase 1 – System Requirements and Novel Concepts, Phase 2 – Novel Concept Modeling Design and Evaluation, and Phase 3 – Subscale System Design, Testing, and Evaluation.

RESULTS

HexCell Prototype

The experimental measurements on the 2-L HexCell prototype using tap density MOF-5 adsorbent at a density of 0.19 g/cc system were completed. Model validation utilizing the experimental results have been carried out for the flow-through system at Savannah River National Laboratory. Table 2 lists the experimental work completed on the HexCell system with data model validation noted.

Figure 1 illustrates the model and experimental data for the HexCell prototype. For each thermocouple measurement, the numerical values closely parallel the experimental data to within 10°C for charging and to within 15°C for discharging. All changes in temperature were fully captured by the models and thus all relevant physical phenomena are taken into consideration. Existing temperature differences are most likely due to thermocouple placement error, and non-uniform packing of the adsorbent media.

In addition to static charging and discharging, dynamic full system cycling was performed to evaluate material capacity over several cycles. A total of 24 consecutive cycles over a pressure range of 5–60 bar were performed with no observed degradation in storage capacity via total standard liters of hydrogen required to reach maximum operational pressure as shown in Figure 2.

TABLE 2. Experimental Work Completed on the HexCell System

	Test	H_2 flow (SLPM)	P_{max} (bar)	Min H_2 Temp (K)	Max Bed Temp (K)
Adsorption	Static charge	200	40, 80	110	
	Flow-through cooling	100*, 500 , 1000	17, 40*, 80*	110	
Desorption	Without heat	11, 25	40, 80		160
	With heat	11*, 25, 50, 100	40*, 80*		160

* HexCell systems with data model validation

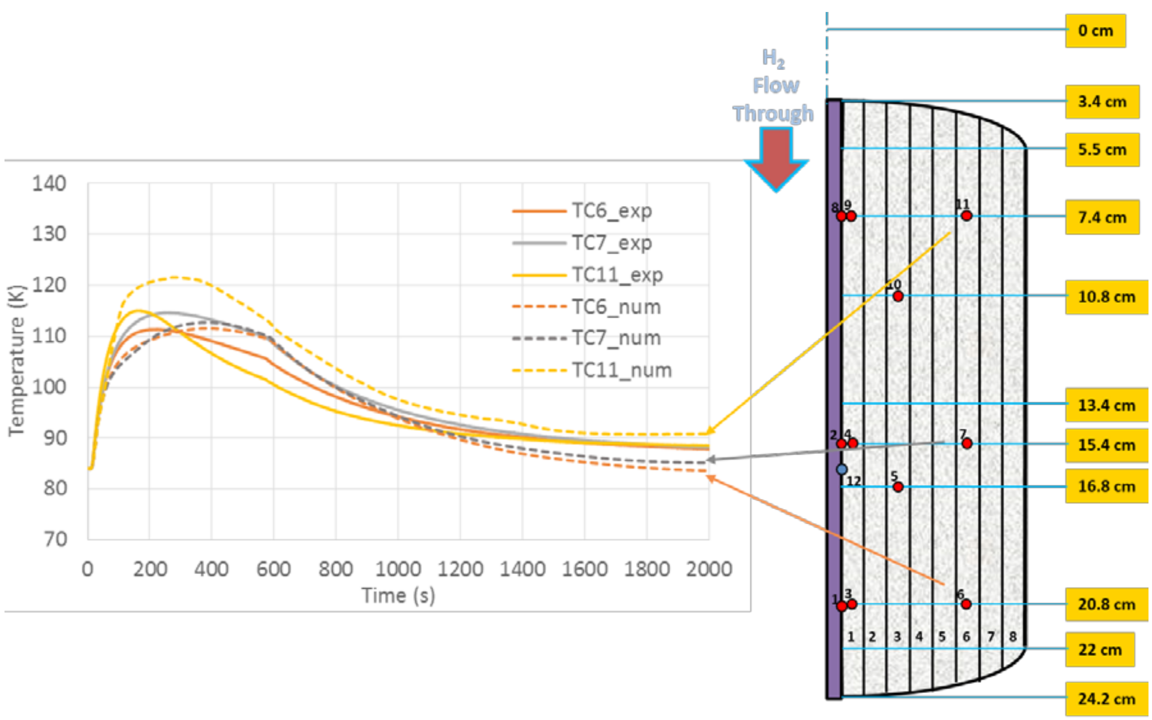

FIGURE 1. Charging of MOF-5 powder in the HexCell flow-through storage system, experimental and numerical data compared

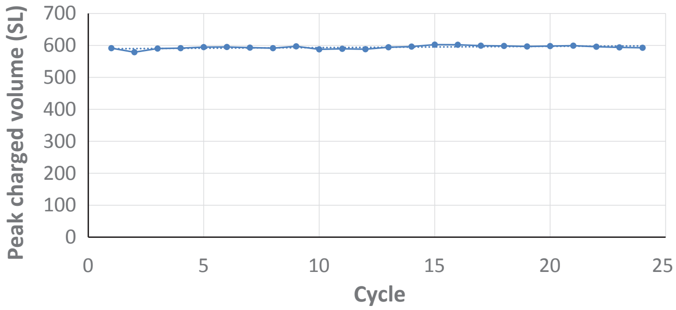

FIGURE 2. Consecutive cycling of the flow-through HexCell MOF-5 hydrogen storage system

MATI Prototype

Final experimental tests were performed on the 2-L MATI prototype system utilizing compacted MOF-5 pucks having a volumetric density twice that of the tap density powder used in the HexCell system at 0.40 g/cc. Table 3 lists the set of half-cycles (charging and discharging) experimental work performed on the MATI prototype system.

In total, over 100 different measurements were performed on the MATI prototype system. In addition, consecutive cycling testing was also conducted, as outlined in Table 4. A representative set of adsorption half cycle data is shown if Figure 3 for hydrogen flows of 150 slpm and 300 slpm. The charging time of technical target of 3 min was achieved at a flow of 300 slpm.

Unlike the HexCell system, the 2-L MATI prototype system could only be run through 9–10 consecutive cycles due to gas volume restrictions within the laboratory. However, the MATI prototype system was cycled not only in the range of 5–60 bar, but also 5–100 bar (100 bar cycling limited the number of consecutive cycles even less). Results for both 60 bar and 100 bar cycling showed similar results. Figure 4 illustrates the cycling capacities for both charging and discharging over eight cycles. No apparent change in capacities was observed through the cycles tested.

Adsorbent System Comparison

Using the experimental and modeling data presented above, the adsorbent storage systems were compared within the vehicle framework. Table 5 shows the subscale prototype experimental results and projected full-scale 5.6 kg hydrogen systems based on the validated models. Note that only the adsorbent and heat exchanger portions of the model were validated using the 2-L prototypes, while the tank sizing tool and the balance of plant estimates were validated/updated based on the latest information from other Hydrogen Storage Engineering Center of Excellence sources.

The adsorbent storage system comparisons are listed in Table 5, which includes columns for the 0.19 g/cc powder MOF-5 HexCell heat exchanger storage system design, and the 0.4 g/cc compacted MOF-5 MATI heat exchanger storage system design. The rows shown in Table 5 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.

TABLE 3. List of the Half Cycle (Charging and Discharging) Experiments Performed on the 2-L MATI Prototype System

Test	P_{min} (bar)	$P_{max(c)}$ (bar)	$P_{max(v)}$ (bar)	H_2 flow (SLPM)	N_2 Flow (SLPM)
Adsorption	1, 5	60, 80, 100	60, 100	0, 50, 100, 150, 200, 300	0, 50, 100, 150, 200
Desorption	1, 5	60, 80, 100		0, 50, 100, 150	0, 50, 100, 150, 200

TABLE 4. List of the Cycling Experiments Performed on the 2-L MATI Prototype System

Test	Consecutive Cycles	Total Cycles	H_2 flow (SLPM)	N_2 Flow (SLPM)
5 to 60 bar cycling	9-10	20	300	150
5 to 100 bar cycling	3	6	130	150

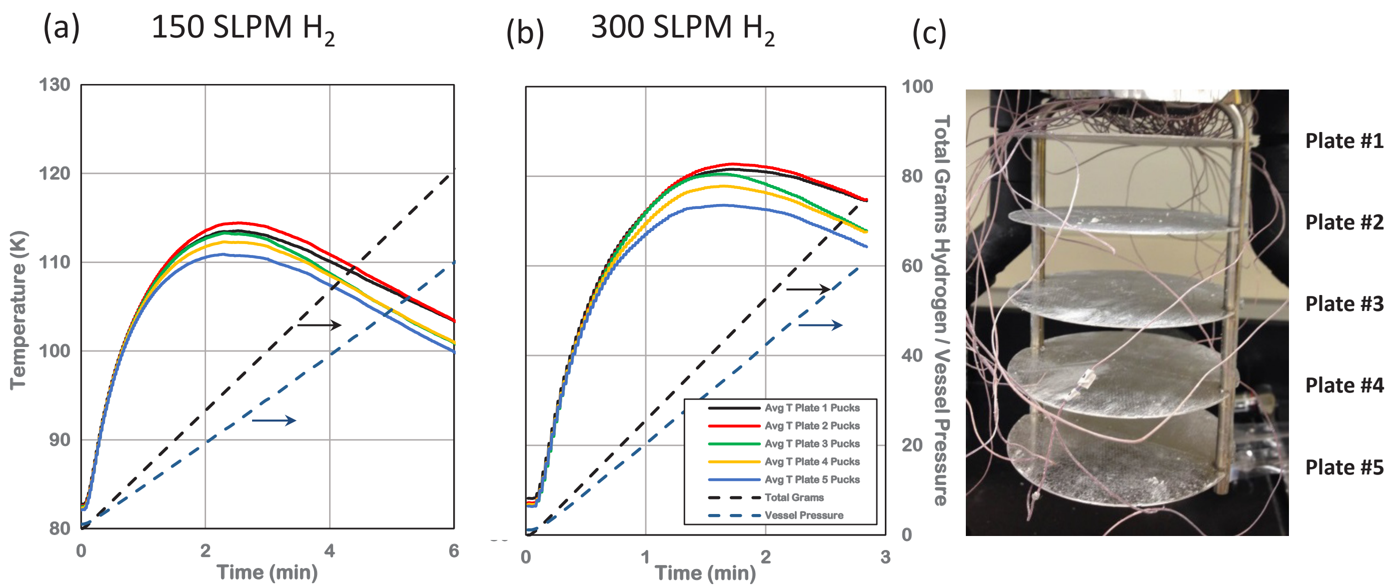

FIGURE 3. Temperature profiles for 2-L MATI prototype charging experiments at hydrogen flows of (a) 150 slpm, (b) 300 slpm, and (c) plate geometry

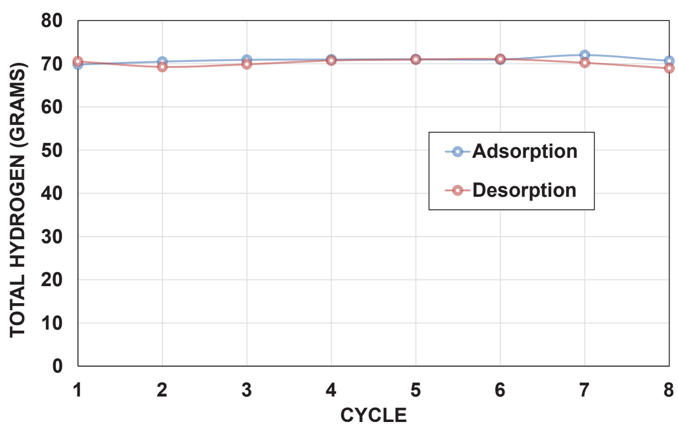

FIGURE 4. Total capacity of hydrogen (in during adsorption or out during desorption) during the 2-L MATI prototype cycling experiments between 5 bar and 60 bar

TABLE 5. HexCell and MATI Adsorbent Storage System Comparisons

	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

HX – Heat exchanger

CONCLUSIONS AND FUTURE DIRECTIONS

The prototype experiments, including the cycling experiments described above, have been completed for both the 2-L HexCell and 2-L MATI prototype systems. The systems performed repeatable and within design specification. The detailed heat and mass transfer computational models for the HexCell system have been validated against experimental data and found to capture all relevant physical phenomena to within 15°C. In addition, the vehicle-level system models for both the HexCell and MATI systems have been used to predict full-scale 5.6 kg H_2 automotive systems. These projections have shown the high density compacted MOF-5 adsorbent utilizing a MATI heat exchanger would surpass a 700 bar Type 4 compressed gas tank in volumetric capacity, and the low density MOF-5 adsorbent system utilizing the HexCell heat exchanger would beat it in cost.

Future technical work will include:

- Characterize the fluid-flow inequality between the five plates of the MATI internal heat exchanger.
- Create and validate detailed models of the MATI prototype system based on the prototype experimental results described above.
- Update the Simulink cryo-adsorbent system models so new materials can be tested within it to predict their full-scale system performance.