IV.D.9 Ford/BASF-SE/UM Activities in Support of the Hydrogen Storage Engineering Center of Excellence

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Fiscal Year (FY) 2011 Objectives

This project addresses three of the key technical obstacles associated with the development of a viable hydrogen storage system for automotive applications:

- (Task 1) Create accurate system models that account for realistic interactions between the fuel system and the vehicle powerplant.
- (Task 2) Develop robust cost projections for various hydrogen storage system configurations.
- (Task 3) Assess and optimize the effective engineering properties of framework-based hydrogen storage media (such as metal-organic frameworks, MOFs).

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
(D) Durability/Operability
(E) Charging/Discharging Rates
(H) Balance of Plant (BOP)
(J) Thermal Management

Technical Targets

The outcomes of this project affect vehicle and system level models, cost analysis, and materials property assessment/optimization. Insights gained from these studies are applied towards the engineering of hydrogen storage systems that meet the following DOE 2010 and ultimately 2015 hydrogen storage targets shown in Table 1.

TABLE. DOE Hydrogen Storage Targets

Storage Parameter	Units	2010	2015
System Gravimetric Capacity	kg·H_2/kg	0.045	0.055
System Volumetric Capacity	kg·H_2/L	0.028	0.040
Storage System Cost	\$/kWh_{net}	To Be Determined	To Be Determined
System Fill Time (for 5 kg H_2)	min	4.2	3.3
Minimum Full Flow Rate	(g/s)/kW	0.02	0.02
Min/Max Delivery Temperature	ºC	-40/85	-40/85
Min. Delivery Pressure (Fuel cell)	atm	4	3

FY 2011 Accomplishments

Below is a list of accomplishments by task:

- Task 1. System Modeling
  - Evaluated and constructed baseline fuel cell model to support the interaction with the vehicle and hydrogen storage system model.
  - Completed classification of the 2010 and 2015 DOE hydrogen storage targets for optimization and tradeoff analysis amongst the storage system concepts.
  - Developed a common set of drive-cycles for vehicle simulation performance evaluations.

- Task 2. Cost Analysis
  - Supported the manufacturing and cost analysis technology team in the evaluation of the initial cost assessments for the hydrogen storage systems.
  - Established initial phase of cost analysis through the development of a component cost matrix.
  - Assisted in the approach of using the component library to decompose the key system elements to evaluate the cost drivers and establishing cost sensitivity items for future trade-offs.
- Task 3. Assessment/Optimization of Framework-Based Storage Media
  - Prepared a set of variable-density *neat* MOF-5 compacts ranging from 0.3 to 0.8 g/cm^3 which have the potential to realize significant volumetric capacity improvement as compared to the powder (ρ=0.13 g/cm^3).
  - Characterized key physical and mechanical properties of MOF-5 compacts including crush strength, Brunauer-Emmett-Teller (BET) surface area, and total pore volume for comparison with known sorbent data (e.g. for AX-21, polyether ether ether ketone [PEEK], MOF-177).
  - Determined excess and estimated total gravimetric and volumetric capacities for MOF-5 compacts and realized a 4× improvement in excess volumetric capacity for 0.5 g/cm^3 compact with only a small decrease (~15%) in excess gravimetric capacity (as compared to powder MOF-5).
  - Evaluated principle thermal property data (i.e. thermal diffusivity, heat capacity, and thermal conductivity) for *neat* MOF-5 compacts (e.g. k at 25°C for 0.35 g/cm^3 is 0.072 W/mK).
  - Prepared a series of variable-density MOF-5 compacts containing expanded natural graphite (ENG; 1, 5, and 10 wt% additions) as a thermal conductivity aid.
  - Evaluated preliminary thermal conductivity and surface area characteristics for ENG-containing MOF-5 compacts, revealing a 5× improvement in thermal conductivity (e.g. 0.56 W/mK for 0.5 g/cm^3 MOF-5 compact w/ 10 wt% ENG as compared to <0.1 W/mK for neat compact).
  - Designed, fabricated hardware, and completed experiment of first-time in situ characterization (via neutron imaging) of hydrogen dynamics in a cryogenic storage vessel on MOF-5 pellets.

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Introduction

Widespread adoption of hydrogen as a vehicular fuel depends critically on the development of low-cost, on-board hydrogen storage technologies capable of achieving high energy densities and fast kinetics for hydrogen uptake and release. As present-day technologies -- which rely on physical storage methods such as pressurization or liquefaction -- are unlikely to attain established DOE targets, interest in materials-based approaches for storing hydrogen have garnered increasing attention. To hasten development of these 'hydride' materials, the DOE has established three Centers of Excellence for materials-based hydrogen storage research as part of a "Grand Challenge" to the scientific community. While the Centers of Excellence have made substantial progress in developing new storage materials, significant challenges associated with the engineering of the storage system around a candidate storage material remain largely unresolved.

Approach

As a partner in the Hydrogen Storage Engineering Center of Excellence, Ford-UM-BASF is conducting a multi-faceted research project that addresses three of the key engineering challenges associated with the development of materials-based hydrogen storage systems.

Systems Modeling (Task 1): Drawing on our extensive expertise in the engineering of fuel cell (FC) and H_2 internal combustion engine (H_2-ICE) vehicles, we are evaluating and developing system engineering technical elements with a focus on hydrogen storage system operating parameters. This effort will result in a set of dynamic operating parameters and a high-level system model describing the interaction of the fuel storage system with the FC (or H_2-ICE) power plant.

Cost Analysis (Task 2): We are leveraging the unique capabilities of the "Ford/Massachusetts Institute of Technology cost model" to develop and perform hydrogen storage manufacturing cost analyses for various candidate system configurations and operating strategies. This analysis facilitates a technology roadmap for potential cost reductions and manufacturing optimization, while providing important feedback to Go/No-Go decisions on prototype design and construction.

Sorbent Media Assessment and Optimization (Task 3): We are evaluating and optimizing the "effective engineering properties" of an important class of sorbent materials (MOFs) and other framework-like materials in order to devise improved packing and processing strategies for their use in a systems context. Various mechanical processing routes are being examined (ranging from powders to pelletization to extrusion) in an effort to simultaneously maximize packing density, heat and mass transfer, and hydrogen uptake characteristics.

This work is expected to impact the broader goals for the DOE and FreedomCAR, leading to a significant advance in the engineering of materials-based hydrogen storage systems, refinement in our understanding of the performance targets of hydride materials, and ultimately, the development of commercially viable hydrogen storage systems.

Results

Following is a description of our technical results for each task and how these results relate to achieving the DOE targets.

Task 1. System Modeling

The Integrated Power Plant/Storage System Modeling Technology Area during the past year focused on the framework elements that were needed to establish simulation modeling parameters for a consistent assessment of the storage systems in support of the phase 1 milestone review. Within this year, the modeling framework was established and fully utilized to assess the multiple storage systems in a consistent manner. Further details in the powerplant models were refined such as the fuel cell stack efficiency and the associated parasitics. The fuel cell stack was sized for 80 kW net operating power at 80°C temperature. In the refinement of the model, the fuel cell system efficiency was evaluated and adjusted to be consistent with the DOE fuel cell system targets for efficiency at rated power (50%) and quarter power (60%) as shown in Figure 1.

The fuel cell model includes the essential elements to interface between the vehicle and the hydrogen storage model blocks. These elements include: the polarization curve to translate requested vehicle power to current and hydrogen flow request, parasitic power from the compressor, and stack temperature to provide the waste heat stream. Each of these elements were integrated and evaluated during this year. The polarization curve transfer functions were compared against the latest results from the general computational (GC) tool. The assessment concluded that an additional effect for temperature would be added to the Hydrogen Storage Engineering Center of Excellence (HSECoE) modeling framework while the GC tool effects to temperature appeared higher due to sensitivity of the future catalyst assumptions. The other activities in the modeling area included confirmation of the maximum flow condition and definition of success criteria for following the flow demand trace within the modeling simulation.

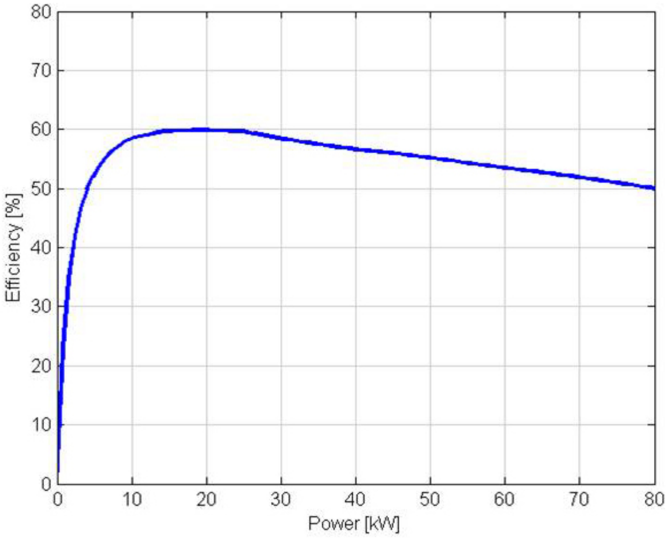
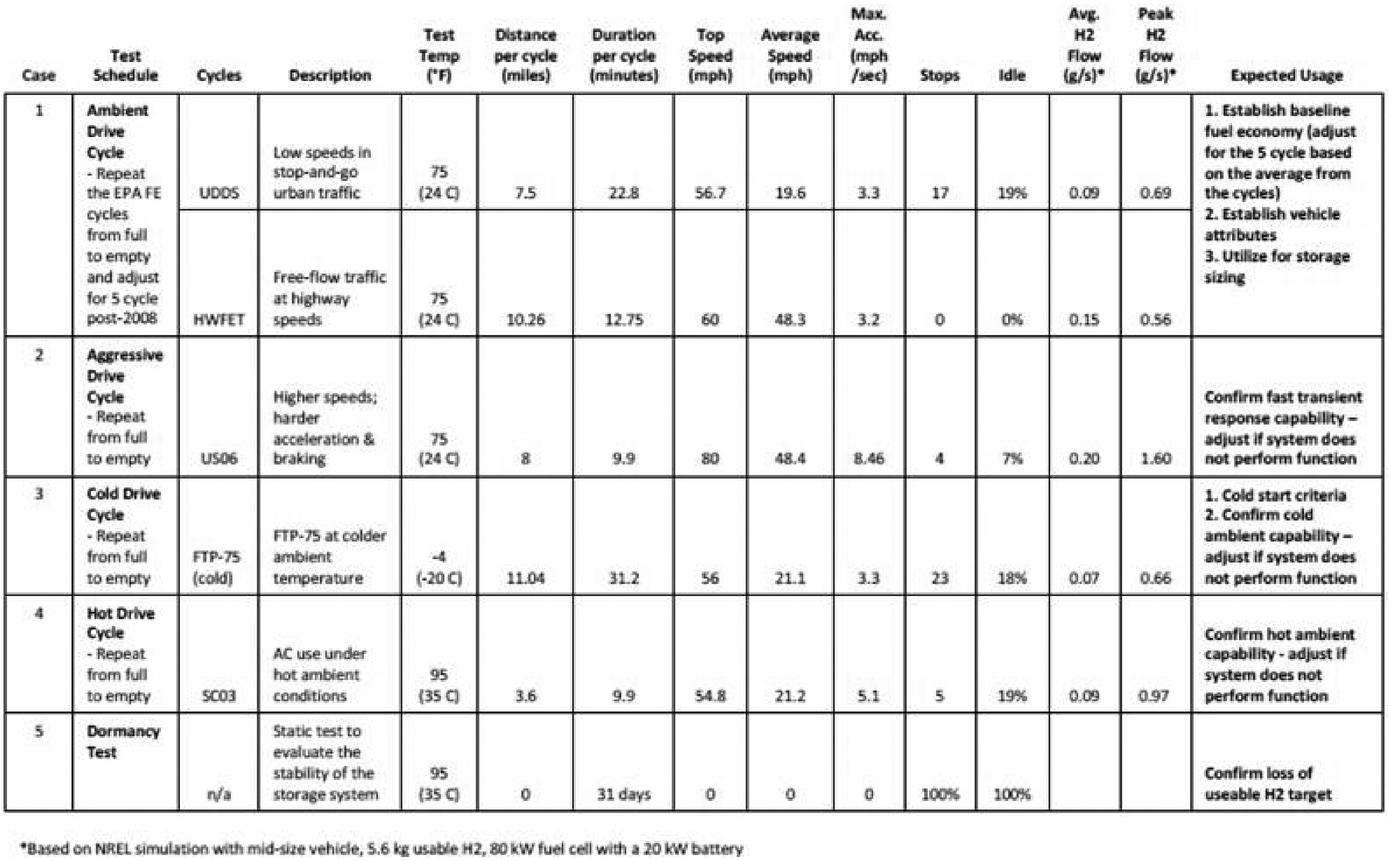


FIGURE 1. Fuel Cell System Efficiency in the HSECoE Universal Framework Model

In this year, a key accomplishment was the establishment of the modeling structure for the baseline vehicle assumptions and drive cycle test cases. In the evaluation of useable hydrogen and other performance attributes, the system architects and storage system modelers had various simulation approaches and assumptions. In order to have a consistent approach, a baseline vehicle and test matrix was developed to establish the storage capacity assessment along with the functional confirmation at the boundary conditions such as high flow, cold cycle, and hot cycle. The initial vehicle proposal was based on the compact vehicle based on a global view of vehicle platforms but was revised to mid-size assumptions to maintain consistency with prior analysis such as those assumed in the Argonne National Laboratory Powertrain Systems Analysis Toolkit model. The emphasis in developing these simulation assumptions was to have consistency and references for the rationale inside of developing unique baseline parameters for the center. The simulation test cases were formulated based on specific needs expected usages to demonstrate a certain performance target. The test case 1 was developed for the basic fuel economy evaluation and confirmation of the usable capacity of the storage systems, which was standardized at 5.6 kg (for consistency with previous studies). The test case 1 utilizes the Environmental Protection Agency (EPA) fuel economy (FE) Urban Dynamometer Driving Schedule (UDDS) and Highway Fuel Economy Test (HWFET) drive cycles and then adjusts them to the post-2008 five-cycle EPA fuel economies from a prior regression correlation in the simulated vehicle fuel economy estimation. The test case 2 consisted of the US06 that simulates aggressive driving and includes the high flow conditions for evaluating the minimum full flow target. The test case 3 is a cold test case with a lower temperature than the EPA cold test to align with the -20°C start-up criteria within the target requirements. The Federal Test Procedure (FTP)-75 was selected for the cold test case since the cycle has low power demand and has idle periods within the drive cycle which would be worst case for systems depending on waste heat or other usage parameters to increase their operating temperatures. The test case 4 is a hot test case based on the drive cycle and consistent with the temperature utilized in the EPA hot condition testing. The final test case 5 was established for the dormancy test case and was based on a month static storage time period at the high EPA temperature. The resulting test cycle matrix is shown in Table 1.

In addition, the HSECoE requested the original equipment manufacturers (OEMs) to assist in the classification of the DOE hydrogen storage targets. The classification of DOE targets was needed for guiding the upcoming phase 1 milestone (i.e. 4 at 100% and remaining at

TABLE 1. HSECoE Simulation and Evaluation Drive Cycle Matrix



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

*Based on NREL simulation with mid-size vehicle, 5.6 kg usable H2, 80 kW fuel cell with a 20 kW battery

40% criteria) and for providing trade-off recommendations to the system architects. The Ford team took the leadership role to brainstorm methods and organize the classification approach. After consideration, the decision was to use a quality function deployment (QFD) method since this tool provides an organized structure to assessing the targets using OEM system engineering disciplines. The system engineering approach uses a cascade from the customer musts/wants to the system requirements/targets. The QFD identifies the priorities of the customer attributes and then ranks the relationships of the system targets to the customer attributes. The cause-effect relationships used a 1 (low effect) to 9 (high effect) scale by evaluating the change in the vehicle attribute based on a 40% reduced target. The priority of the customer attributes utilized the analytic hierarchy process which a series of pairwise comparison judgments to express the relative strength or impact of the element compared to another.

The results of this classification process produced the ranking of the 2010 targets as shown in Figure 2. As indicated by the color codes, the OEM team classified the targets as safety, performance musts (required for basic function), environmental factors (not actual targets), and design choices. The targets classified as design choices were viewed as the attributes that should be utilized by the system architects to emphasize the development of the higher ranked items. The lower ranked design choice targets are still important but could be deemphasized in the system design (at a 40% lower limit). It is important to recognize the analysis was conducted based on the DOE phase 1 milestone criteria that allowed a hydrogen storage system to meet a 40% target level. Therefore, this ranking approach is only valid to a 40% lower limit of the existing DOE target. When considering this assumption, certain targets were relatively immune to a 40% setting of the value. The process was repeated for the 2015 targets at a 50% lower limit and the top five target priorities remained the same with only minor changes in the absolute classification levels.

Task 2. Cost Analysis

The Manufacturing and Cost Analysis Technology Team during the past year established the HSECoE component library foundation to provide the cost evaluation and initial assessment of overall system weight and volume attributes. The HSECoE component library was populated to provide the system architects with the elements needed for the system assessments to support phase 1 milestone review. The system architects utilized the library for the system references for the milestone to ensure the common assumptions are being used throughout the HSECoE. Alignment of the library and the structure of cost evaluation analysis were completed during this year. The component library progressed through various reviews and industry

2010 Target Rank

1. Gravimetric Density

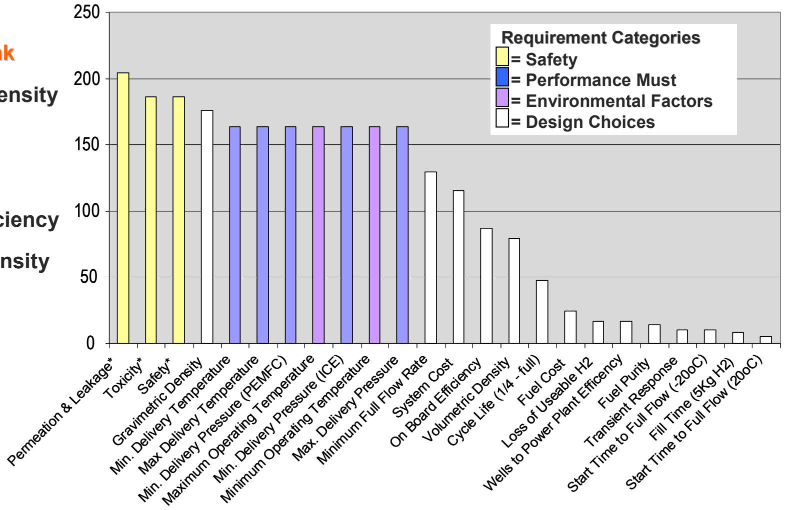
2. Min. Full Flow

3. System Cost

4. On-board Efficiency

5. Volumetric Density

6. Cycle Life



Disclaimer for the approach

1. All targets are important and must be achieved.
2. Input from OEM individuals (not company perspectives) within HSECoE along with FreedomCAR
3. Assessment is only valid based on a **40% lower limit of the 2010 target values** when assessing the rank
4. Guidance provided for HSECoE system architects to determine research and development focus

FIGURE 2. HSECoE Hydrogen Storage Target Classification Pareto Assessment

sources. The effort in developing the library was led by the Pacific Northwest National Laboratory along with input from Ford and other HSECoE partners to ensure the required data for the phase 1 milestone was available. The benchmarking and comparison of other cost models were conducted during this year and will continue as the cost approach advances from catalog components to enhanced manufacturing assessments of key components.

Task 3. Sorbent Media Assessment and Optimization

During the previous year (FY 2010), the HSECoE collaboratively selected MOF-5 as the initial framework material of interest. Therefore during last year a complete set of its fundamental and engineering materials properties were assessed and the primary properties for *powder* MOF-5 deduced including thermal properties (e.g., thermal conductivity, heat capacity), bulk properties (e.g., density, surface area, particle size, pore volume), and isotherm properties. These engineering properties were submitted and distributed to the HSECoE to aid in the creation of preliminary system models for *powder* MOF-5.

Based on preliminary performance modeling data, two principle materials property deficiencies were identified for the *powder* MOF-5 system: 1) low volumetric capacity and 2) poor thermal conductivity. This year's focus aimed at addressing these gaps through both materials compaction and the incorporation of thermal conductivity additives. A series of six *neat* MOF-5 pellets were initially prepared with varying densities from 0.31 to 0.79 g/cm^3. For reference, the loose powder and single crystal densities for MOF-5 are 0.13 and 0.61 g/cm^3, respectively. The goal of MOF-5 compaction is to sufficiently compress the powder to eliminate interparticle voids without compressing the internal (micropores) pores of the MOF structure (i.e. not going beyond the single crystal density). Unlike many other sorbents (e.g. AX-21 or PEEK), addition of a binder is not necessary to form stable MOF-5 compacts, as cohesion within the pellet is high. MOF-5 compacts were fabricated using a manual arbor press with pressing pressures ranging from approximately 30 MPa up to 100 MPa to construct pellets with densities of 0.31 to 0.79 g/cm^3, respectively.

Select physical properties, in particular, phase characterization, BET surface area, and total pore volume of variable density MOF-5 pellets were determined. The phase characterization of each compact was analyzed by powder X-ray diffraction (XRD) to investigate to what extent the original crystal structure of MOF-5 was maintained (i.e. qualitatively evaluate any increase in amorphous content). Based on the XRD data, it was evident that as the pellet density is increases, the intensity of MOF-5 diffraction peaks decreases along with a concomitant increase in the amorphous content (i.e. low angle diffuse scattering). This behavior becomes more pronounced as density is increased from 0.51 g/cm^3 to 0.65 g/cm^3 (i.e. beyond the single crystal density). Thus this data confirms that to simultaneously improve the volumetric efficiency while preserving the MOF-5 structure, it is necessary to use densities slightly below the MOF-5 single crystal density of 0.61 g/cm^3.

Mechanical strength is also an important consideration in determining optimum compact density. To evaluate the mechanical properties of pelletized MOF-5, radial crush strengths of several sets of MOF-5 pellets were determined. These data reveal that compacts with a density of 0.31 g/cm^3 show almost no resistance to compressive loads applied along their radius. However, tablets with larger densities have greatly improved crush strength. For 0.41 g/cm^3 pellets, the average crush strength was 24 N. This increases to 71 N and 106 N for pellets having densities of 0.51 g/cm^3 and 0.60 g/cm^3, respectively.

The BET surface areas and total pore volumes of the variable density MOF-5 compacts were also determined (Figure 3). These data indicate that as one initially begins to compress MOF-5 from a loose powder density of 0.13 g/cm^3 to 0.3 g/cm^3, the BET surface area and total pore volume remain roughly constant at approximately 2,700 m^2/g and 1.4 cm^3/g, respectively. Beyond 0.3 g/cm^3, the BET surface area and total pore volume decrease linearly with increasing density. The linear decrease in surface area with increasing density is an effect also observed for activated carbon (AX-21). Since the storage of hydrogen in sorbents such as MOFs and activated carbons relies on physisorption of hydrogen onto the surfaces of the host sorbent (i.e. MOF), the hydrogen capacity typically scales with surface area. Based on Figure 3, going to a MOF-5 density of 0.51 g/cm^3 results in a 20% decrease in BET surface area (and total pore volume). One must evaluate the hydrogen storage uptake to determine if the reduction in surface area results in a corresponding 20% reduction in hydrogen capacity.

The excess hydrogen adsorption isotherms for MOF-5 powder and compacts are shown in Figure 4 along with fits to the empirical data (Figure 4, symbols) using the modified D-A model (Figure 4, lines). Similar to the surface area results above, the maximum gravimetric uptake is unchanged in the 0.31 g/cm^3 pellet relative to the powder. However, a 15% or 41% decrease in gravimetric uptake is observed for the 0.51 g/cm^3 or 0.79 g/cm^3 samples; these reductions are comparable to the respective 20% and 50% loss in surface area. This suggests that some of the surface area lost upon compression was not active in uptake of hydrogen. The maximum volumetric excess adsorption is increased by a factor of 2.5 for the 0.31 g/cm^3 sample relative to the powder. The increase is a factor of 3.7 for the 0.79 g/cm^3 sample.

The total amount of hydrogen storage at 77 K by MOF-5 compacts is defined as the excess adsorption plus the gas phase H_2 within the void space of the pellets. Relative to the MOF-5 powder, total storage at 80 bar is increased by 26% in the 0.31 g/cm^3 sample and by 40% in the 0.51 g/cm^3 sample. On the other hand, if desorption occurs isothermally at 77 K by a pressure decrease from 80 bar to 3 bar, then the total hydrogen delivery is increased by 13% in the 0.31 g/cm^3 sample, versus 17% for the 0.51 g/cm^3 sample. The total *materials-based* volumetric capacity for the 0.51 g/cm^3 MOF-5 compact at 80 bar and 77 K is 40 g/L, a 150% improvement as compared to powder (0.13 g/cm^3). (For reference the 2015 DOE *system-based* volumetric capacity target is 40 g/L.[1].)

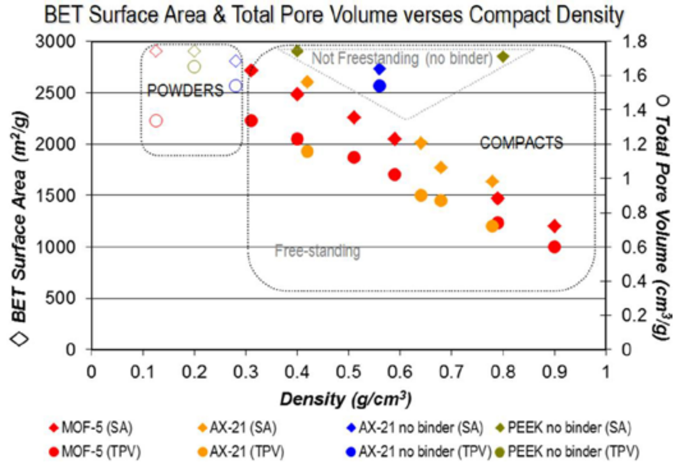


FIGURE 3. BET surface area (◊, primary *y*-axis) and total pore volume (○, secondary *y*-axis) verses compact density for powders (open symbols) of MOF-5 (red), AX-21 with binder (orange), AX-21 without binder (blue) and PEEK without binder (green).

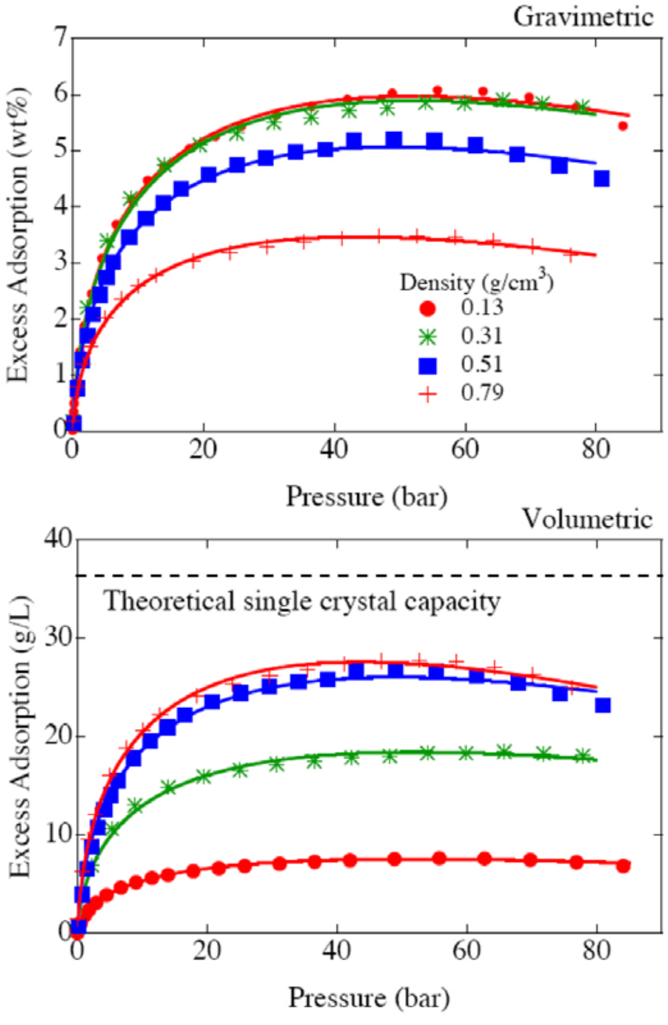


FIGURE 4. Excess hydrogen adsorption at 77 K from 0 to 80 bar by MOF-5 powder (ρ=0.13 g/cm^3) and MOF-5 compacts with ρ=0.31–0.79 g/cm^3. Excess gravimetric adsorption (top) and excess volumetric adsorption (bottom) expressed as a mass fraction (i.e. $m_H/m_{sample} \times 100$). Fits of empirical data (symbols) to the modified D-A model (lines) are shown.

The thermal conductivity of most microporous materials (e.g. MOFs) is expected to be low due to their large pore size (>20 Å in diameter) and high free volume (>90%). For example, the measured thermal conductivity of a single crystal of MOF-5 was previously determined to be 0.3 W/mK between 70 and 300 K [2]. The thermal conductivity (k) for *neat* MOF-5 compacts with densities from 0.35 to 0.69 g/cm^3 were determined over the temperature range of 25 to 65ºC from the measured thermal diffusivity (α), heat capacity (c_p), and density (ρ) using the equation, $k = \alpha \times c_p \times \rho$. Thermal conductivity verses temperature data are shown in Figure 5. Increasing pellet density from 0.35 g/cm^3 to 0.52 g/cm^3 (33% increase) results in only a modest increase in thermal conductivity, from 0.072 to 0.095 W/mK (at 25ºC). We speculate that this small improvement in k arises from a decrease in the amount of inter-particle void space within the pellet volume. Despite this improvement, the neat MOF-5 compact conductivities are all uniformly low and well below the single crystal value of 0.3 W/mK at room temperature. Since hydrogen uptake in sorbents is an exothermic process, low thermal conductivity could restrict the design of efficient MOF-5 based storage systems. In order to achieve targeted refueling times (2015 DOE target is 3.3 min for 5 kg H_2 [1]), and maximize the amount of hydrogen stored, this heat of adsorption must be removed from the storage bed in order to quickly reach the desired operation temperature (e.g. 77 K). Therefore, the identification of methods to augment the thermal conductivity of MOF-5 is desirable; moreover such techniques could be generally applicable to other MOFs as well as the broader class of framework materials (e.g. zeolitic imidizolate frameworks and covalent organic frameworks).

To achieve greater improvements in thermal conductivity, we prepared a series of MOF-5 compacts containing ENG as thermal conductivity enhancer. Analogous to the neat MOF-5 compacts, the MOF-5/ENG composites explored also had densities between 0.35 g/cm^3 and 0.69 g/cm^3 with the ENG mixed at varying mass ratios of 1%, 5% and 10% (by weight). Thermal conductivity verses temperature data are also given in Figure 5. Over the examined temperature range of 25 to 65ºC, there is no systematic temperature dependence, consistent with previous data for MOF-5 [2]. Adding 1 wt% ENG to MOF-5 with compaction up to 0.69 g/cm^3, does not significantly enhance thermal conductivity. However, increasing the ENG content to 5 wt% reveals a 300% enhancement relative to the neat MOF-5 compact of comparable density. For example, at a density of approximately 0.5 g/cm^3, the 5 wt% ENG MOF-5 compact has thermal conductivity of 0.3 W/m·K at 25ºC as compared to the neat MOF-5 compact which has a value of 0.1 W/m·K. Similarly, for a 10 wt% ENG addition, a 600% enhancement is observed. In particular, for the 0.5 g/cm^3 density at 25°C, a thermal conductivity of almost 0.6 W/m·K is observed. Therefore, ENG additions do appear to be effective at increasing the thermal conductivity of MOF-5. Future work (described below) will focus on understanding the impact (tradeoffs) of ENG on other properties such as hydrogen uptake, permeability, crush strength, surface area, etc.

Conclusions and Future Directions

- Task 1. System Modeling
  - Benchmark the system modeling results in comparison to other hydrogen vehicle and storage analysis (i.e. Argonne National Labatory) and identify the areas of differing assumptions or modeling approaches.
  - Enhance the framework and validate the elements of the universal HSECoE Simulink model with the objective of stabilizing the vehicle and fuel cell model blocks within the universal model for the storage optimization analysis.
  - Further refine the fuel cell model to ensure the waste heat and temperature polarization effects are representative of future integration with the hydrogen storage systems and evaluate additional

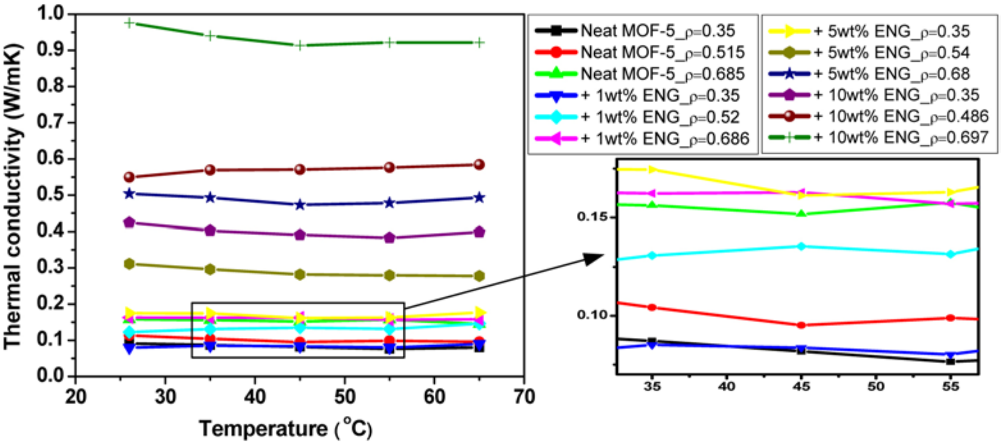


FIGURE 5. Thermal conductivity of pellets of neat MOF-5 and MOF-5/ENG composites with varying densities (from 0.35 to 0.69 g/cm^3) and ENG content (1, 5, or 10 wt%) as a function of temperature (T = 26 to 65°C).

  - opportunities of vehicle and storage system integration.
  - Assess any needed revisions in the test matrix and modeling assumptions based on the feedback from the phase 1 milestone review.
- Task 2. Cost Analysis
  - Enhance the component library information through the development of the manufacturing model structure of the key components.
  - Evolve the cost and weight estimates in the component from available industry catalog items to projected attributes that are representative of automotive designed systems.
  - Decompose the components for the purpose of detailed system design trade-offs and component optimization in addition to the pursuit of equivalent data sources and sensitivity cost assessments.
  - Develop cost estimating resource tools to be utilized for the manufacturing models with additional cost estimation capability based on an agreed set of manufacturing assumptions of the key cost drivers.
- Task 3. Sorbent Media Assessment and Optimization
  - Validate powder MOF-5 isotherm model parameters at higher pressure (i.e. up to 200 bar), and at temperatures within the anticipated operating window.
  - Continue to assess impact of thermal conductivity aids on other principle hydrogen storage engineering properties (e.g., gravimetric capacity, gas permeability, crush strength, etc.); identify correlation between densification conditions, microstructure, and conductivity.
  - Collaboratively with HSECoE modeling efforts, determine required materials property values which are necessary to yield desired system performance.
  - Establish relationship between density and gas transport; collaboratively with HSECoE modeling teams, determine required value to optimize compact dimensions and shape.
  - Continue to support the experimental validation of sorbent bed and system models through neutron imaging and/or other experimental characterization efforts.

Special Recognitions & Awards

Mike Veenstra received a Special Recognition Award from USCAR for his proactive leadership role as a liaison between the Hydrogen Storage Tech Team and the Hydrogen Storage Engineering Center of Excellence.

FY 2011 Publications/Presentations

1. A. Sudik, Ford/BASF/UM Activities in Support of the Hydrogen Storage Engineering Center of Excellence, Invited Presentation, 2010 American Institute of Chemical Engineers Meeting, Salt Lake City UT, October 2010.

2. J.J. Purewal, Hydrogen Storage by MOF-5 Monoliths and Composites: Materials Processing, Thermal Conductivity, and Neutron Imaging, 2011 Materials Research Society Meeting, San Francisco CA, April 2011.

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