IV.D.1a Hydrogen Storage Engineering Center of Excellence

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- United Technologies Research Center, E. Hartford, CT
- General Motors, Warren, MI
- Ford Motor, Dearborn, MI
- The National Renewable Energy Laboratory, Golden, CO
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- California Institute of Technology, Pasadena, CA
- Oregon State University, Corvallis, OR
- Lincoln Composites LLC, Lincoln, NE
- BASF GmbH, Ludwigshafen, Germany
- Université du Québec à Trois-Rivières, Canada

Project Start Date: February 1, 2009
Project End Date: Project continuation and direction determined annually by DOE

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 on-board storage energy management requirements.
- Develop innovative on-board system concepts for metal hydride, chemical hydride, and adsorption hydride 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).

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
(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

This project is directing the modeling, design, build and demonstration of prototype hydrogen storage systems for each metal hydride, chemical hydride and hydrogen sorption materials meeting as many of the DOE technical targets for light-duty vehicular hydrogen storage. The current status of these systems vs. the onboard hydrogen storage system technical targets are given in Table 1.

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Introduction

The Hydrogen Storage Engineering Center of Excellence (HSECoE) brings together all of the materials and hydrogen storage technology efforts to address onboard hydrogen storage in light-duty vehicle applications. The effort will begin with a heavy emphasis on modeling and data gathering to determine the state-of-the-art in hydrogen storage systems. This effort will span the design space of vehicle requirements, power plant and balance of plant requirements, storage system components, and materials engineering efforts. These data and models will then be used to design components and sub-scale prototypes of hydrogen storage systems which will be evaluated and tested to

TABLE 1. System Status vs. Technical Targets

Parameter	Units	Target			System		
		2010	2015	ultimate	Metal Hydride	Adsorbent	Chemical Hydride
Gravimetric Density	*(Kg H_2/Kg system)*	0.045	0.055	0.75	0.0118	0.0295	0.03246
Volumetric Density	*(Kg H_2/liter)*	0.028	0.04	0.07	0.0122	0.0103	0.02083
Minimum Operating Temperature	*(^{o} C)*	-30	-40	-40	-30	-30	-30
Maximum Operating Temperature	*(^{o} C)*	50	60	60	50	50	50
Min. Delivery Temperature	*(^{o} C)*	-40	-40	-40	-40	-40	-40
Max Delivery Temperature	*(^{o} C)*	85	85	85	85	85	250
Cycle Life (1/4 - full)	*(N)*	1000	1500	1500	100	1000	1000
Cycle Life	*(% mean)*	90%	99%	99%	90	90	100
Min. Delivery Pressure (PEMFC)	*(bar)*	4	3	3	4		4
Max. Delivery Pressure	*(bar)*	12	12	12	12	12	12
On Board Efficiency	*(%)*	90%	90%	90%	75%	90%	97%
Fill Time (5Kg H_2)	*(min.)*	4.2	3.3	2.5	10.5	4.2	15
Minimum Full Flow Rate	*([g/s]/KW)*	0.02	0.02	0.02	0.02	0.02	
Start Time to Full Flow (20^{o}C)	*(sec,)*	5	5	5	5	5	3.75
Start Time to Full Flow (-20^{o}C)	*(sec,)*	15	15	15	15	15	7.5
Transient Response	*(sec,)*	0.75	0.75	0.75	0.75	0.75	0.75
Fuel Purity	*(%)*	99.97%	99.97%	99.97%	100%	100%	85%
Permiation & Leakage*		1	1	1	1	1	0.5
Toxicity*		1	1	1	0.25	1	0.5
Safety*		1	1	1	0.25	1	1
Loss of Useable H_2	*([g/hr]/Kg H_2)*	0.1	0.05	0.05	0.1		2.2

** indicates qualitative assessment*

determine the status of potential system against the DOE 2010 and 2015 technical targets for hydrogen storage systems for light-duty vehicles.

Approach

A team of leading national laboratories, universities, and industrial laboratories, each with a high degree of hydrogen storage engineering expertise cultivated through prior DOE, international, and privately sponsored programs has been assembled to study and analyze the engineering aspects of condensed phase hydrogen storage as applied to automotive applications. This diverse group will bring creativity and originality to the HSECoE, where innovative concepts must be identified to develop hydrogen storage systems capable of meeting the stringent DOE goals. The technical activities of the HSECoE are divided into three system architectures: adsorbent, chemical hydride and metal hydride matrixed with six technologies areas: Performance Analysis, Integrated Powerplant/Storage System Analysis, Materials Operating Requirements, Transport Phenomena, Enabling Technologies and Subscale Prototype Construction, Testing and Evaluation.

Results

The following technical accomplishments were achieved by the partners in the HSECoE during the course of the past year. These accomplishments were the result of intense inter-organizational communication and interfacing through the existing technology area lead organization for the Center. These accomplishments are:

- The positions of system architects were formulated to give prime responsibility to individuals for driving technical solutions to identified technology gaps in storage system development.
- Completed programming of the Hydrogen Storage SIMulator to aid in prediction of impact of technical targets.
- Completed baseline fuel cell power plant models with physical storage fuel sources.
- Completed finite element models on metal hydrides and adsorbent system.
- Completed initial metal hydride hydrogen storage system models with various configurations of pressure vessels, buffer tanks, hybridization schemes, pumps and heat exchangers.

- Completed initial chemical hydride hydrogen storage system models with various configurations of mass transport mechanisms, spent fuel reservoirs and reactors.
- Completed initial adsorbent hydrogen storage system models with various configurations of heat exchangers, pressure vessels, buffer tanks and pumps.
- Completed coupling of vehicle modeling, fuel cell modeling and storage system modeling in a MATLAB/Comsol/Simulink environment.
- Identified acceptability criteria and UP/DOWN select methodology for metal hydrides, chemical hydrides and adsorbent materials.
- Completed identification of parametric models to be used for metal hydride, chemical hydride and adsorbent system thermal models.

Chemical Hydrides: $$\left(\frac{dC}{dt}\right) = A\exp\left(-\frac{E}{RT}\right)(C)^{z}$$

Metal Hydrides: $$\left(\frac{dC}{dt}\right) = A\exp\left(-\frac{E}{RT}\right)\left(\frac{P_e - P}{P_e}\right)(C)^{z}$$

Adsorbents: $$n_{ex} = n_{\max}\exp\left[-\left[\frac{RT}{\alpha+\beta T}\right]^2 \ln^2\left(\frac{P_0}{P}\right)\right] - \rho_g V_a$$

- Compiled a data base for each of the materials to be modeled and identified technical data gaps in the data with plans to fill these gaps as shown in Table 2.

TABLE 2. HSECoE Materials Matrix

	Tier 1 Developed Materials	*Tier 2* Developing Materials	Down-selected Materials
Adsorbents	AX-21	Pt/AC-IRMOF 8	MOF 177
	MOF 5		
Chemical Hydrides	$NH_3BH_{3(s)}$	$NH_3BH_{3(l)}$	
	AlH_3	$LiAlH_4$	
Metal Hydrides	$NaAlH_4$	$Mg(NH_2)_2+MgH_2+2LiH$	MgH_2
	$2LiNH_2+MgH_2$	$TiCr(Mn)H_2$	Mg_2NiH_4

- Completed an acceptability envelope for metal hydrides to aid in determination of the critical thermochemical characteristics required for storage system consideration:

$$\left(\frac{1}{L^2}\right)\left(\frac{k\ M_{Hyd\_eff}\ \Delta T}{-\Delta H_{overall}\ \rho_{Hydride}}\right) = \frac{1}{mM_{H2}}\frac{\Delta m_{H2}}{\Delta t}$$

- Identified critical technologies for pressure vessels, sensing, insulation, thermal generation and fuel purity required to enable use of various storage system materials.
- Determined the current system technical target status of metal hydrides based on $NaAlH_4$ and technology gaps (gravimetric density, cycle life, safety and toxicity) needing to be addressed to meet the 2010 and 2015 technical targets (see Figure 1).

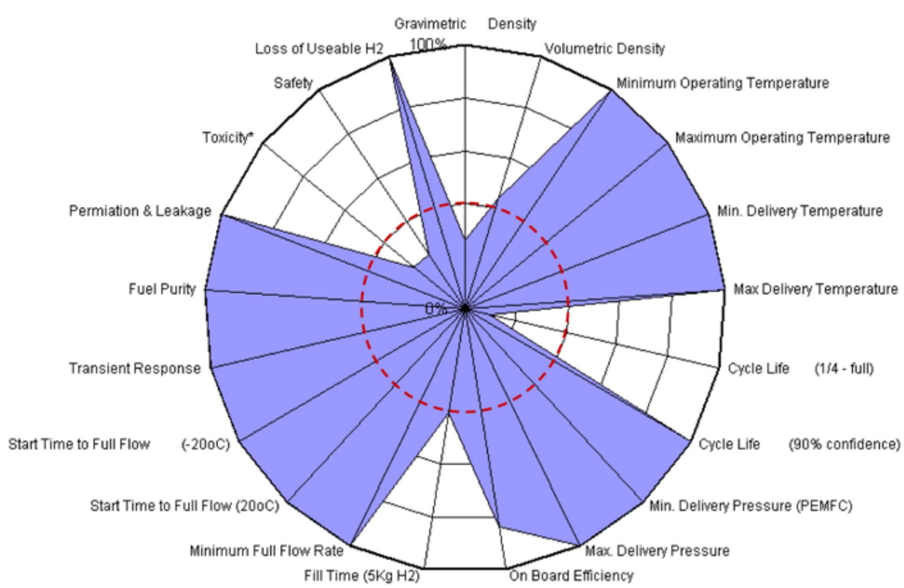

FIGURE 1. Spider chart against DOE 2010 targets for sodium aluminum hydride metal hydride system showing technical gaps in gravimetric density, cycle life, safety and toxicity.

- Determined the current system technical target status of chemical hydrides based on solid NH_3BH_3 and technology gaps (fuel purity, fill time, minimum full flow rate and loss of useable hydrogen) needing to be addressed to meet the 2010 and 2015 technical targets (see Figure 2).
- Determined the current system technical target status of adsorbents based on super-activated carbon and technology gaps (volumetric density, minimum delivery pressure and loss of useable hydrogen) needing to be addressed to meet the 2010 and 2015 technical targets (see Figure 3).

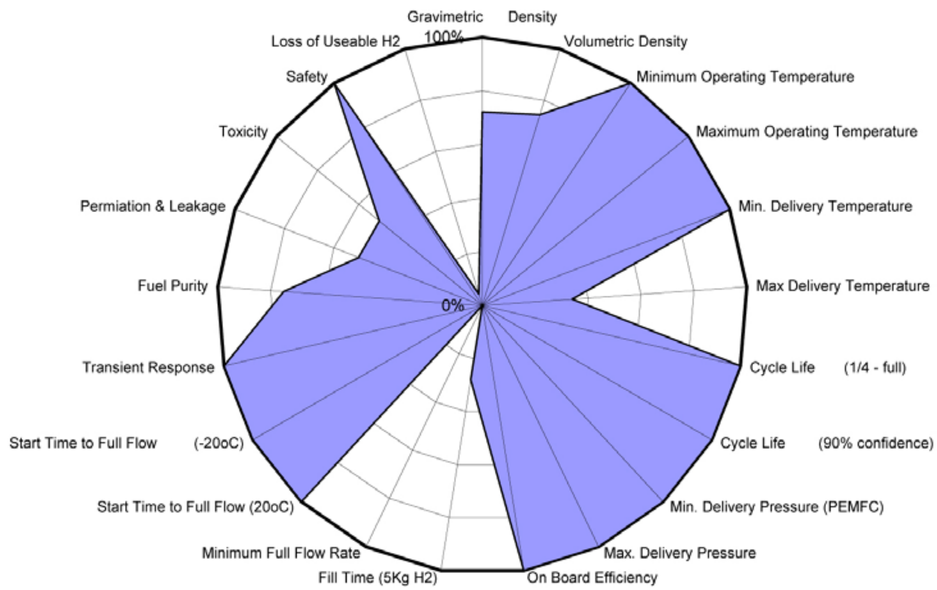

FIGURE 2. Spider chart against DOE 2010 targets for solid ammonia borane chemical hydride system showing technical gaps in fuel purity, fill time, minimum full flow rate and loss of useable hydrogen.

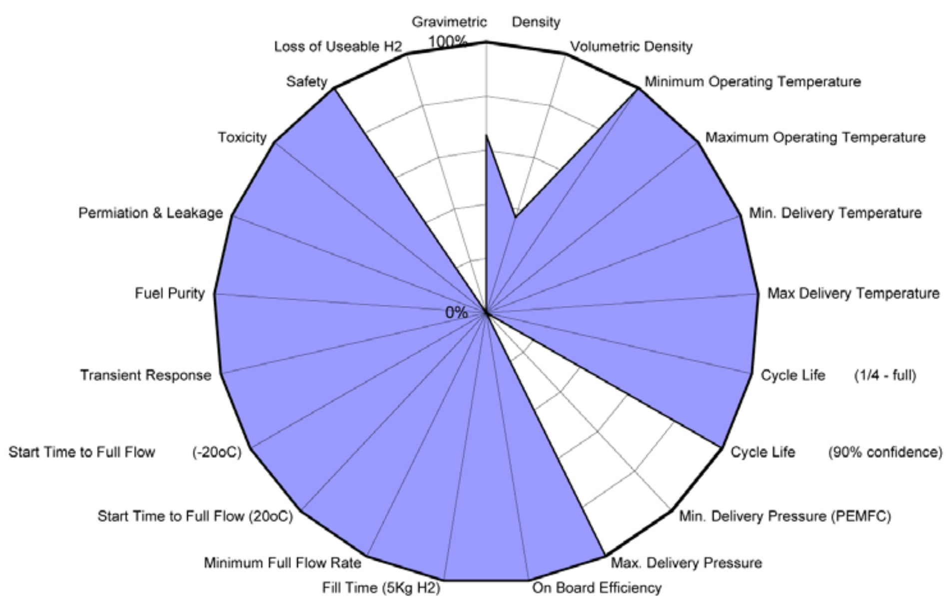

FIGURE 3. Spider chart against DOE 2010 targets for super activated carbon (ax-21) adsorbent system showing technical gaps in volumetric density, loss of useable hydrogen and minimum delivery pressure.

Conclusion and Future Directions

For each of the storage system types, many of the technical targets have been fully met with a number more met to at least the 40% level. The technical directions to achieve the Phase 2 Go/No-Go decision are set by the technical gaps noted in the spider charts. Furthermore, the technical targets will be prioritized in the coming year give guidance as to the technical gaps requiring further work.

For metal hydride systems, approaches must be proposed which have been shown minimally through modeling that:

- Gravimetric targets can be met through characterization of LiMgN materials systems.
- Cycle life of materials can be estimated through accelerated testing.
- Acceptable toxicity and safety risk levels can be achieved through mitigation strategies.

For chemical hydride systems, approaches must be proposed which have been shown minimally through modeling that:

- Fuel purity can be achieved through impurity trapping and materials development.
- Fill time can be achieved through solid mass flow concepts and novel system designs.
- Minimum full flow rate can be achieved through solid mass flow and solid reactor designs.
- Loss of useable hydrogen can be minimized through materials characterization.

For adsorbent systems, approaches must be proposed which have been shown minimally through modeling that:

- Volumetric densities can be achieved through compaction methods with minimal loss of gravimetric density.
- Minimum delivery pressures can be achieved through novel thermal designs.
- Loss of useable hydrogen can be minimized through utilization of novel low-cost insulation schemes.

As Phase 2 is entered, experimental validation of modeling will take precedence. Heat and mass flow experiments will be detailed constructed and performed to validate modeled performance. The modeling and empirical validation cycle will be used to obtain enhanced performance.

FY 2010 Publications/Presentations

Presentations

1. D. Anton, Materials for Hydrogen Storage Systems Development, IEA HIA TASK 22 Meeting Fundamental and Applied Hydrogen Storage Materials Development, Oct 10–17, 2009 Paris, France.

2. D. Anton, Materials for Hydrogen Storage Systems Development, IEA HIA TASK 22 Meeting Fundamental and Applied Hydrogen Storage Materials Development, April 11–15, 2010 Death Valley, California.