IV.D.1c Systems Engineering of Chemical Hydride, Pressure Vessel, and Balance of Plant for On-Board Hydrogen Storage

Darrell R. Herling
Pacific Northwest National Laboratory (PNNL)
902 Battelle Blvd.
P.O. Box 999, MS: K2-03
Richland, WA 99354
Phone: (509) 375-6905; Fax: (509) 375-4448
E-mail: darrell.herling@pnl.gov

DOE Technology Development Manager:
Monterey Gardiner
Phone: (202) 586-1758; Fax: (202) 586-9811
E-mail: Monterey.Gardiner@ee.doe.gov

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Objectives

PNNL's objectives address some of the critical engineering challenges that currently limit design optimization and commercialization of on-board hydrogen storage systems. Each of these objectives and corresponding tasks have been established to advance the state-of-the-art in design and engineering for chemical hydride storage, pressure/containment vessel construction, and component miniaturization to achieve PNNL, Hydrogen Storage Engineering Center of Excellence (HSECoE), and DOE goals.

- Demonstrate a high level of performance that meets DOE targets for key components (reactor, solids handling, and heat exchanger) of a solid chemical hydrogen storage system.
- Optimized the design of a structured storage bed and system performance through engineering, including establishment of bulk storage media and system kinetics data to aid in design activities.
- Reduce system volume and weight and optimizing system storage capability, fueling, and dehydriding performance through application of microtechnology and associated architectures to the design of high-efficiency heat exchangers and balance-of-plant (BOP) components.
- Mitigate materials incompatibility issues associated with hydrogen embrittlement, corrosion, and permeability though suitable materials selection for vessel materials, heat exchangers, plumbing, and BOP components.
- Demonstrate the performance of economical, compact, lightweight vessels for a hybrid pressurized metal-hydride and adsorbent system, and containment vessel for a chemical hydride system.
- Guide design and technology down-selection, Go/No-Go decision-making, and address vehicle and market impact through cost modeling and manufacturing tradeoff assessments of the three HSECoE prototype storage systems.

Achieving the objectives will enable PNNL, Savannah River National Laboratory (SRNL), and other HSECoE partners to demonstrate on-board hydrogen storage with the potential to meet 2015 DOE technical targets. This technology and design knowledge will be transferred to the participating automotive original equipment manufacturers (OEMs), thus advancing the hydrogen market sector and production of future hydrogen-powered vehicles.

Technical Barriers

This project addresses the following technical barriers from the Hydrogen Storage section of the Hydrogen, Fuel Cells and Infrastructure Technologies Program Multi-Year Research, Development and Demonstration Plan:

General to All Storage Approaches:

(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 (BOP) Components
(I) Dispensing Technology
(J) Thermal Management
(K) System Life-Cycle Assessments

Off-Board Regenerable Specific:

(S) By-Product/Spent Material Removal

Technical Targets

The Center activities being conducted at PNNL range from process modeling and component design/engineering to technology application and prototypical demonstration. The final ultimate goal of the Center is to demonstrate a (100 g) scaled storage system that meets all sixteen of the DOE storage performance targets. No progress toward these technical targets has been made to-date, since the Center is new and just getting underway. Technical work and modeling that will address the Technical Targets was recently initiated in the 3rd quarter of Fiscal Year 2009.

Accomplishments

The Center activities, and by extension PNNL activities, commenced in the 2nd quarter of FY 2009. To-date the Center partners have completed the initial project planning and award contracting. In addition, the Center Technical Areas and Teams have been established. PNNL accomplishments to-date includes:

- Establishment of the Materials Requirements Technical Area, including establishment of liaisons and connections with the Hydrogen Storage Materials Centers of Excellence.
- Down-selection of candidate hydrogen storage materials an initial set of materials to be used for modeling activities. Part of this down-selection process was to initiate data collection on materials. This data collection is currently in-progress.
- Initiation of a sensitivity study on pressure vessel design that includes construction of materials and cost factors.
- Initiation of process flow diagram and model development for a solid chemical hydride storage system.
- Established common modeling approaches and platform for use among Center partners.

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Introduction

To-date there has been multiple on-board vehicle-scale hydrogen storage demonstrations, including several studies to examine phenomena and characteristics that impact the engineering of hydrogen storage systems. However, none of these demonstrations have simultaneously met all of the DOE hydrogen storage program goals. Additionally, engineering of new chemical hydride approaches specifically is in its infancy, with ample opportunity to develop novel systems capable of reaching the DOE targets for storage capacity. Toward this goal, PNNL is proposing to contribute to the HSECoE led by SRNL. The goal of this virtual Center and PNNL's role is to develop and demonstrate low-cost, high-performing on-board solid-state hydrogen storage through a fully integrated systems design and engineering approach.

PNNL will target six key objectives to optimize performance characteristics and reduce the size, weight, and cost of a solid-state hydrogen storage system. This will be accomplished through a carefully engineered and integrated design approach, including application of advanced materials (structural and hydrogen storage), use of micro-scale enhancements of heat and mass transfer, better understanding and tailoring of bulk storage media and system kinetics, and assessments of manufacturing and cost impact based on established models/approaches for technology tradeoff studies. PNNL will also serve multiple leadership roles within the HSECoE to help facilitate collaboration across the Center partnership.

Approach

PNNL will actively contribute to the five Technology Areas proposed as part of the HSECoE led by SRNL. The goal of this virtual Center, and PNNL's role, is to develop and demonstrate low-cost, high-performing, on-board solid-state hydrogen storage through a fully integrated systems design and engineering approach. PNNL will focus scope on six technical tasks:

1. Low Volume Storage Systems for Solid Chemical Hydrides
2. Kinetics and Reactor Design and Testing
3. System Miniaturization Using Efficient Microachitectures
4. Materials Compatibility and Selection
5. Containment and Pressure Vessels Construction
6. Manufacturing and Cost Analysis.

The outcomes from these six technical development tasks will ultimately feed into the overall Center objectives, prototyping and demonstration activities, including design and construction of the solid chemical hydride prototype system and pressurized composite storage tanks for the metal hydride and absorbent systems.

Achieving the objectives will enable PNNL, SRNL, and other HSECoE partners to demonstrate on-board hydrogen storage with the potential to meet 2015 DOE technical targets. This technology and design knowledge will be transferred to the participating automotive OEMs, thus advancing the hydrogen market sector and production of future hydrogen-powered vehicles.

In addition, the Center is structured around six Technical Areas, with leads for each of: Performance, Cost & Energy Analysis; Integrated Power Plant/Storage System Modeling; Materials Requirements; Transport Phenomena; Enabling Technologies; Subscale Prototyping. These Technical Areas and subsequent Technology Teams have been established, with technical objectives and task planning now complete for each. PNNL is responsible for coordinating the Materials Requirements Technical Area, as well as various Technical Teams within the Center and among all the partners.

Results

The HSECoE kicked off planning and scope refinement discussions among the partners in the 2nd quarter of FY 2009. PNNL initiated technical development activities in the 3rd quarter of FY 2009 and as a result of the short period of time elapsed, no significant or conclusive data has been generated as of yet.

All PNNL tasks have, however, been initiated, and work in underway. The follow is a description of those tasks and objectives of each:

Low Volume Storage Systems for Solid Chemical Hydrides – As part of the Chemical Hydrogen Storage Center of Excellence (CHSCoE) activities, PNNL recently discovered additives for ammonia borane that completely suppress foaming without affecting the hydrogen release chemistry, which solves a problem that has plagued this material system for some time. This is a significant finding because these new fuel formulations allow consideration of engineered monolithic fuel systems that may have effectively no void volume in the fuel tank, presenting a significant advantage over pelletized systems. As part of the work scope PNNL is working toward engineering and demonstration of a monolithic fuel system can be achieved where the fuel is divided into elements that pack with nearly 100% volume efficiency into a fuel tank. This allows the opportunity to employ an elemental volume-exchange fuel management approach, which potentially makes refueling fairly easy as portions of the tank can be refueled based on how much fuel has been used and further increasing volumetric capacity. This is a paradigm shift in chemical hydride system fueling that will require significant engineering efforts to develop a viable and optimized system design. Much of the necessary ancillary technology already exists; PNNL's objective will be to engineer a complete integrated system. Solid chemical hydride storage with non-foaming solid fuel elements, coupled with a volume-exchange approach in the fuel tank, can likely meet the challenging 2015 volumetric capacity target of 0.8 kg/L for a system. It should also meet the gravimetric density target of 9 wt%, with kinetics properties capable of meeting the rate target of ~1.6 g H_2/s for an 80 kW fuel cell.

Kinetics and Reactor Design and Testing – Studies on reaction kinetics are valuable when engineering the size of a device that might be used to release hydrogen from solid hydrogen carriers. For example, bench-scale data and proven reactor models for chemical hydride systems are invaluable when working toward a competent design. PNNL has initiated activities to develop models for a solid chemical hydride system, taking into account geometrical effects of the reactor on combined heat and mass transfer. Bench-scale kinetics measurements obtained from the CHSCoE will be used as input parameters to these three-dimensional reactor models, which will ultimately provide predictions on the hydrogen release rate under varying operating conditions. Test data on small-scale chemical reactors will be used to validate the component models, and the models will be used to assist in the design of larger-scale reactor systems. Component models and process-flow diagrams will be integrated to form system-level models for assessing BOP components. This work will result in new methods for mechanical fuel handling systems to enable the release of hydrogen with efficient thermal management. There is strong potential for microarchitectures to be developed as part of Task 3 to support this activity as well to reduce reactor volume.

System Miniaturization Using Efficient Microarchitectures – Microchannel processing technology uses component architectures consisting of small channels and reaction chambers having a characteristic dimension of 0.1 to 1 millimeter that enable rapid heat and mass transfer. This facilitates process intensification (high processing capacity per unit volume), permitting system volumes that are typically an order of magnitude smaller than conventional technologies. In addition, these same attributes can improve component efficiency and promote rapid transients. Established PNNL microchannel design approaches are being applied to the development of the chemical hydride reactor and integrated heat exchanger systems to achieve the system size and performance objectives. Likewise, PNNL is applying its microchannel modeling and design methodologies to investigate the potential for integration of a heat exchanger inside of a hybrid storage tank for applications in compact, highly efficient metal hydride and adsorbent systems. The results of this task will enable significant advancement in meeting system volumetric targets. The benefit in component miniaturization through the application of microtechnology has been demonstrated by PNNL and others previously; therefore, with proper adaptation of the technology, DOE volumetric targets should be within reach.

Containment and Pressure Vessel Development – There are a number of challenges in designing a contained hydride or adsorbent system, such as simultaneously maximizing volumetric and gravimetric hydrogen storage capacity, effective thermal management during refueling and hydrogen release, and mitigating hydride or adsorbent decrepitation during cycles resulting in degradation of the storage bed integrity and thermal conductivity. The best solution to address these challenges is likely to be one that integrates a structured storage bed approach and tank construction that can accommodate a wide range of operating conditions. PNNL has initiated activities, in conjunction with HSECoE partners SRNL, United Technologies Research Center, and University of Quebec at Trois-Rivières to integrate the structured bed design they develop as part of their respective tasks for metal hydride and adsorbent storage materials with an appropriately engineered hybrid pressurized storage vessel. The principal technical focus will be to design the vessel to mitigate the major engineering concern of dealing with the volumetric expansion/contraction during hydriding/dehydriding and thermal management.

Manufacturing and Cost Analysis – To support the HSECoE and ensure a holistic down-selection approach to system design and engineering, PNNL has initiated work toward creating a cost model to perform economic and impact assessments of viable manufacturing methods and technology options. This task is focused on the economics of the three prototype on-board hydrogen storage systems and will including modeling and analysis of fuel costs, cost per unit or configuration, component costs, and manufacturing costs. In addition, a manufacturing-cycle analysis is planned for out-year assessments that will be performed together with a value/impact assessment of technology versus the level of objectives accomplished. Successful completion of this task will provide the necessary financial and technology assessment analyses to enable the selection of the best overall hydrogen storage system.

Conclusions and Future Directions

The HSECoE has been established and research activities recently commenced at PNNL, as well as at other Center partner locations. To date the Center partners have completed the initial program planning and award contracting. In addition, the Center Technical Areas and Teams have been established. PNNL is underway in executing the scope of work as defined in previous sections of this report.

Future planned activities include the scope of work as defined in the results section of this report and presented at the DOE Annual Merit Review.

FY 2009 Publications/Presentations

1. Materials Requirements and PNNL Activities in Support of the HSECoE, USCAR Technical Team Review, Washington, D.C., December 11, 2008.

2. 2009 DOE Hydrogen Program Annual Merit Review, Washington, D.C., May 20, 2009, Presentation STP07.