IV.D.1d Advancement of Systems Designs and Key Engineering Technologies for Materials Based Hydrogen Storage

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Objectives

- Collaborate closely with the Hydrogen Storage Engineering Center of Excellence (HSECoE) partners to advance materials-based hydrogen storage system technologies.
- Develop vehicle/power plant/storage system integrated system modeling elements to improve specification of storage system requirements and to predict performance for candidate designs.
- Establish detailed heat and mass transfer modeling and apply to design improved internal heat exchange configurations.
- Design and evaluate compacted/structured hydride powder beds including integration into the above heat exchange configurations.
- Assess the viability of on-board purification for various storage material classes and purification approaches.
- Conduct risk assessments during the progression of the phased HSECoE efforts to evaluate concepts regarding the "Environmental Health and Safety" target.

Technical Barriers

This project is concerned with assessing and developing all aspects associated with viability of storage systems and therefore addresses a broad set of technical barriers from the Storage section (3.3.4) of the Hydrogen, Fuel Cells and Infrastructure 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 (BOP) Components
(I) Dispensing Technology
(J) Thermal Management
(K) System Life-Cycle Assessments

Technical Targets

The goals of this project mirror those of the HSECoE which by the end of the first two-year Phase I seek to define systems configurations which can fully meet four of the DOE 2010 numerical system storage targets as outlined in the Multi-Year Research, Development and Demonstration Plan and partially meet the remaining numerical targets to at least 40% of the target or higher.

Accomplishments

This and other HSECoE projects are in their initial stage, having started nominally in February. Given the close coordination and interdependence of many of the activities, a portion of the efforts to date have involved refinement of the partners' roles and task scopes. Accomplishments of the current project include:

- Refined structure of integrated system modeling. Developed simplified model of an on-board reversible storage system for inclusion in vehicle level modeling.
- Developed detailed modeling methods. Applied these tools to examine potential improvements in heat exchanger effectiveness.
- Constructed modeling framework for preliminary analysis of membrane separation methods. Compiled materials and impurities of interest.

- Developed compaction design concept which offers greater flexibility in optimization for heat transfer, simple/low cost manufacturing and good potential for effective mass transport and durability.

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Introduction

Physical storage of hydrogen through compressed gas and cryogenic liquid approaches is well established, but has drawbacks regarding weight, volume, cost and efficiency which motivate the development of alternative, materials-based methods of hydrogen storage. Recent worldwide research efforts for improved storage materials have produced novel candidates and continue in the pursuit of materials with overall viability. While the characteristics of the storage materials are of primary importance, the additional system components required for the materials to function as desired can have a significant impact on the overall performance. Definition, analysis and improvement of such systems components and architectures, both for specific materials and for generalized material classes, are important technical elements to advance in the development of superior methods of hydrogen storage.

Approach

The most significant aspect of the approach is the HSECoE structure through which ten prime organizations will collaborate. The partner activities have been coordinated from the initial planning and continue to be refined. The center is comprised of six technology areas:

- Performance, Cost & Energy Analysis
- Integrated Power Plant/Storage System (IPPSS) Modeling
- Materials Requirements
- Transport Phenomena
- Enabling Technologies
- Subscale Prototyping

UTRC's approach involves a broad set of tasks which leverage prior experience, coordinate with other UTRC projects and extend to new areas of concept development. These activities include:

1. Develop system engineering technical elements to understand vehicle/power plant/storage system integrated performance. Coupled modeling of these higher level system aspects is needed to determine the requirements for storage systems and to predict vehicle performance for candidate designs.
2. Determine the thermal, physical and chemical properties of hydrogen storage and component materials to support modeling and experimental investigations of heat transfer, mass transfer and durability with a focus on the key material behaviors in other UTRC tasks.
3. Conduct safety risk assessments at various levels of fidelity during the progression of the phased HSECoE efforts in order to pursue the concepts with the greatest potential for complete viability including the "Environmental Health and Safety" target. This will include coordination with the three DOE Material Reactivity projects.
4. Support HSECoE partner development of detailed heat and mass transfer modeling and derive simplified component/system performance models.
5. Assess on-board purification methods for their potential to meet minimum fuel flow requirements with acceptable weight, volume and cost. If successful, this would broaden the number of storage materials that are viable for fuel cell applications.
6. Build upon prior storage system prototype heat exchanger designs and examine enhancements to thermal conductivity, integration with compaction of task 7 and tubing configurations.
7. Design and optimize compacted forms of hydride powder to improve volumetrics, significantly improve safety, increase thermal conductivity and if properly designed, improve hydrogen mass transfer.
8. Address material handling challenges for solid chemical storage through refinement of novel concepts in collaboration with HSECoE partners.
9. Support development of overall system design and fabrication including component integration and assembly procedures, focusing on components developed by UTRC.

Note that several of the above tasks in the approach have close synergy, most notably tasks 2, 4, 6 and 7. The project is divided into three phases with the first covering two years. A Go/No-Go decision at the end of Phase I will guide activities and concepts for deeper evaluation in Phase II.

Results

The framework for integrated vehicle/power plant/storage system modeling was refined. Connections of the more detailed component design modeling to the higher level vehicle modeling are diagrammed in Figure 1. The computational framework Matlab was selected as a common language to bridge across the different levels of modeling.

As part of the connection between the simulation levels, a simplified model for on-board reversible hydride storage system behavior for use in vehicle level studies was developed using results produced from

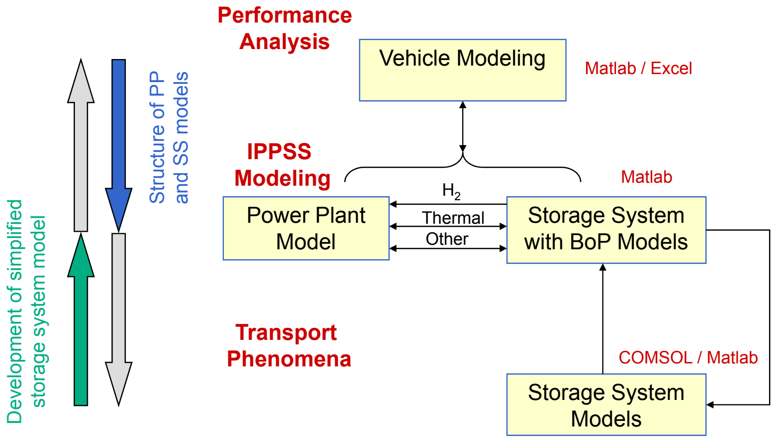

FIGURE 1. Diagram of Multi-Level HSECoE Modeling

detailed simulations. This simplified model captures the transient effects of heat transfer and the temperature/pressure dependent reaction kinetics, approximating the temperature, pressure and composition fields as being homogeneous (lumped parameters). The kinetics model is taken directly from the detailed COMSOL simulation tool developed by Savannah River National Laboratory (SRNL) with support from UTRC. The transient heat transfer representation was constructed with thermal results from COMSOL simulations of a $NaAlH_4$-based prototype design developed in a prior DOE contract (DE-FC36-02AL67610).

In order to have a common detailed simulation environment across the center partners, the COMSOL multi-physics package mentioned above was installed at UTRC and verified with three dimensional, single fin models developed by SRNL. Solver methods were modified, resulting in over a 4X reduction in execution time. Figure 2 gives a contour plot of temperature during rehydrogenation for a symmetrical sector of the storage system cross section that is representative of the modeling. Additional configurations were constructed for studying behavior and sensitivities of heat exchanger designs including a two dimensional, axisymmetric model running longitudinally along the tubing. In collaboration with SRNL, concepts to reduce temperature differentials across the hydride bed were developed and evaluated, focusing on minimizing the large gradients which inherently occur near the heat exchanger tubing.

Detailed models were developed to study the various rate limiting steps that can occur in thin film metallic hydrogen purification membranes. In addition to performance, cost is a critical target for large scale impact of hydrogen in light-duty vehicles. To give some perspective on cost, a simple model was developed with the results shown in Figure 3. Inputs include one refueling of 5 kg per week over a 10-year life. Thus, in order to achieve a level of less than \$0.50 added cost per kg of refueled hydrogen, the purification subsystem must have a cost of less than \$100 per square foot of membrane material which can achieve better than 300 standard cubic feet per hour per square foot of hydrogen flux. This effort is being leveraged with a separate DOE project at UTRC aimed at developing low cost, high flux membranes. Additional modeling examining the pressure and temperature dependencies of hydrogen flux were also conducted, supporting the conclusion that on-board purification has the greatest potential for chemical storage materials which can provide higher desorption pressures and temperatures than are likely for on-board reversible materials. From the HSECoE storage material candidates, the initial impurities on which to focus were identified as borazine and ammonia.

Experimental capabilities for conducting well controlled uniaxial compaction at elevated temperatures

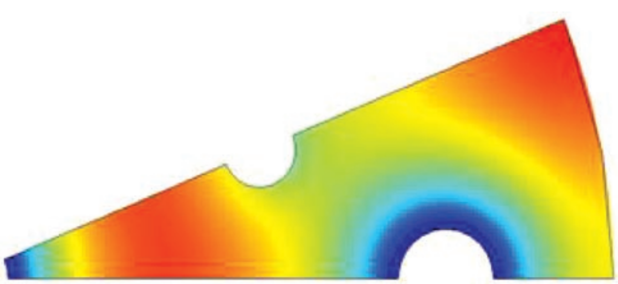

FIGURE 2. Temperature Contour of a Single Fin Sector Model

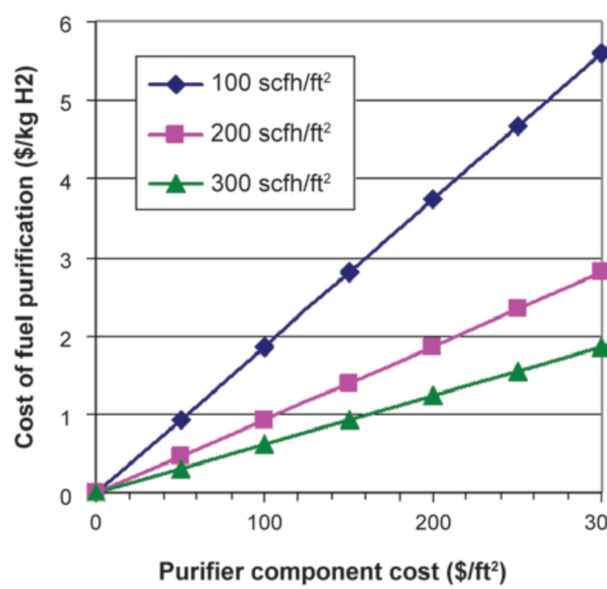

FIGURE 3. Added Fuel Cost for On-Board Purification

within a glove box environment have been specified and partially procured/constructed. Concepts for how the compacted forms will be integrated with the heat exchanger configurations have been generated and down-selected. The prime approach involves distributed, low cost conduction enhancement, low loss coupling to the heat exchanger tubing and a relatively simple compaction geometry. Initial experiments will be conducted with $NaAlH_4$ as a representative ball-milled/catalyzed advanced hydride material.

Conclusions and Future Directions

The initial activities within the HSECoE have established collaborative efforts along a number of technical lines including integrated systems analyses, detailed heat/mass transfer modeling, hydrogen quality/purification and compacted structured forms of powdered storage material. Future efforts in these areas will involve:

- Refinement of simplified storage system models to include integration with power plant and vehicle level models.
- Evaluation of forecourt requirements and communication to relevant hydrogen delivery efforts.
- Through detailed COMSOL modeling, evaluate sensitivities and optimize the conduction enhancement level and distribution for the configuration conceived under the compacted structured bed efforts. Develop response surfaces to American Society of Mechanical Engineers pressure vessel code requirements and include guidance from partner Lincoln Composites when including pressure in the optimizations.
- Continue to assess the viability of membrane purification as well as alternate methods including adsorbents and scrubbers. Any future experiments for on-board purification will focus on borazine and ammonia, and involve premixed gases rather than actual discharged hydrogen.
- Produce planar compacted forms of $NaAlH_4$ and test for thermal and kinetic performance as well as reduction of adverse reactivity in air and water environments.