IV.D.5 SRNL Technical Work Scope for the Hydrogen Storage Engineering Center of Excellence: Design and Testing of Metal Hydride and Adsorbent Systems

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Subcontractor:
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Projected End Date: July 31, 2014

Fiscal Year (FY) 2011 Objectives

The Savannah River National Laboratory (SRNL) and its sub-recipient the Université du Québec à Trois-Rivières (UQTR) will:

- Collect property data for select metal hydrides and adsorbents.
- Compile list of available analytical techniques to support materials property data requirements.
- Develop and evaluate the acceptability envelope for storage media and vessels.
- Develop numerical models to adequately predict storage system behavior for metal hydride and adsorbent based storage systems.
- Use the models to design optimized storage systems based on $NaAlH_4$, other metal hydrides, AX-21, and other potential absorbent materials.
- Direct metal hydride system testing and evaluations as the Metal Hydride System Architect for the Center.

Technical Barriers

This project addresses the following technical barriers from the Hydrogen Storage section (3.3) of the Hydrogen, Fuel Cells and Infrastructure Technologies Program Multi-Year Research, Development and Demonstration Plan:

(A) System Weight and Volume
(C) Efficiency
(E) Charging/Discharging Rate

Technical Targets

The goal of the entire Hydrogen Storage Engineering Center of Excellence (HSECoE) is to provide a system model for each material sub-class (metal hydrides, adsorption, chemical storage) which meets the "Technical System Targets: On-Board Hydrogen Storage for Light-Duty Vehicles", Table 3.3.2 in the DOE Multi-Year Research and Development Plan – April 2009. The end-of-Phase I, Go/No-Go milestone which is set for February 2011 for the entire HSECoE project is that:

1. Four of the DOE 2010 numerical system storage targets are fully met and that,
2. The status of the remaining numerical targets must be at least 40% of the target or higher.

For SRNL's specific technical portion of HSECoE, SRNL will:

- Direct the testing and evaluations necessary for the specific Go/No-Go milestones for metal hydride systems.
- Compile thermochemical data.
- Bound media operating characteristics for metal and adsorption hydride material.
- Develop and apply numerical models that couple mass, momentum and energy balances with chemical kinetics and/or isotherms to simulate hydrogen uptake and discharge.
- Develop and run system models for candidate adsorbent material systems.
- Identify technology gaps.
- Identify preliminary system designs to achieve DOE 2015 hydrogen storage goals.

FY 2011 Accomplishments

- Collected material operating data for LiMg-amide metal hydride materials including developing engineering kinetic expressions.
- Applied Acceptability Envelope to select metal hydride materials and systems.
- Studied 50 bar, 100 bar, and 150 bar sodium alanate optimal systems.
- Estimated isenthalpic (Joule-Thompson) temperature change for hydrogen flow through a throttling valve, which can be as large as an 18 K drop.
- Developed methodology and estimated pressure drop losses for flow in piping of cryo-adsorbent system for a range of conditions (mass flow rates, temperatures, and pressures) for use in system models.

- Developed improved methodology to estimate heat transfer coefficient for turbulent (radial) flow in micro-channel between cooling plates for analysis and COMSOL optimization of modular cryo-adsorbent designs.
- Studied in-line heat exchangers for hydrogen feed to fuel cell.
- Completed System Architect analysis of sodium alanate as a model material vs. DOE 2010 Go/No-Go Decision.

Introduction

SRNL and its subrecipient, UQTR, are involved in several critical aspects of the HSECoE. SRNL is focused primarily on modeling, validating, and optimizing hydrogen storage designs for metal hydrides, adsorbents, and, to a lesser extent, chemical hydrides, and System Architect Analyses of metal hydride systems. SRNL is applying its expertise in modeling dynamic transport phenomena and chemical processes, materials testing, and system modeling to accomplish its objectives in the proposed effort– developing and applying models to identify viable subscale prototype designs, performing design calculations sufficiently accurate for engineering application, and defining the scope and required measurements for experiments with the selected prototypes.

UQTR is developing thermodynamic formulations for adsorbent isotherms that can be easily and efficiently implemented by SRNL into a numerical model that accurately predicts the behavior of an adsorption-based storage system over a range of operating conditions and system configurations. UQTR is extending its thermodynamic model, which currently applies to adsorption on activated carbons, to other adsorbents.

Relevance

The ultimate goals of the HSECoE are the design and testing of prototype hydrogen storage vessels, the interpretation of test data, and the implementation for full-scale vessels. Within the HSECoE, the Transport Phenomena Technology Area is responsible for the development and application of analyses for storage systems that are necessary to identify and design prototype media and vessel configurations having the best performance relative to the DOE Technical Targets. Storage vessel models developed by this Technology Area will be essential to interpret data obtained from prototype testing and to relate it to full scale systems.

Approach

In Phase I, SRNL and UQTR will:

- Evaluate, interpret, and assimilate data for media and vessel components.
- Develop and apply an "Acceptability Envelope" based on DOE targets.
- Develop, validate and test general models for scoping and detailed evaluation of storage system designs.
- Obtain material operating requirements for metal hydride and AX-21 materials.
- Perform System Architect analysis on candidate metal hydride systems for Phase I Go-No-Go decision.

Results

SRNL and its subrecipient UQTR to date have met and or exceeded their Phase I objectives for all of their major technical areas for the HSECoE. These major technical areas include: Transport Phenomena, Adsorbent Systems Modeling, Material Operating Requirements and System Architecture. Transport Phenomena and Adsorbent System Modeling results are shown below for adsorbents systems. Results for activities under Material Operating Requirements and System Architecture are shown for metal hydrides systems.

Transport Phenomena

- Developed Detailed and Thermodynamic Models for Adsorbent-Based Storage Vessels
  - Applied to MaxSorb™ (MSC-30™) and MOF-5™ (Basolite Z100-H)
  - Validated MaxSorb™ model against test data
- Applied Models for Charging and Discharging of Storage Vessel
  - Charging characteristics (see Figure 1)
    - Charging models were applied for DOE 2015 Technical Target time of 198 seconds (3.3 minutes)

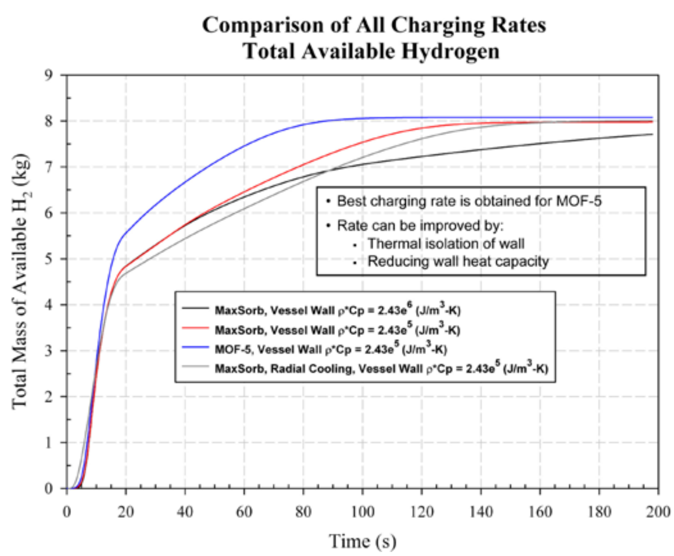


FIGURE 1. Comparison of system charging rate for different adsorbent materials and different wall thermal isolating conditions.

- Considered stored energy in vessel wall
- Heat removal by axial and radial convection via flow-through cooling
- Contributions of pressure work and heat of adsorption

– Discharging characteristics (see Figure 2)
  - Resistance heater
  - Flow-through cooling

Adsorbent System Modeling

- Developed and ran baseline system models for four adsorbent systems (AX-21 at 60 and 200 bar and MOF-5 at 60 and 200 bar) in support of the baseline Adsorbent System Go/No-Go decision (see Figure 3)
- Evaluated several tank heating input methods using the adsorbent system model
  – Hot hydrogen recirculation line
  – Heat switches
  – Internal resistance heater (currently the base case system option)
- Evaluated various heat exchanger options
  – None other than the exposed hydrogen piping
  – Air-to-hydrogen vessel heat exchanger
  – Air-to-fuel cell coolant heat exchanger (currently the base case system option)

Material Operating Requirements: Metal Hydrides

- Selected sodium aluminum hydride ($NaAlH_4$) material as initial baseline hydride candidate material for transport phenomena and system modeling development.
- Database updated for:
  – $NaAlH_4$ (with and without catalysts)
  – TiCrMn
  – Mg_2Ni
  – $8LiH{:}3Mg(NH_2)_2$
- Additional data added for:
  – 2:1 $LiNH_2{:}MgH_2$
  – 1:1 $LiNH_2{:}MgH_2$
  – MgH_2 (without catalysts)

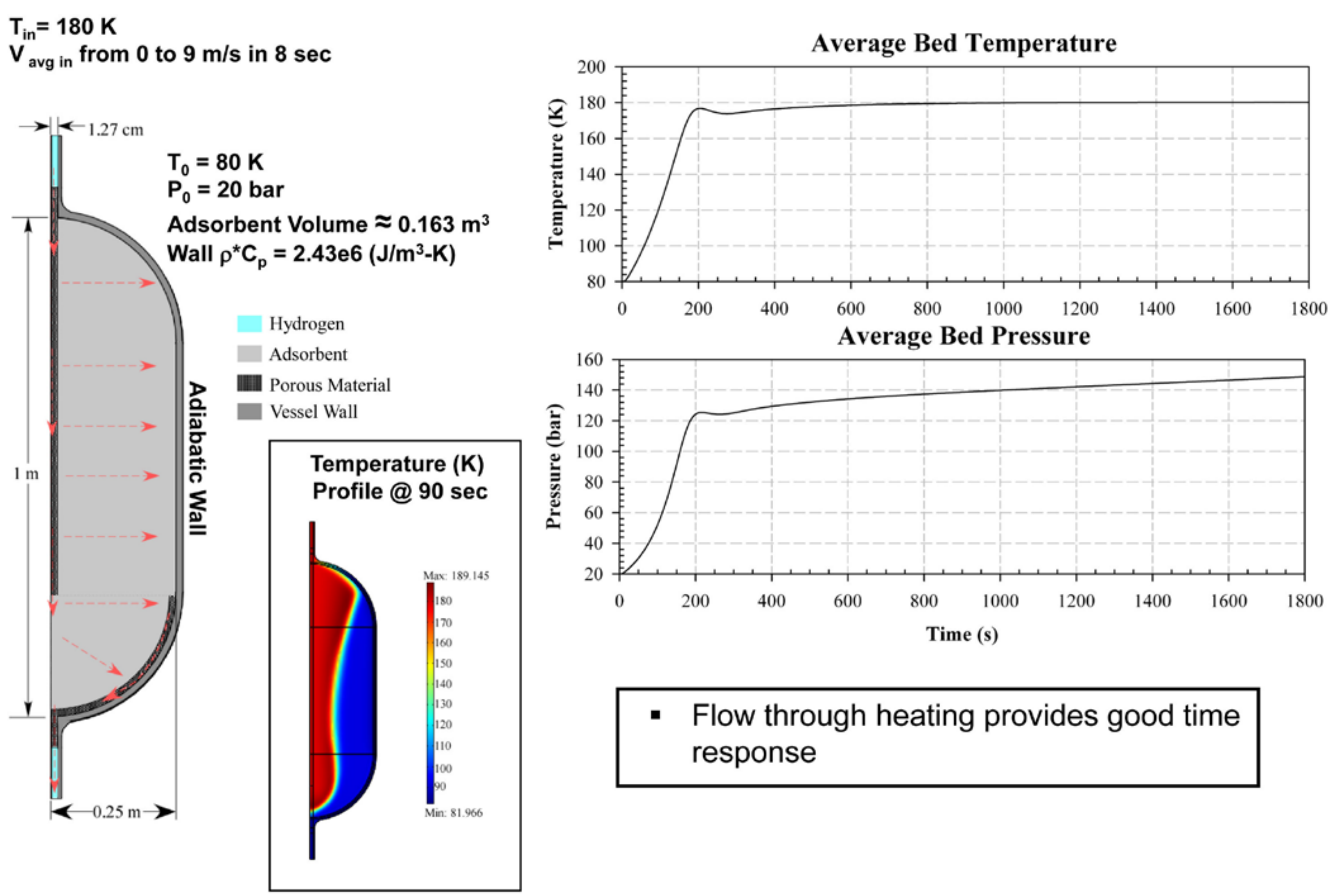


FIGURE 2. Average adsorbent bed temperature and pressure profiles with radial flow-through heating.

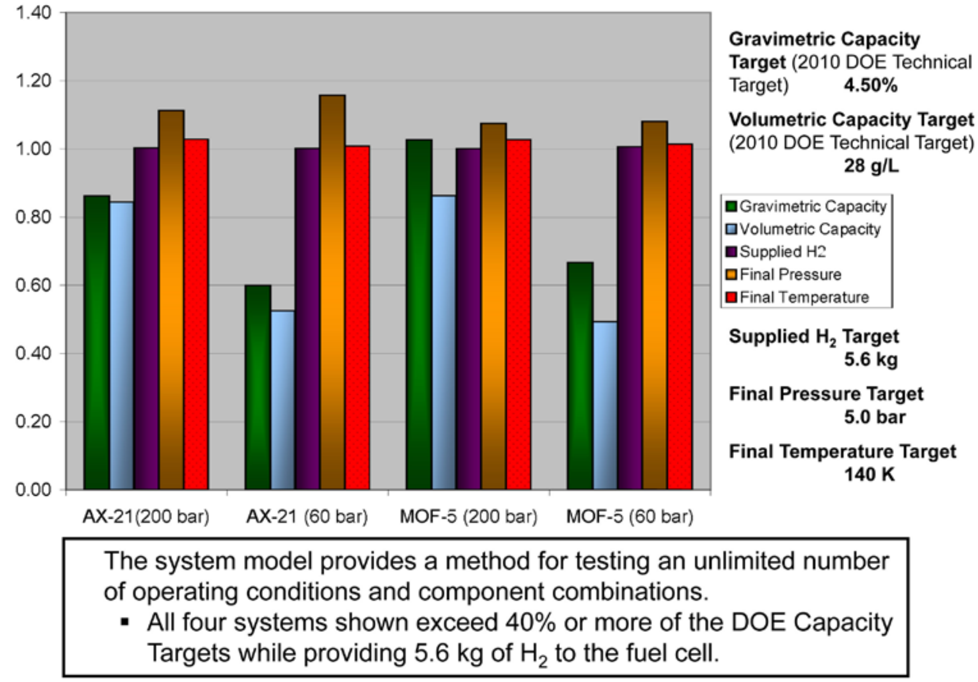


FIGURE 3. Adsorbent system modeling results compared to DOE 2010 system targets.

- Developed preliminary kinetic expressions for 2:1 $LiNH_2$:MgH_2 and 1:1 $LiNH_2$:MgH_2 to support system modeling analyses.
- Updated and improved the Acceptability Envelop to evaluate metal hydride materials for the Go/No-Go decision.

System Architect Analyses: Metal Hydride

- Selected Metal Hydride System for baseline Phase 1 Go/No-Go decision (see Figure 4).
- Documented selection criteria and assumptions for Metal Hydride Systems with respect to 2010 targets and Phase 1 Go/No-Go decision.
- Identified deficiencies and improvement areas for Metal Hydride Systems for Phase 2 development plan.

Conclusions and Future Directions

- Continue Metal Hydride System Architect analyses.
- Provide analyses for Phase 2 Go/No-Go decision.
- Investigate thermal and structural effects of bed expansion.
- Improve bed heat transfer for metal hydrides and adsorbents (expanded natural graphite addition and honeycomb lattice) - experiments will be guided by models.
- Investigate viability of flow-through concept for adsorbent systems.
- Optimize adsorbent system with respect to pressure work, enthalpy of hydrogen discharge flow, dormancy conditions and thermal interaction with container wall.

FY 2011 Publications/Presentations

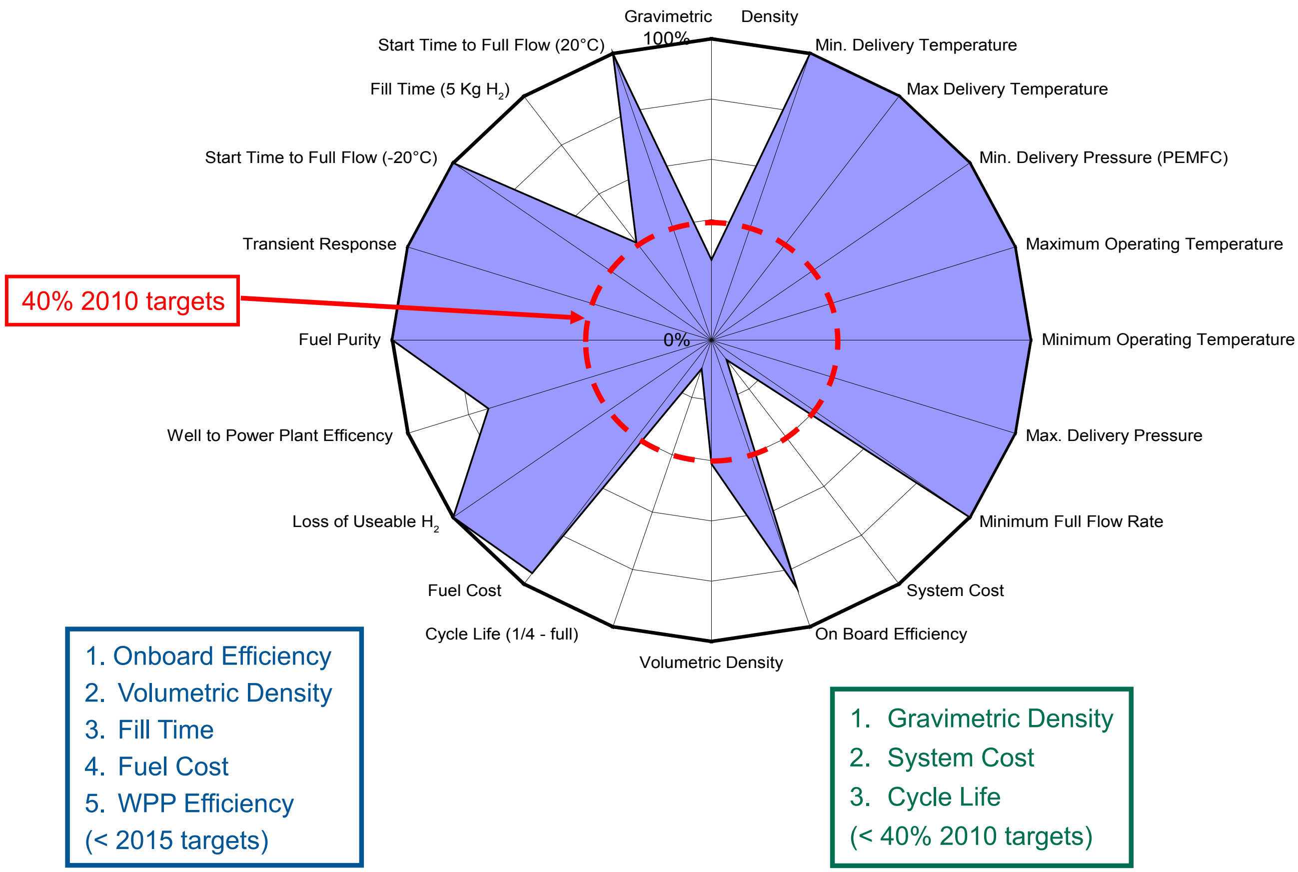
1. M. Bhouri, J. Goyette, B.J. Hardy, D.L. Anton. "Sensitivity study of alanate hydride storage system." International Journal of Hydrogen Energy 36 (2011) 621-633.

2. C. Corgnale, B. Hardy, D. Anton. "Development of an acceptability envelope for metal hydrides: a system analysis", IEA HIA TASK 22 Meeting, January 2011, Australia.

3. S.L. Garrison; C. Corgnale; B.J. Hardy; D.A. Tamburello; T. Motyka; D.L. Anton. "Automatic optimization of metal hydride storage tanks and analysis of material property envelopes." Presented at the Pacifichem 2010 conference Dec.15–20, Honolulu, HI.

4. B. Hardy, C. Corgnale, R. Chahine, M-A Richard, D. Tamburello, S. Garrison, D. Anton. "Modeling of Adsorbent Based Hydrogen Storage Systems." Presented at the special session Hydrogen Storage System Engineering and Applications: Heat and Mass Transfer, of the AIChE 2010 Annual Meeting Nov 7–12 in Salt Lake City, Utah.

5. C. Corgnale, B. Hardy, D. Tamburello, S. Garrison and D. Anton. "Evaluation of Acceptability Envelope for Materials-Based H2 Storage Systems." Presented at the special session Hydrogen Storage System Engineering and Applications: Heat and Mass Transfer, of the AIChE 2010 Annual Meeting Nov 7–12 in Salt Lake City, Utah. Full paper submitted to the IJHE and currently in review.



PEMFC - proton exchange membrane fuel cell

FIGURE 4. “Spider” chart showing baseline metal hydride case for the sodium alanate system versus DOE 2010 targets.

6. S. Garrison, M. Gorbounov, D. Tamburello, B. Hardy, C. Corgnale, D. Mosher and D. Anton. “Automatic Optimization of Metal Hydride Storage Tanks and Novel Designs.” Presented at the special session Hydrogen Storage System Engineering and Applications: Heat and Mass Transfer, of the AIChE 2010 Annual Meeting Nov 7–12 in Salt Lake City, Utah. Full paper submitted to the IJHE and currently in review.

7. R. Chahine, “Evaluation of Sorption System for Hydrogen Storage” Presented at the special session Hydrogen Storage System Engineering and Applications: Heat and Mass Transfer, of the AIChE 2010 Annual Meeting Nov 7–12 in Salt Lake City, Utah. Full paper submitted to the IJHE and currently in review.