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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Projected End Date:  July 31, 2014

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.

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-50™) 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)

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.
- 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

\[ T_{in} = 180 \text{ K} \]
\[ V_{avg, in} \text{ from 0 to 9 m/s in 8 sec} \]

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

**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\(_2\)Ni
  - 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)
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 Envelope 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

- 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


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 Pacificchem 2010 conference Dec.15–20, Honolulu, HI.

