System Design and Media Structuring for On-board Hydrogen Storage Technologies

Darsh Kumar
General Motors
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Project ID: STP_12_Kumar
Overview

Timeline
Project start – Feb 1, 2009
   Phase I end – Jan 31, 2011
   Phase II end – Jan 31, 2013
Project end – Jan 31, 2014

Barriers Addressed
• System weight and volume (A)
• Energy efficiency (C)
• Charging/discharging rates (E)
• Thermal management (J)

Budget
DOE: $2,954,707
GM match: $738,677
Budget spent: < 5%

Partners
• SRNL
• UTRC
• Ford
• UQTR
• Other HSECoE partners
Major Objectives

• Develop system simulation models for on-board rechargeable (metal hydride and adsorbent) hydrogen storage systems

• Develop models for mass and energy transport in metal hydride and adsorbent beds

• Optimize mechanical stability, thermal properties, and hydrogen uptake of metal hydride and adsorbent media

• Design and build a vessel for adsorbent bed model validation and determination of fast-fill and discharge characteristics of an adsorption system

• Participate in prototype designs, data analysis and model validation
Systems Engineering

Integrated Power Plant / Storage System Modeling

D. Mosher, UTRC

Framework Development & Power Plant Modeling
Ford
UTRC, GM

On-Board Rechargeable System Modeling & Integration
GM
Ford, UTRC

Off-Board Rechargeable System Modeling & Integration
UTRC
Ford, GM
Technology Area: Integrated System Modeling  
Technology Team: On-Board Rechargeable Systems  
Date: March 17, 2009

**Objectives:**
- Develop representations for on-board rechargeable adsorbent and hydride storage systems consistent with a common simulation platform and power plant model.
- Determine storage system baseline requirements.
- Establish representations consistent with the modeling strategy for vehicle level optimization studies.
- Develop system simulation models for the prime material candidates and system configurations.
- Conduct simulations of integrated power plant / storage system performance for key operational conditions.

**Accomplishments:**
- Identified MATLAB/Simulink as the common platform for building FC and storage system simulation models

**Key Milestones:**
1. Identify materials and baseline configurations for hydrogen storage system simulation. (6/09, GM/Ford)
2. Develop initial representations of system models. (9/09, GM)
3. Identify baseline hydrogen storage system requirements. (12/09, All)
4. Develop detailed representation consistent with power-plant and vehicle level models. (3/10, GM)
5. Establish generic operating profiles and conduct interaction evaluation of models. (6/10, Ford/GM)
6. Provide initial model method and results for Phase 1 Go/No-Go deliverables. (10/10, All)

**Issues:**
- Objectives requires close cooperation with FC modeling team and vehicle level modeling team to identify appropriate interactions with their modeling efforts.
**On-Board Rechargeable Systems**

**Compressed H₂ Storage**

Storage as compressed gas or cryogenic liquid

\[ T \approx 25 \, ^\circ\text{C} \]
\[ P \approx 350-700 \, \text{bar} \]

**Liquid H₂ Storage**

\[ T \approx -253 \, ^\circ\text{C} \]
\[ P \approx 1-2 \, \text{Bar} \]

**Solid State Storage**

Complex metal hydrides (reaction)

\[ \text{NaAlH}_4 \rightarrow \frac{1}{3}\text{Na}_3\text{AlH}_6 + \frac{2}{3}\text{Al} + \text{H}_2 \]
\[ \text{Na}_3\text{AlH}_6 \rightarrow 3\text{NaH} + \text{Al} + \frac{3}{2}\text{H}_2 \]

**Interstitial metal hydrides (absorption)**

\[ T \approx -196 \, ^\circ\text{C}, P \approx 20 \, \text{bar} \]

\[ T \approx 85 \, ^\circ\text{C}, P \approx 350 \, \text{bar} \]

**Cryo-adsorption**

\[ T \approx 200 \, ^\circ\text{C}, P \approx 125 \, \text{bar} \]

Source: www & literature

DOE Annual Merit Review
Transport Phenomena

B. Hardy, SRNL

Mass Transport
- SRNL
  - LANL, OSU, PNNL, GM, UTRC, UQTR, Ford

Thermal Transport
- SRNL
  - LANL, JPL, OSU, PNNL, UQTR, UTRC, GM, Ford

Bulk Materials Handling
- PNNL
  - LANL, UTRC, HSM, UQTR, Ford, GM

Media Structure and Enhancement
- GM
  - Ford, SRNL, PNNL, UQTR, UTRC

DOE Annual Merit Review
**Technology Area:** Transport Phenomena  
**Technology Team:** Media Structuring & Enhancement  
**Date:** March 17, 2009

**Technology Team Lead:** S. Kumar  
**Team Members:** GM, Ford, UTRC, UQTR, SRNL

<table>
<thead>
<tr>
<th>Objectives:</th>
<th>Accomplishments:</th>
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</table>
| • Select metal hydride (MH), activated carbon (AC) and framework materials (FM) for structured material studies  
• Test binders, additives, and processing schemes for enhanced mechanical stability, thermal properties and kinetics  
• Optimize composition and processing methods for thermal properties and H2 uptake/discharge rates  
• Measure engineering properties and durability of optimized structural materials | |

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<thead>
<tr>
<th>Key Milestones:</th>
<th>Issues:</th>
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| • Literature review of metal hydride, AC and FM for structured material studies (All) (5/01/09)  
• Select metal hydride (GM, UTRC), AC (GM, UQTR) and FM (Ford, GM) materials for experimental investigation (07/01/09)  
• Coordinate characterizing powder MH, AC, and FM materials for thermal properties and hydrogen uptake with materials requirements team(08/01/09)  
• Preliminary experiments with respective binders, additives, and processing schemes for enhanced mechanical stability, thermal properties, and hydrogen uptake (GM, Ford, UTRC) (11/01/09) | • Coordinate efforts with bulk transport Tech Team |
Phase I – Storage System Simulation Models

- Identify common modeling framework and develop initial representation of hydrogen storage system models
- Develop preliminary simulation models
- System integration with generic FC model
- Analysis of storage system ability to meet fuel cell hydrogen flow requirements
  - Adsorption system
  - Metal hydride system
- Use of realistic fuel cell drive cycles
  - Typical urban drive cycle
  - Extreme drive cycle
MH System – H₂ Absorption Schematic

**Control Block**
- Bed Temp
- Concentrations
- Coolant Temp
- H₂ Pressure
- H₂ Supply Pressure

**Hydride Bed**
- Bed Temperature
- H₂ Supply Pressure
- Species Concentrations
- Kinetics
  - a + b ⇄ c + d

**Heat Transfer**
- Bed Temperature
- Concentrations
Adsorption System - Modeling Approach & Hierarchy

Refueling << Discharge << Dormancy << Venting
minutes << hours << days << weeks

Fast process

Slow processes

Mass balance
Momentum balance
Energy balance
Adsorption kinetics
Thermodynamics

0-D model
Slow processes
1-D model
Refueling
2-D model
Flow maldistribution
Tank design
System model
Drive cycle response
System integration with fuel cell model

Refueling << Discharge << Dormancy << Venting minutes << hours << days << weeks

HSECoE

DOE Annual Merit Review 12
A lumped parameter model will be used to study the system dynamics during discharge and to:

- Identify the operating regimes where hot gas recirculation is necessary
- For a typical drive cycle hydrogen demand, study the storage system response and identify the optimal control strategy.
Status of Adsorption Bed Simulations

- A lumped parameter model for simulation of all four tank processes has been developed
- For the slower processes (discharge, dormancy and venting) a lumped parameter model is expected to be sufficient
- For refueling - the fastest process - higher dimensional models may be required because of significant temperature gradients expected in the tank
- Storage system model will be developed using the lumped parameter model for the adsorption system tank as well as the balance of plant components (pump, heater and controller)
- A hierarchy of models will be developed to study refueling and other issues associated with the adsorption system storage tank
Phase I – Mass and Energy Transport in Storage Beds

- Assessment of the ability of existing metal hydrides and adsorbents to meet DOE technical targets
- Initial models of storage system designs with generic materials; Lumped parameter and 1-D models for
  - Adsorbent material systems (AM)
  - Metal hydride systems (MH)
- Performance sensitivity studies
- Refueling studies
- Dormancy and boil-off analysis for adsorption system
- Select designs that hold promise to meet DOE 2015 goals for further analysis
Phase I – Media Structuring and Enhancement

• Develop MH and adsorbent material composites with enhanced thermal properties
  – Pellets, disks, and similar shapes
  – Metal hydride/adsorbent material, heat transfer enhancing materials, and binders
  – Goal of increasing thermal conductivity by 10 X with minimal impact on hydrogen absorption/adsorption characteristics

• Measure hydrogen uptake and engineering properties as a function of H₂ content for metal hydrides and adsorbent materials
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<tr>
<th>Date</th>
<th>Milestone Description</th>
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<tbody>
<tr>
<td>Sep ’09</td>
<td>Identify materials and develop initial representations of system simulation models</td>
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<td>Sep ’09</td>
<td>Preliminary assessment of the ability of existing media to meet 2010 and 2015 DOE targets</td>
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<tr>
<td>Nov ’09</td>
<td>Preliminary experiments to develop structured media with enhanced thermal properties</td>
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<td>Nov ’09</td>
<td>Lumped parameter models suitable for MH and AM system simulations</td>
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<tr>
<td>Nov ’09</td>
<td>Design of a small cryogenic adsorbent material vessel for model validation studies</td>
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<tr>
<td>Mar ’10</td>
<td>System simulation model studies</td>
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Phase II – System Simulation Models

- Refine storage systems models for metal hydride and adsorbent material systems
- Integration with fuel cell model to meet requirements
- Forecourt requirements determination through modeling and analysis for energy efficient refueling
- Participate in subscale prototype designs for metal hydride and adsorbent bed technologies
Phase II: Mass and Energy Transport in Storage Beds

- Refine 2-D storage system models for MH and adsorbent bed technologies
  - Include specific geometry
  - Enhanced mass, energy, and momentum transfer as appropriate
  - Refueling and discharge studies
  - Dormancy and boil-off studies for adsorbent bed systems

- Simulations and validation of selected systems

- Evaluation of systems with potential future materials and compare to DOE goals
Phase II: Adsorbent Materials Systems Kinetics, Refueling and Discharge Characteristics

- Validate mass and energy transport models and study adsorption characteristics of various cryoadsorbents in a cryoadsorbent vessel
- Measure axial and radial temperature profiles in the bed
- Pressure drop across bed
- Vessel capable of material exchange to test various materials
Phase III

- Design of experiments for subscale prototype tests
- Analysis and evaluation of data from subscale tests
- Storage system model validation and refinement based on test data
Collaborations

- System simulation models – UTRC, Ford
- Media structuring and enhancement – UTRC, Ford, UQTR
- Mass and thermal energy transport – SRNL

GM Team

- Darsh Kumar – Principal Investigator
- Senthil Kumar V.
- Michael Herrmann
- Jerry Ortmann
- Mei Cai
- Scott Jorgensen