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

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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%

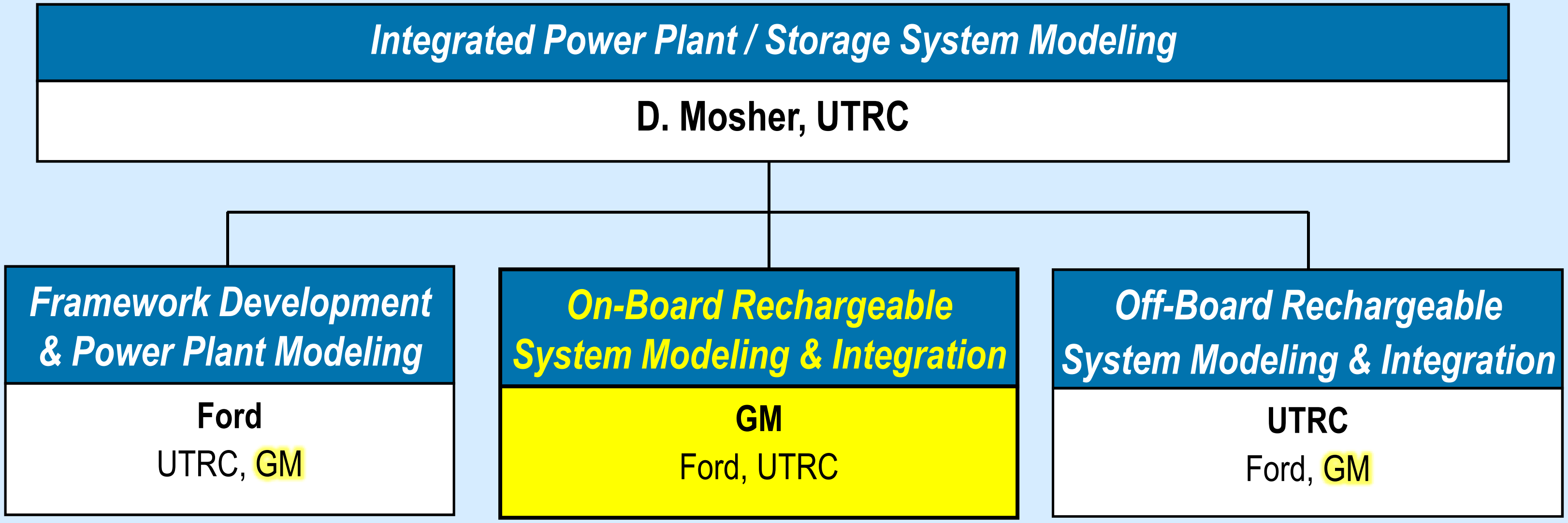
Partners

- 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



Technology Area: Integrated System Modeling

Technology Team Lead: S. Kumar

Technology Team: On-Board Rechargeable Systems

Team members: GM, Ford, UTRC

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 H_2 Storage

T ~ 25 °C
P ~ 350-700 bar

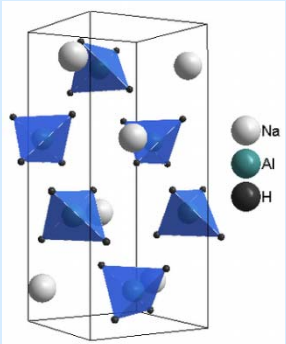
Storage as compressed gas or cryogenic liquid

Liquid H_2 Storage

T ~ -253 °C
P ~ 1-2 Bar

Solid State Storage

Complex metal hydrides (reaction)

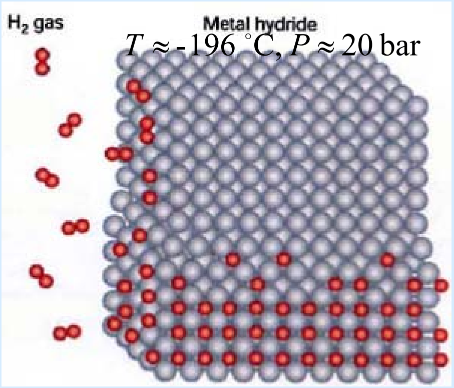


$$NaAlH_4 \rightarrow \tfrac{1}{3}Na_3AlH_6 + \tfrac{2}{3}Al + H_2$$

$$Na_3AlH_6 \rightarrow 3NaH + Al + \tfrac{3}{2}H_2$$

$T \approx 200\ ^{\circ}C, P \approx 125$ bar

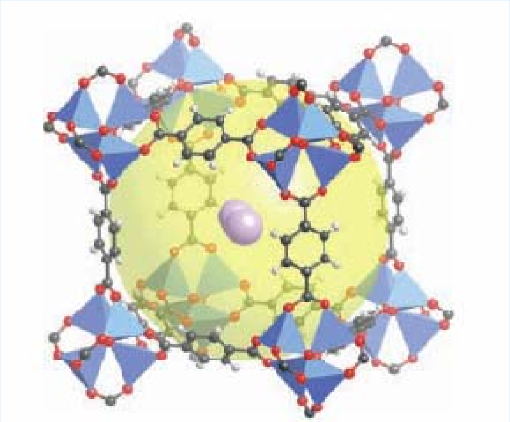
Interstitial metal hydrides (absorption)



$Ti_{1.08}Cr_{1.04}\ Mn_{0.96}$

$T \approx 85\ ^{\circ}C, P \approx 350$ bar

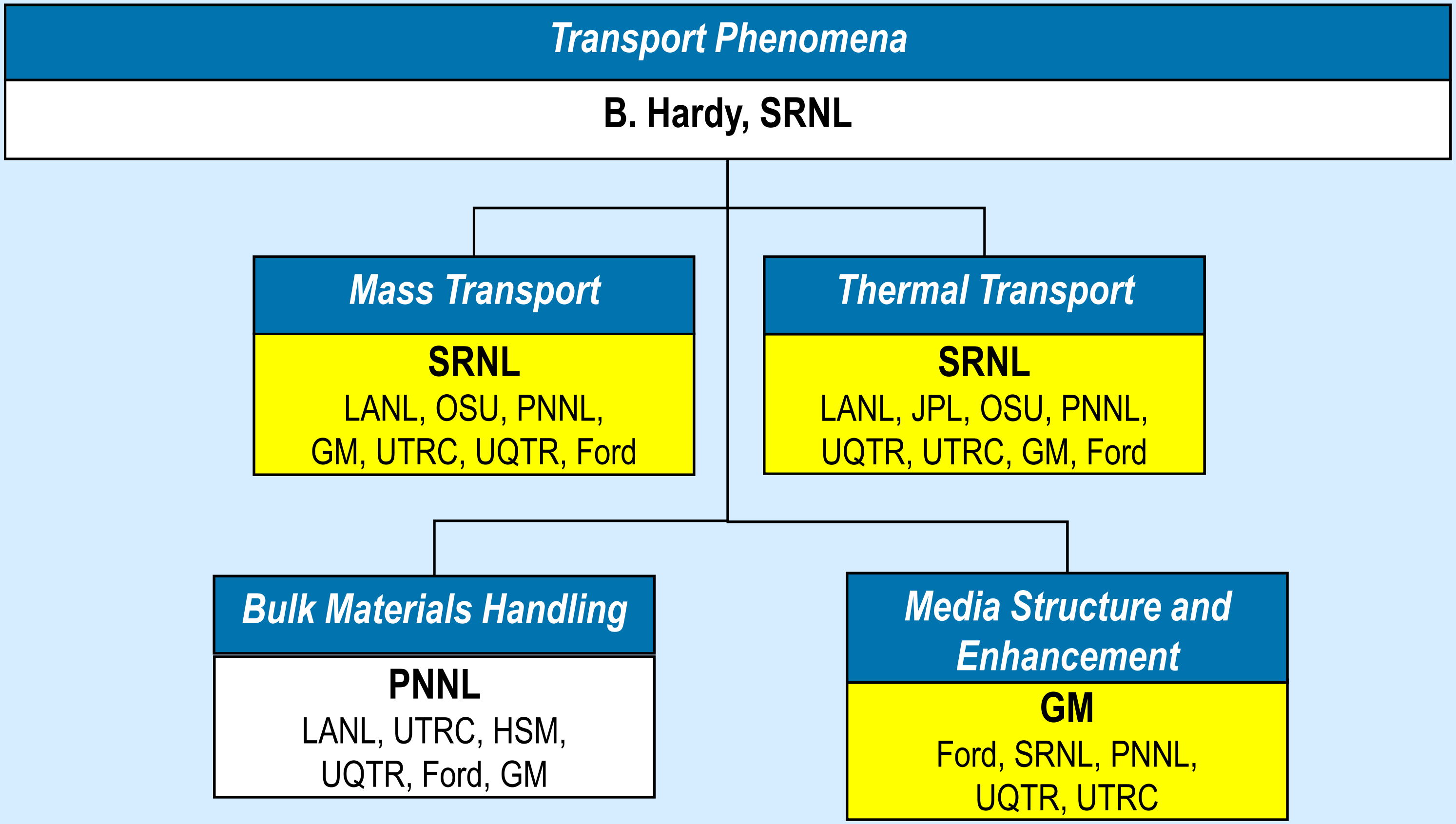
Cryo-adsorption



MOFs, ACs

Source: www & literature

Transport Phenomena



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

Objectives:

- 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

Accomplishments:

Key Milestones:

- 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)

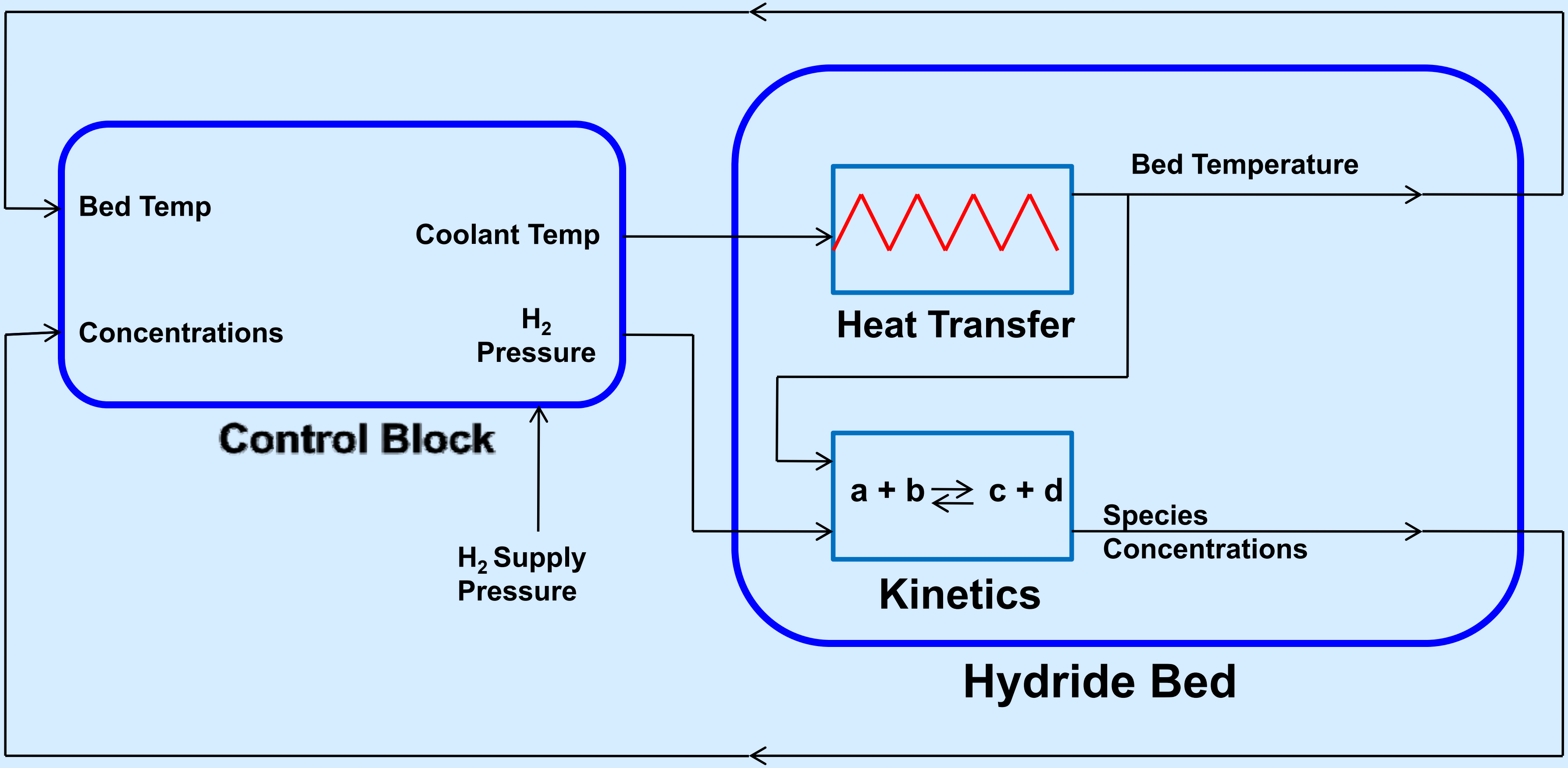
Issues:

- **Coordinate efforts with bulk transport Tech Team**

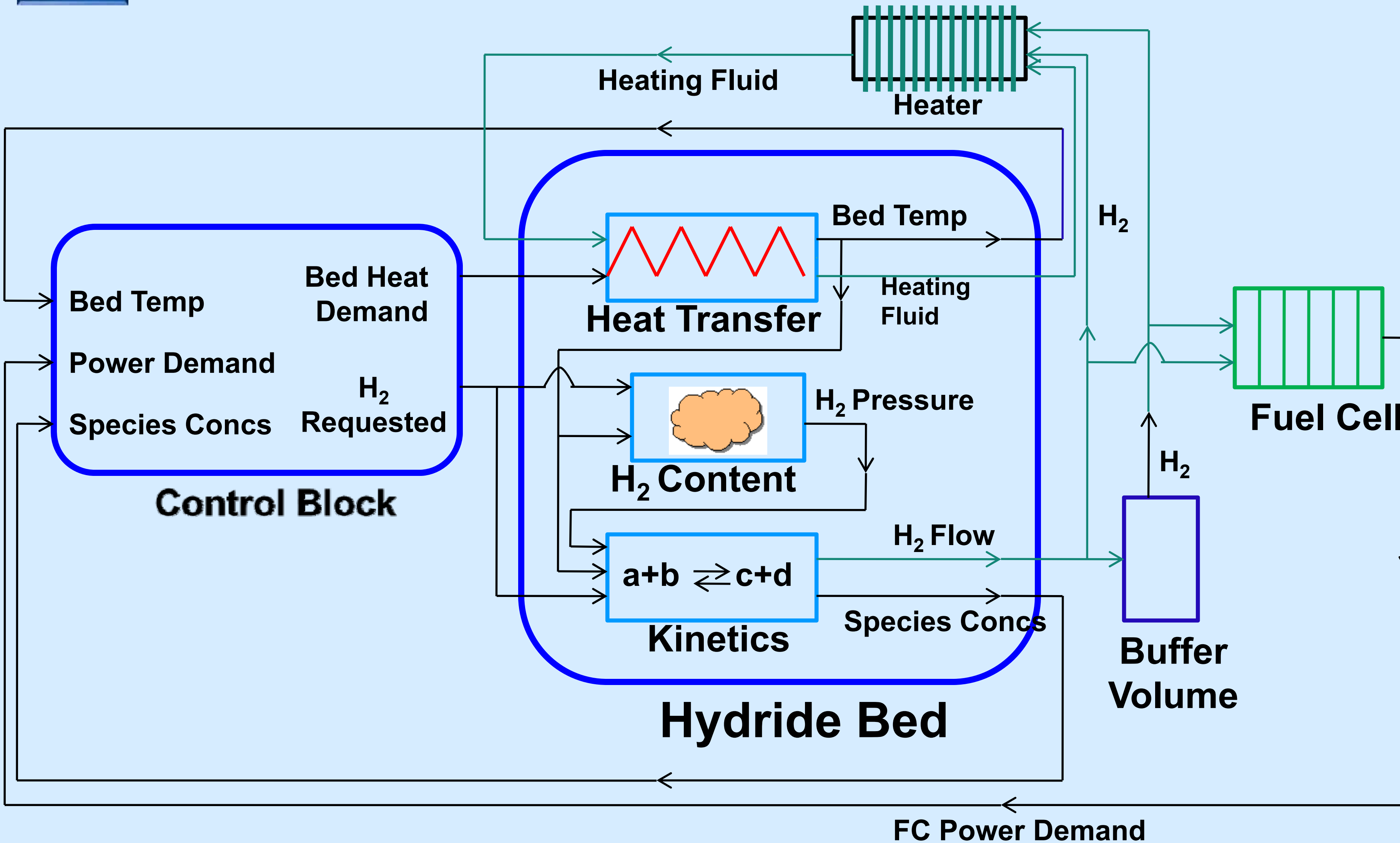
Phase I – Storage System Simulation Models

- 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 – H_2 Absorption Schematic



MH System – H_2 Desorption Schematic



Adsorption System - Modeling Approach & Hierarchy

Refueling << Discharge << Dormancy << Venting

minutes << hours << days << weeks

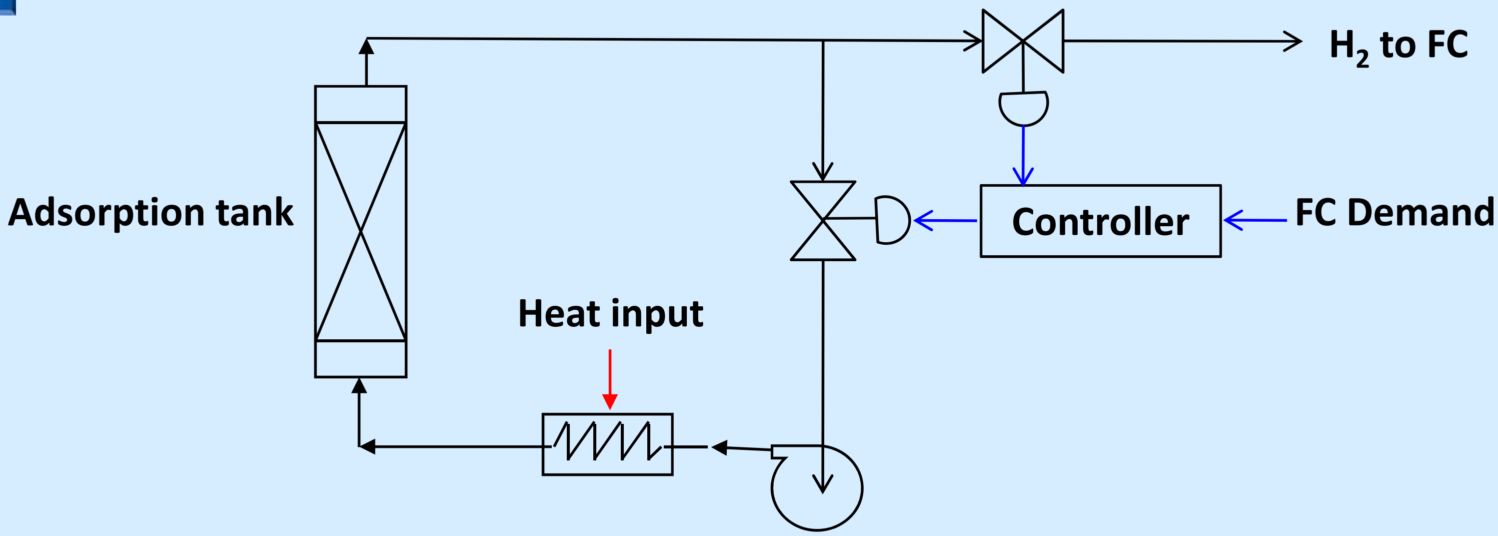
Fast process | Slow processes

- Mass balance
- Momentum balance
- Energy balance
- Adsorption kinetics
- Thermodynamics

→

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

System Modeling - Adsorption System



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 H_2 content for metal hydrides and adsorbent materials

Planned Milestones

Sep ’09	Identify materials and develop initial representations of system simulation models
Sep ’09	Preliminary assessment of the ability of existing media to meet 2010 and 2015 DOE targets
Nov ’09	Preliminary experiments to develop structured media with enhanced thermal properties
Nov ‘09	Lumped parameter models suitable for MH and AM system simulations
Nov ‘09	Design of a small cryogenic adsorbent material vessel for model validation studies
Mar ‘10	System simulation model studies

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