Optimization of Heat Exchangers and System Simulation of On-Board Storage Systems Designs

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General Motors Company

Project ID: ST009

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Overview

Timeline

- Project Start: February 2009
- Phase I end: Mar 2011
- Phase II end: July 2013
- Project end: June 2014
- % complete: 35%

Relevance/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
- Funding in FY 10: $750,000
- Funding for FY 11:$475,000

Partners

United Technologies Research Center

JPL

Ford

SRNL Savannah River National Laboratory

Pacific Northwest National Laboratory

NREL National Renewable Energy Laboratory

Lincoln Composites

Plan and Approach

System Simulation Models and Detailed Transport Models for Metal Hydrides:

- System simulation models for metal hydrides, incorporate in the integrated framework
- Build detailed 2-D models to include heat transfer, chemical rxns, guide system models
- Novel heat exchanger designs
- Optimization of heat exchanger designs
- Test simulation models for system performance, performance metrics in relation to DOE targets

System Simulation Models and Detailed Transport Models for Adsorbent Systems (with SRNL):

- System simulation models for activated carbon and MOF-5
- Build 2-D models to include adsorption and heat transfer to guide system models
- Identify system operating conditions for high gravimetric density
- Test simulation models for system performance, performance metrics in relation to DOE targets

Pelletization of AX-21 and sodium alanate (with UTRC):

- Binders and additives for pelletization
- Test various binders and additives for pelletization
- Measure hydrogen uptake, thermal conductivity, and pellet strength

Other Tasks (with HSECoE partners):

- OEM Team's prioritization of DOE Technical targets
- Development of an integrated framework including the vehicle, fuel cell, and H_2 storage system models
- Integration of hydrogen storage models in a common framework

Introduction

- **Metal Hydride Systems:**
  - For known materials, system capacity too low to meet on-board system performance goals. Surrogate materials: a complex MH (sodium alanate) and a high-pressure MH ($Ti_{1.1}CrMn$)
  - System models developed focus on system design and engineering improvements
  - Models built to evaluate performance of different systems on a common HSECoE Framework using same set of 4 drive cycles
- **Heat exchanger designs and optimization – Detailed models**
  - MH in bed with cooling tubes and interconnected aluminum fins
  - Helical coil heat exchanger design
  - MH in tubes and coolant in shell
  - Each design optimized by varying the geometric parameters
- **System operation for 4 Drive Cycles**
  - Mass balance for hydrogen
  - System performance in relation to DOE targets
- **Cryo-adsorbent systems (with SRNL)**
  - System design and simulations
- **Pelletization of storage media**
- **Other contributions to the HSECoE**

Metal Hydride Systems

For modeling, it is necessary to choose a surrogate material

Sodium alanate chosen as the surrogate material because of data availability

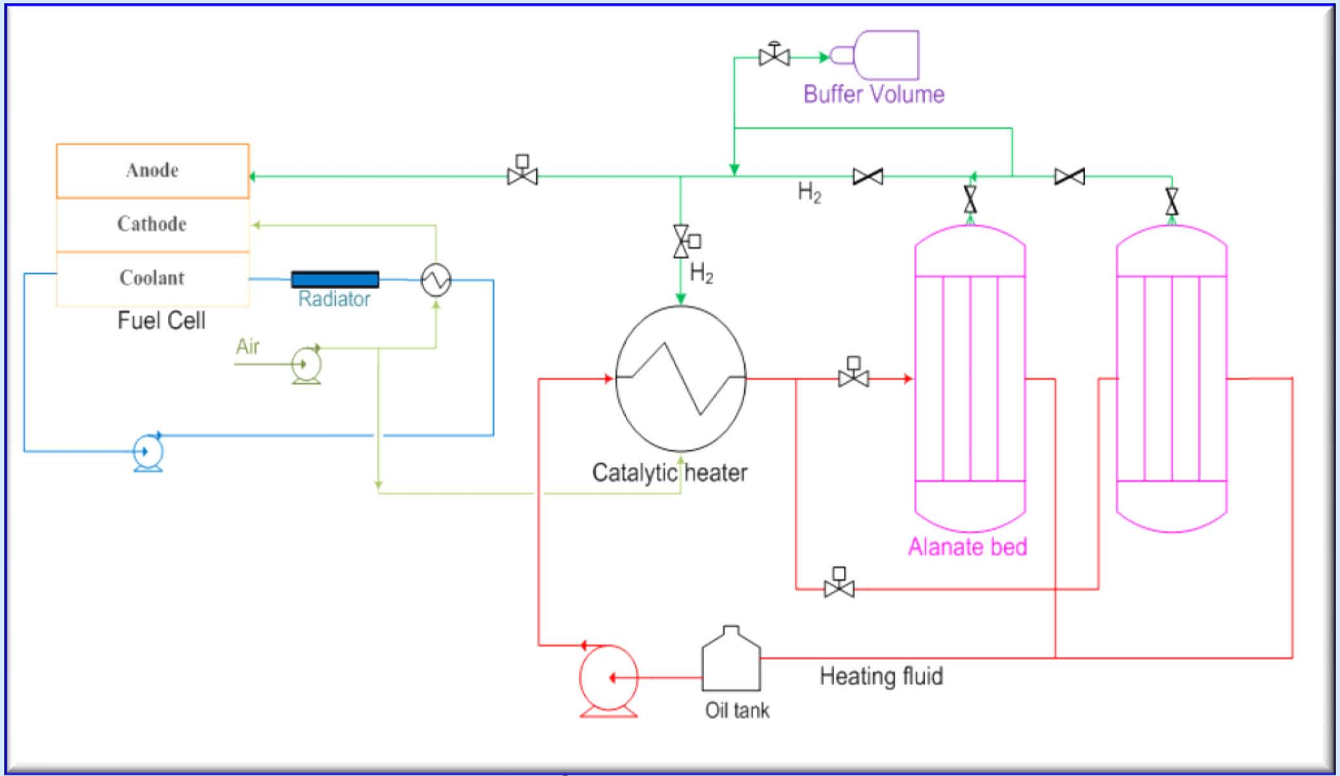
- Complex metal hydrides characterized by high heat of absorption/desorption
- Reactions proceed significantly only at high temperatures
- Thermal management of the system during refueling is challenging
- *Need to explore optimized heat exchanger designs*

$$NaAlH_4 \leftrightarrow 1/3\ Na_3AlH_6 + 2/3\ Al + H_2 \qquad \Delta H = -37\ \text{kJ/mole}\ H_2$$

$$1/3\ Na_3AlH_6 \leftrightarrow NaH + 1/3\ Al + \tfrac{1}{2}\ H_2 \qquad \Delta H = -47\ \text{kJ/mole}\ H_2$$

Multiple Bed Storage System for MH Systems

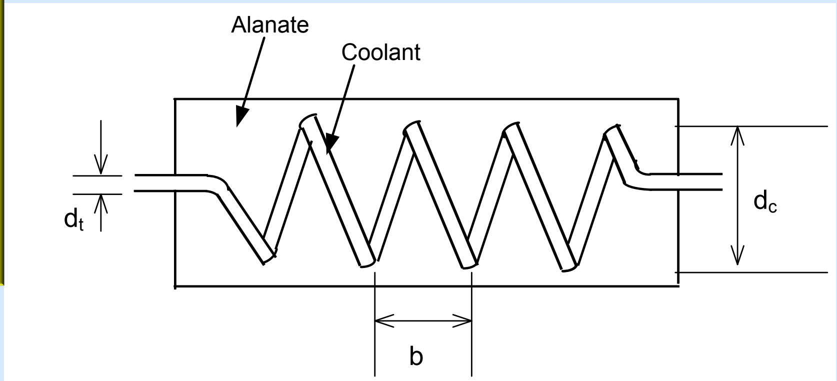
- System models necessary for evaluation of system performance relative to DOE targets
- Multiple bed design considered – important because of vehicle architecture , energy efficiency , or heat exchanger design
- Beds sized for 5.6 kg deliverable H2
- A catalytic burner to supply heat of desorption and a buffer volume possibly necessary for cold starts
- System model must include control scheme to transfer control among the beds and buffer



Heat Exchanger Designs

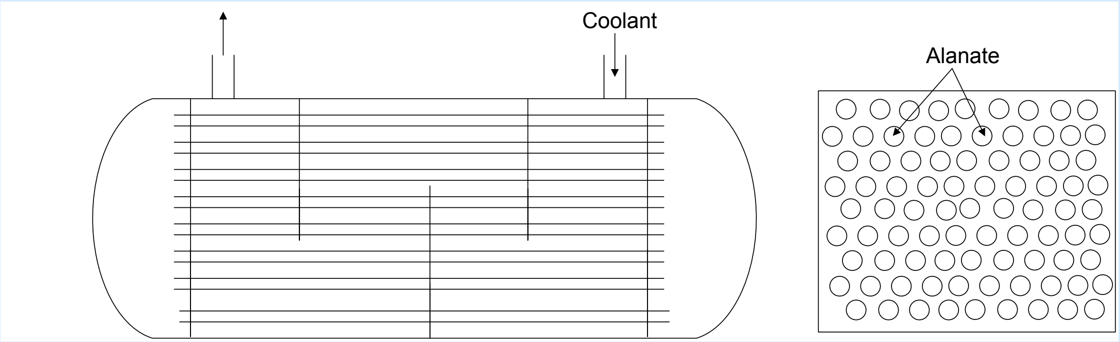
- Heat exchangers very important part for system mass and volume
- Multiple heat exchanger designs
- Optimize each type of heat exchanger design
- Choose the best

Design - II

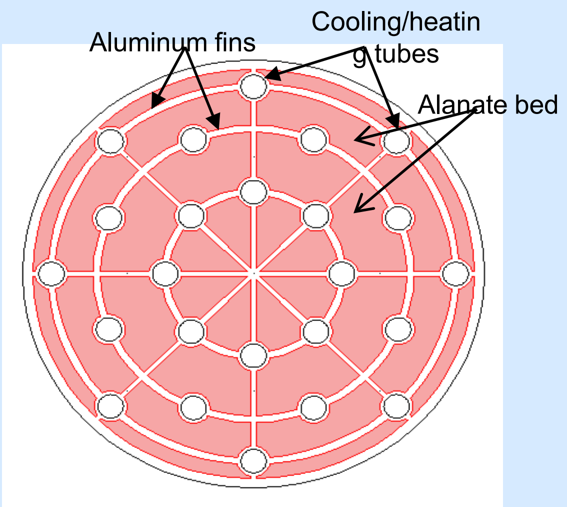


HELICAL COIL HEAT EXCHANGER WITH ALANATE IN SHELL

Design - III



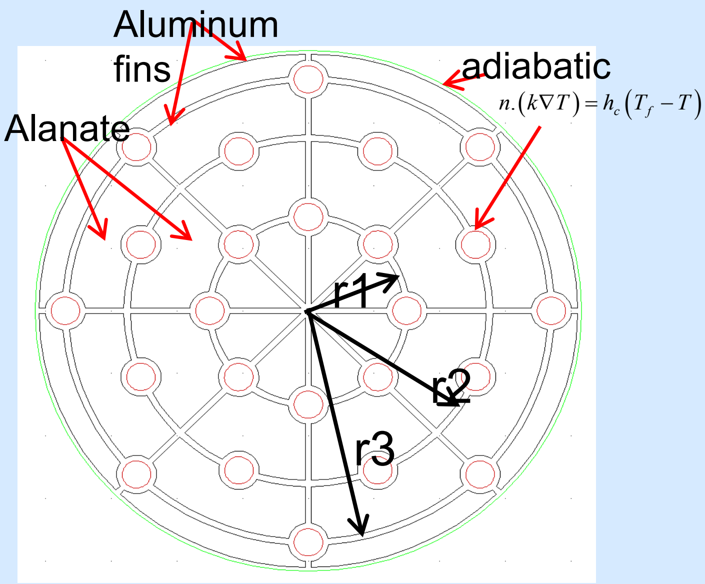
SHELL AND TUBE HEAT EXCHANGER WITH ALANATE IN TUBES



Design - I

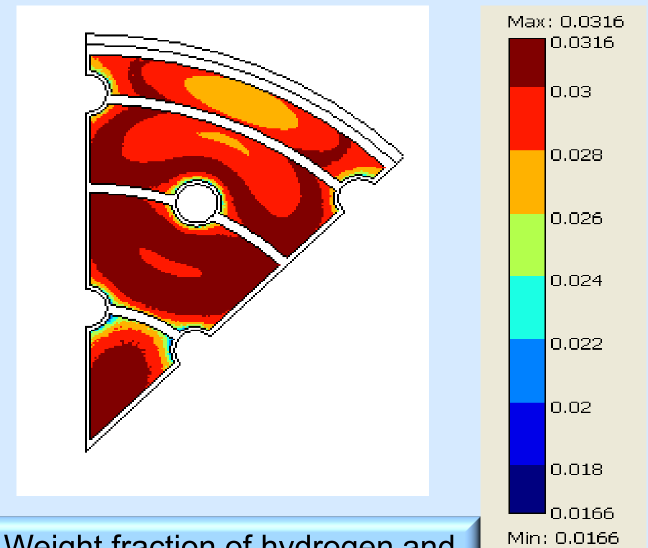
SHELL AND TUBE HEAT EXCHANGER WITH ALANATE IN SHELL

Heat Exchanger Design - I: Dual Bed Design

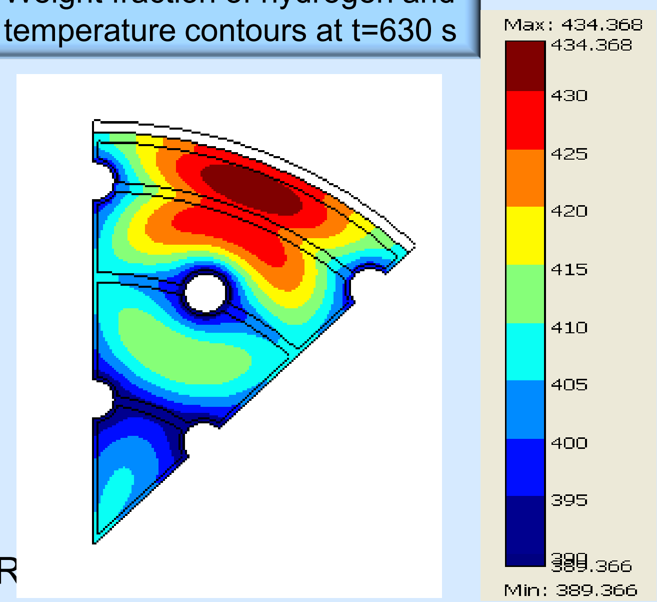


- For this design 2-beds necessary
- Control scheme to be devised for transfer of control between beds and buffer
- For design optimization, parameters varied
  - Bed diameter, r1, r2, and r3
  - Fin and tube thickness
  - Tube diameter

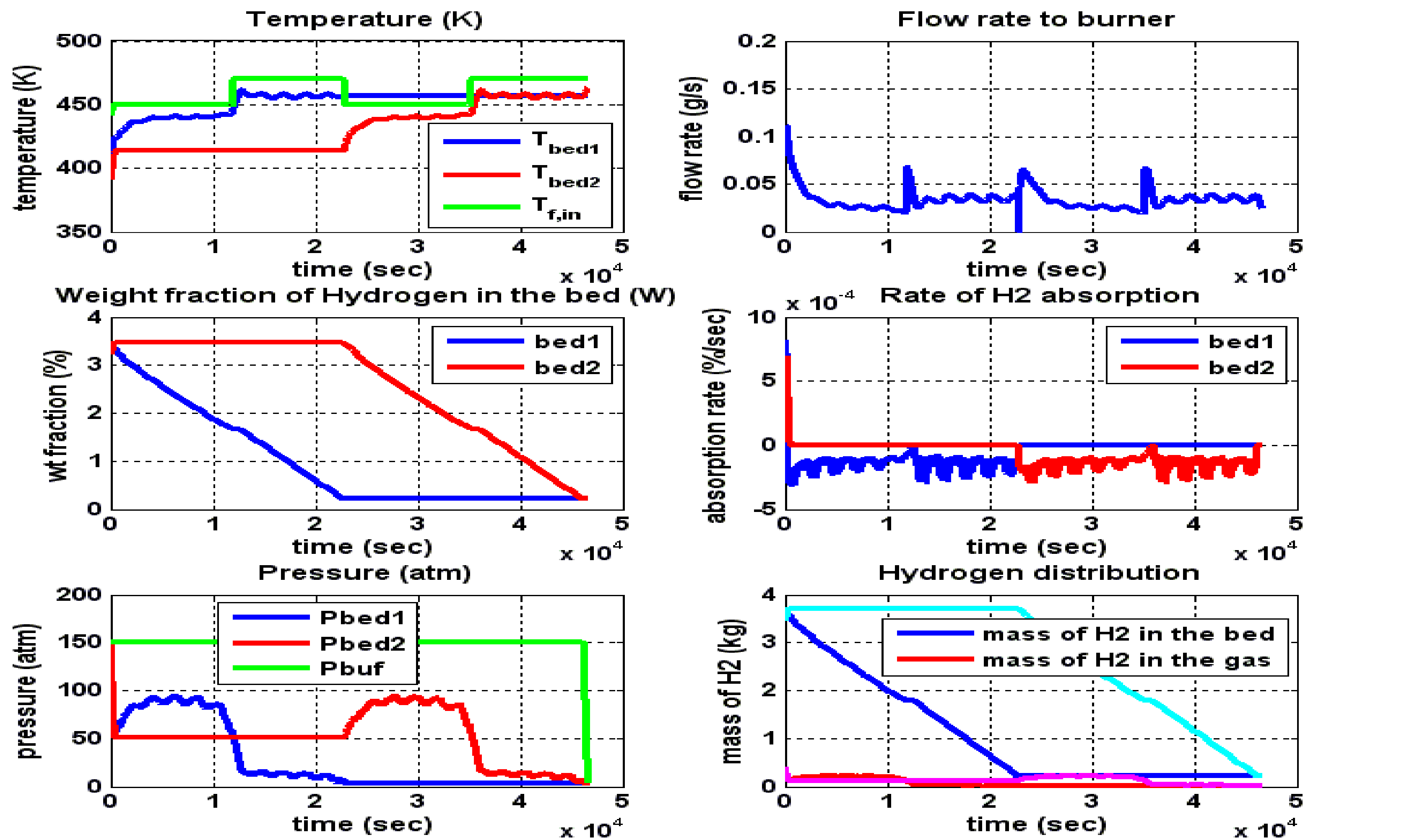
System Charging: 2-D COMSOL Simulation



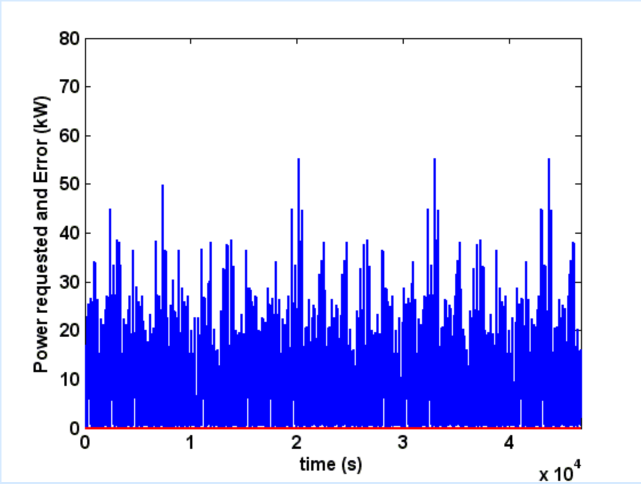
Weight fraction of hydrogen and temperature contours at t=630 s

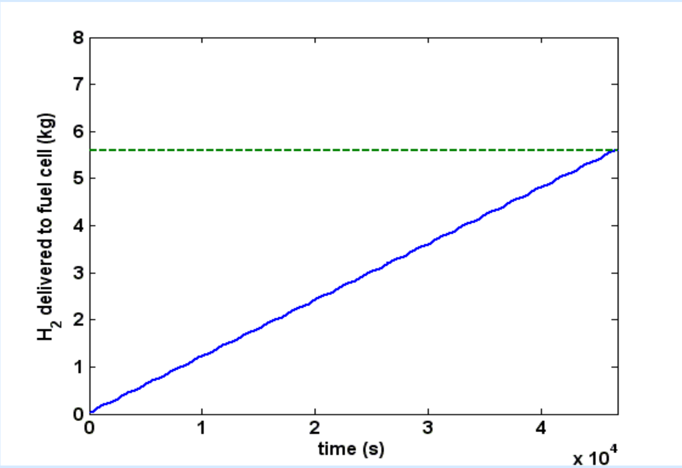


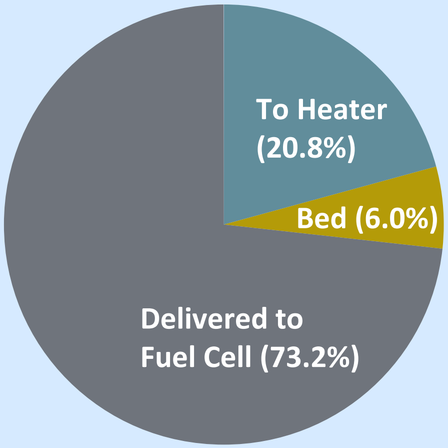
Dual Bed Design Results for Drive Cycle 1



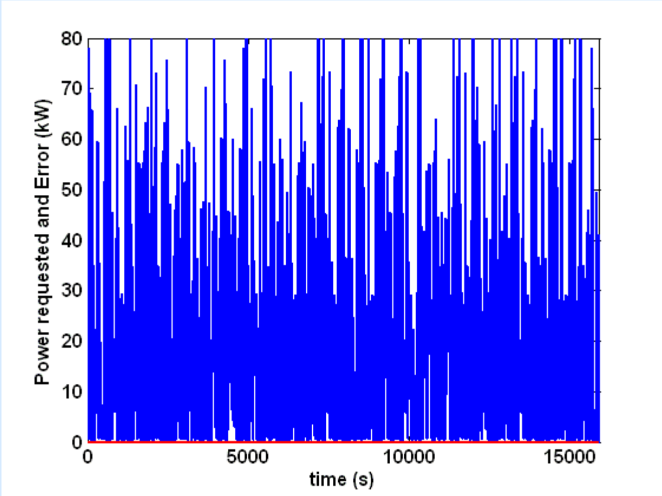
Drive Cycles 1 (Ambient) and 2 (Aggressive)

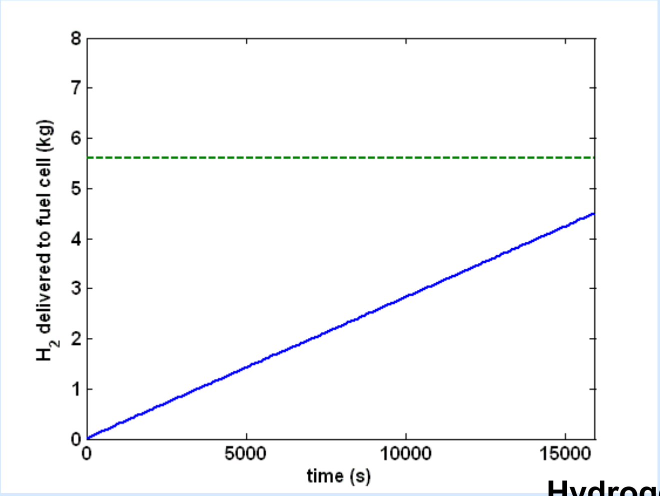


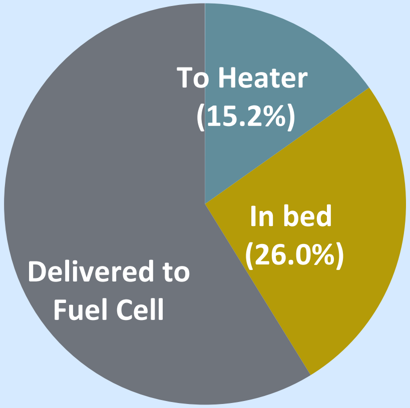




Hydrogen distribution: end of DC1



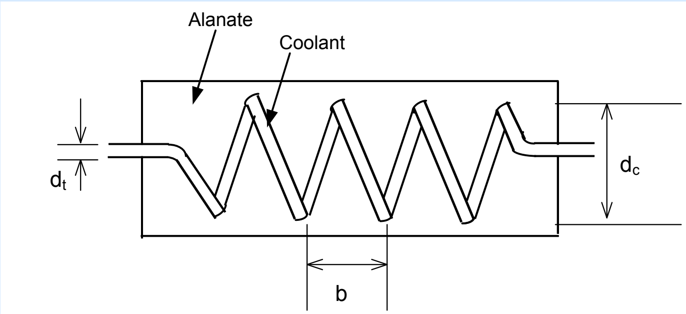




Hydrogen distribution: end of DC2

- ***Drive Cycles 3 and 4 test operability at cold and hot ambient T – not shown***

Design – II
(Helical Coil Heat Exchanger with Alanate in Shell)

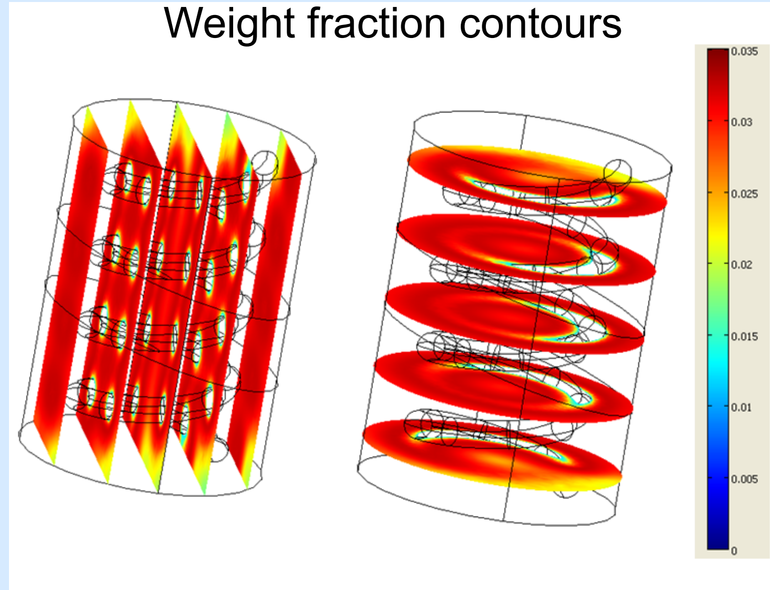


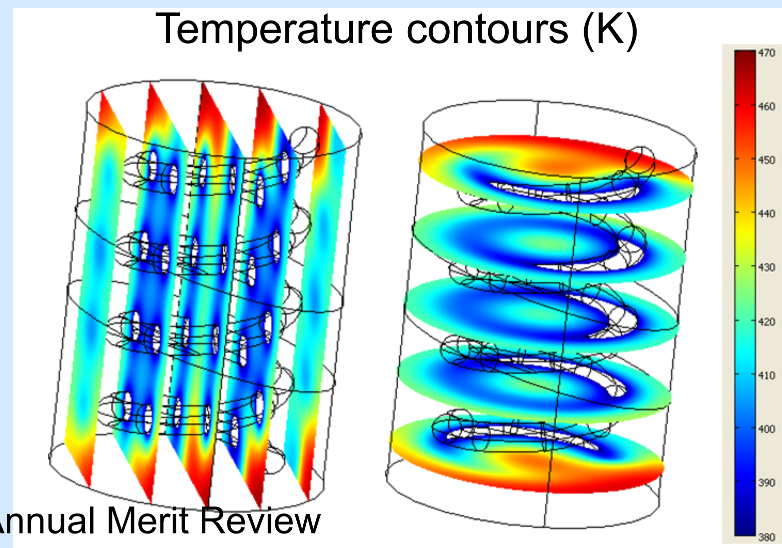
- Helical coil heat exchanger works well with systems with internal heat generation, has higher heat transfer coefficient than straight tubes because of higher turbulence

- For effective heat transfer, coil radius and pitch can be determined as a function of system properties – ΔH, k, ΔT, w, ρ_b, t_f

- Optimized the design by changing vessel diameter, coil diameter, and pitch for sodium alanate system

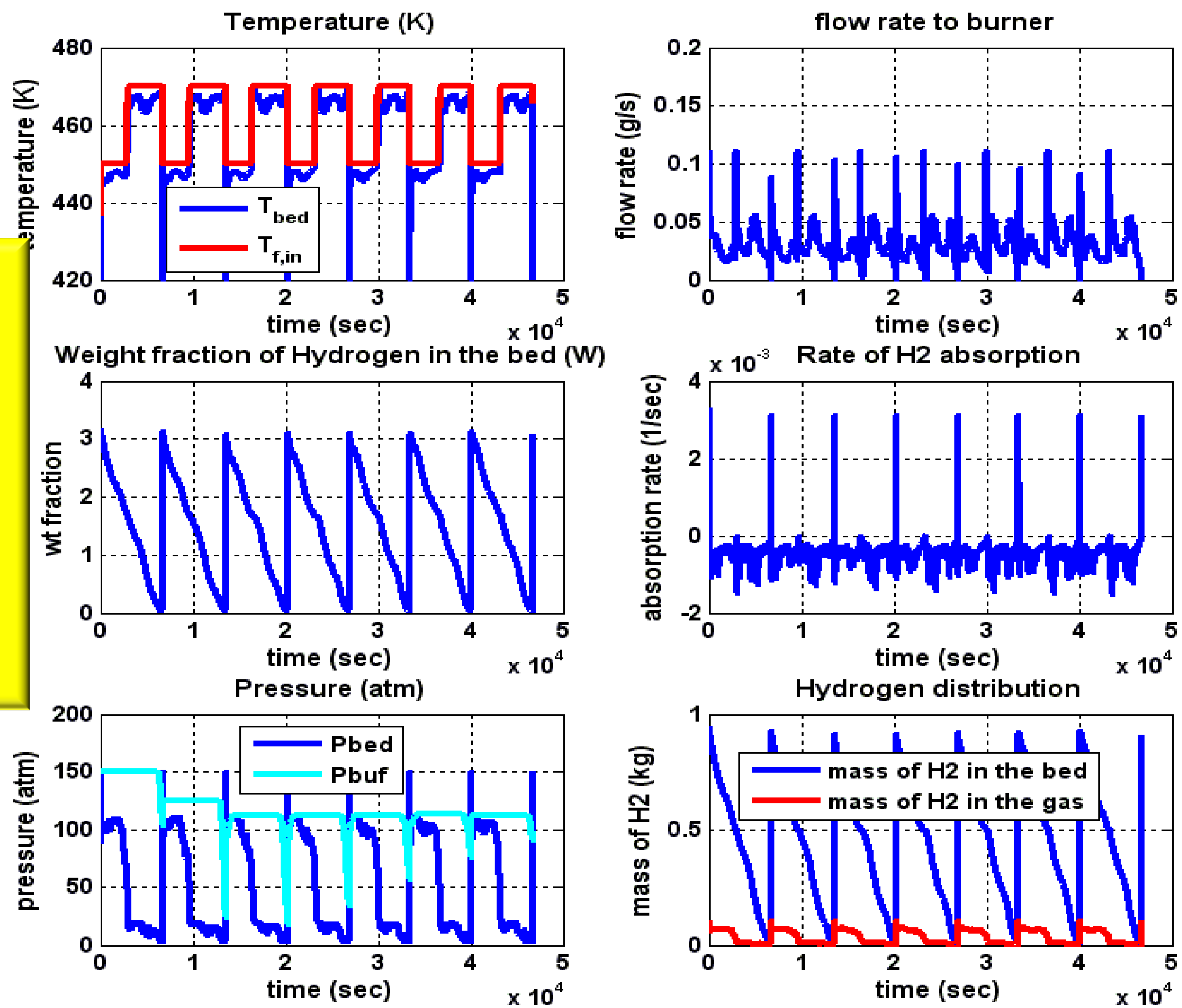
- **Heat exchanger mass is roughly 1/3 that in conventional design.**



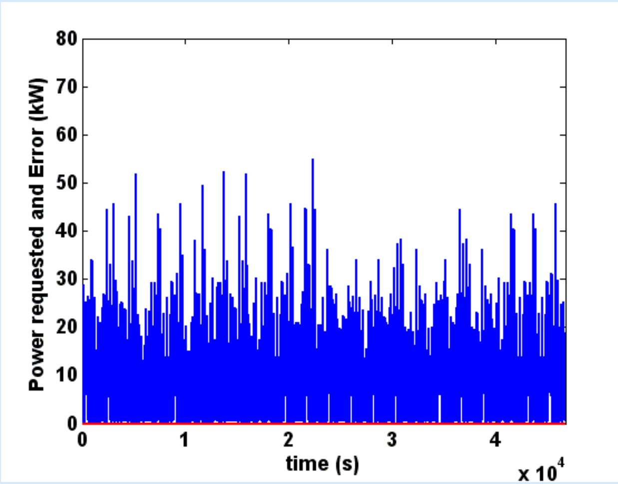


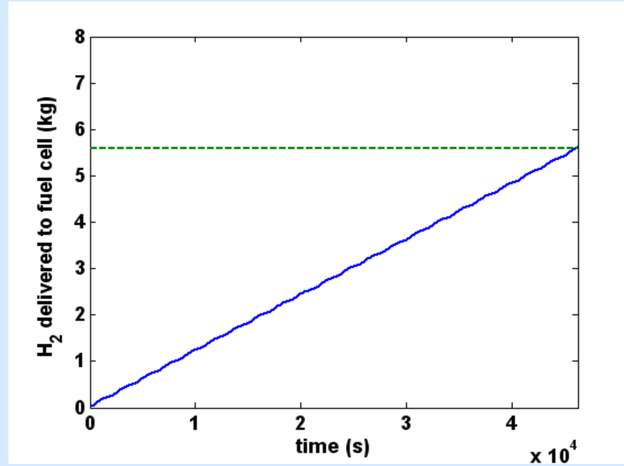
Helical coil design – 7 beds

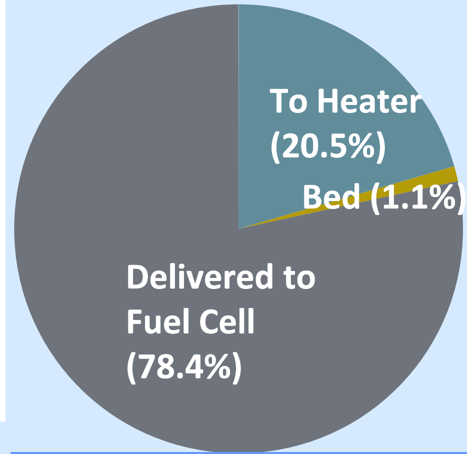
- Helical coil hex weight is about 1/3 of the previous system, but for $NaAlH_4$, 7 vessels are needed
- But this design is very promising for a high capacity material with somewhat lower ΔH



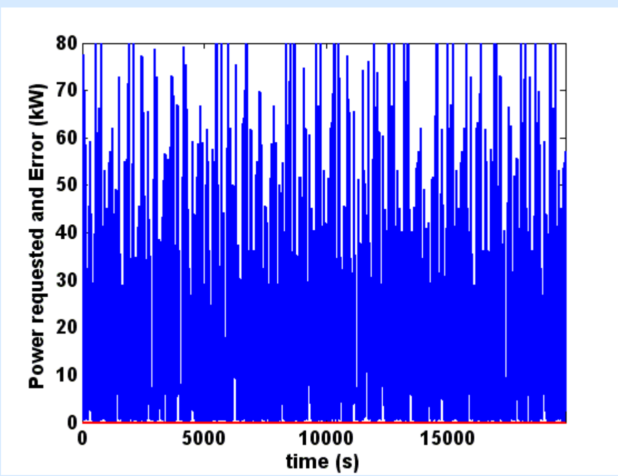
Helical Coil Design – Ambient and Aggressive Cycles

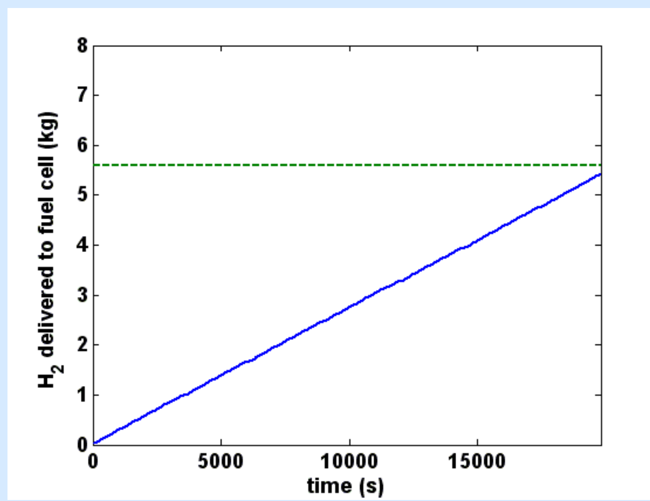


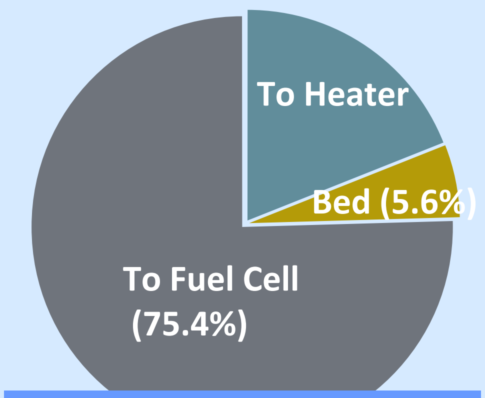




H2 distribution at the end of DC1



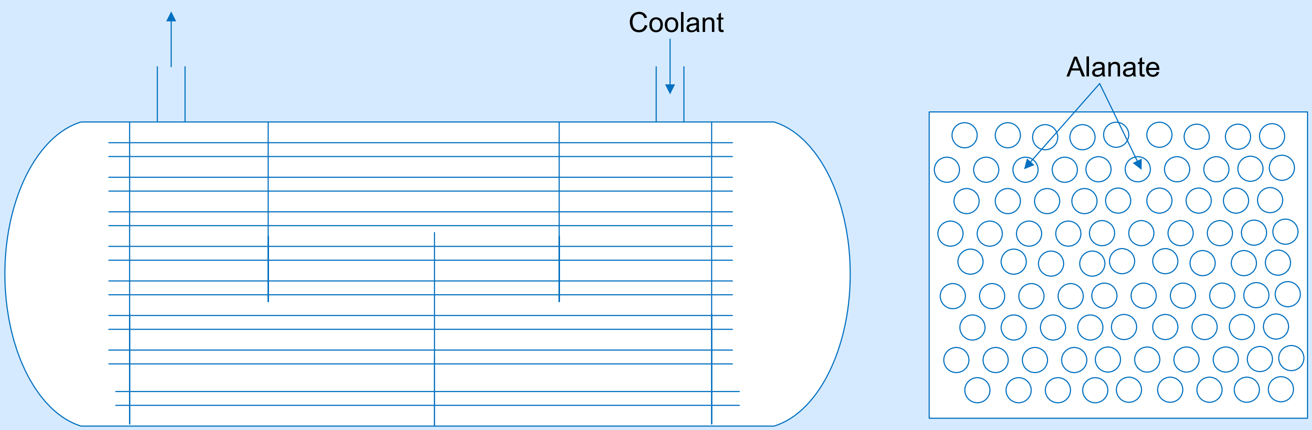




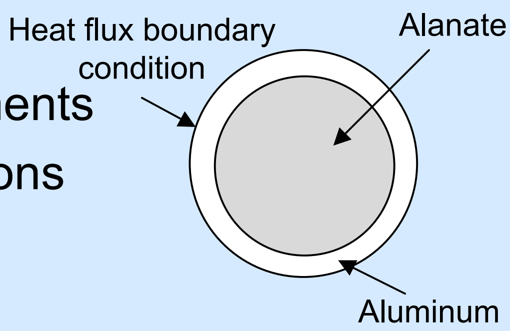
H2 distribution at the end of DC2

- ***Drive Cycles 3 and 4 test operability at cold and hot ambient T – not shown***

Design III – Alanate in Tubes Design



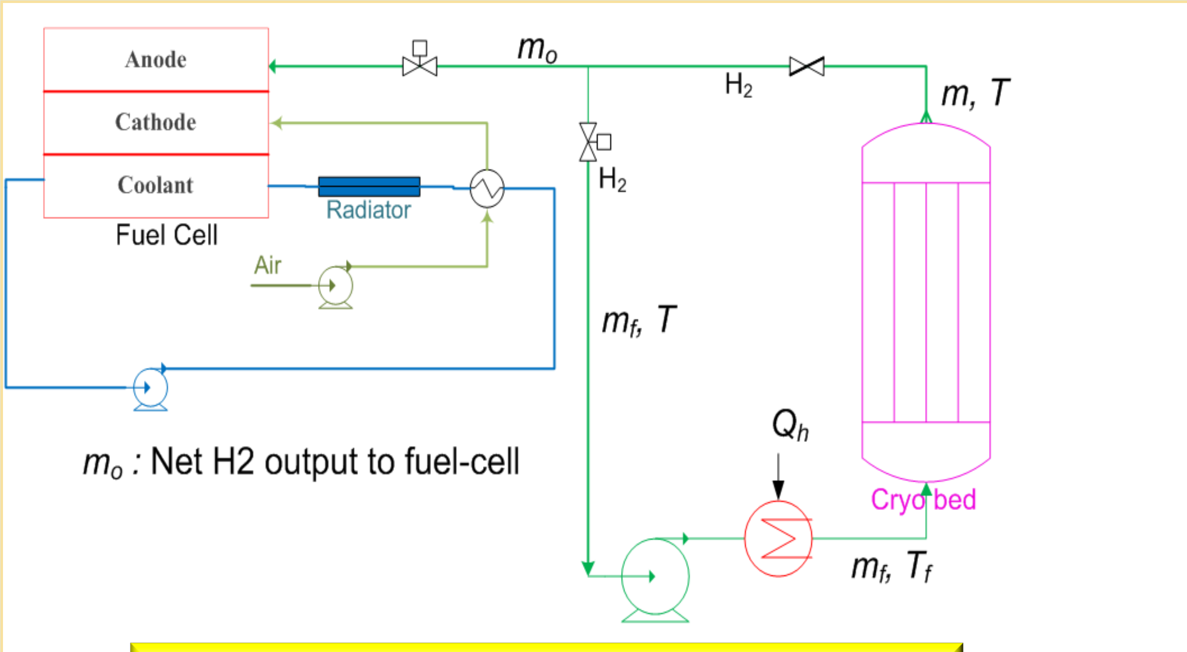
- 81 tubes, 9x9 arrangement, possibly modular arrangement
- Coolant flow in the shell
- Tube diameter determined by heat transfer requirements
- Tube thickness determined by structural considerations
- Limited optimization opportunities



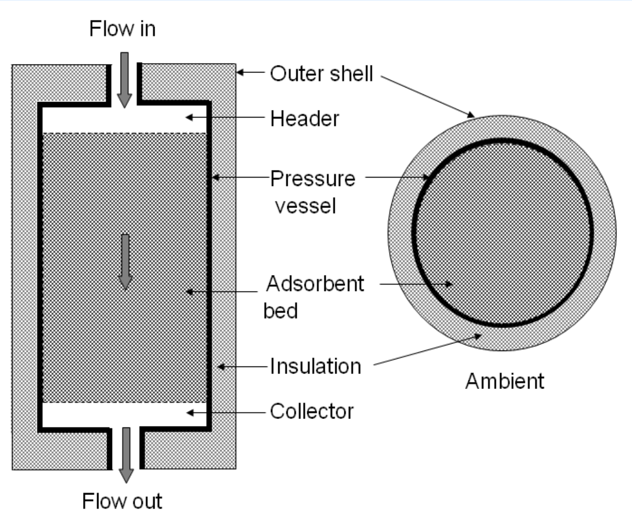
Cryoadsorption System Modeling
(in cooperation with SRNL)

- During refueling, heat of adsorption is removed by passing excess cold H_2 through the bed
- Cold H_2 used to refuel the tank, cools it as well as remove the heat of adsorption
- Similarly, during discharge heat can be supplied via a heated H2 stream, electrically, or via radiator fluid

SRNL will discuss cryo-adsorption system models in detail



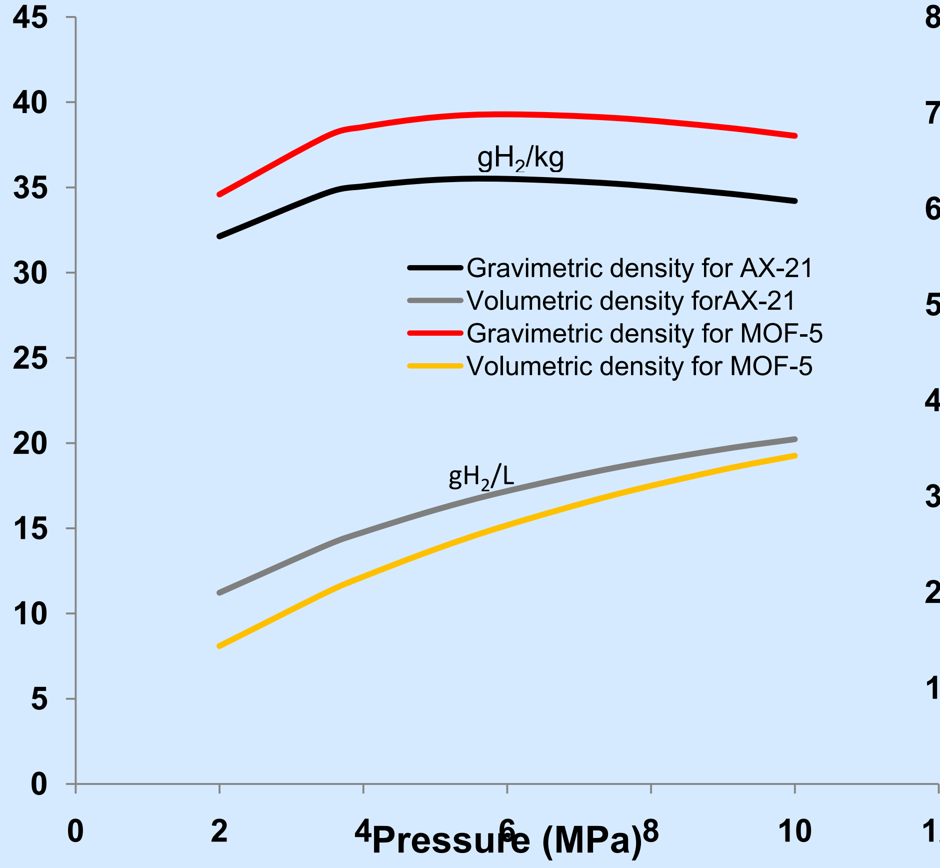
Cryo-adsorption system – discharge schematic

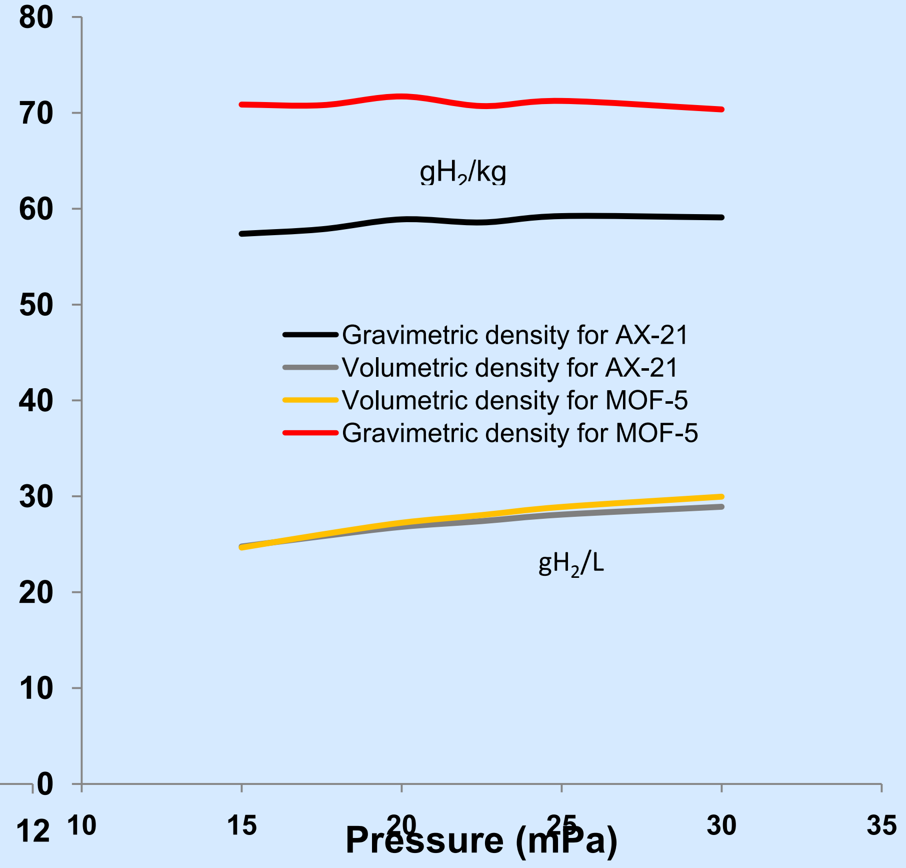


System Pressure Considerations

- For pressures less than 100 bar, aluminum tanks are a cost-effective option
- For pressures 100 bar or greater, considered a composite tank.
- Conducted calculations for 20 -100 bar assuming an inner aluminum vessel and calculations for 60-300 bar assuming a composite vessel
- Assumptions
  - 5.6 kg usable H_2
  - Convective cooling assumed, no in-tank heat exchanger
  - 1” MLVSI wrapped around the inner vessel, outer vessel aluminum
  - Inner vessel thickness from Lincoln Composites
  - 5% extra adsorbent, additional 10% volume provided for manifolds and piping
  - Fixed BOP mass included
- Technical gaps for composite tanks for cryo applications:
  - Off-gases evolved during curing of the resin will destroy the vacuum in MLVSI
  - Development of resins that do not emit off-gases or a way to capture them necessary to maintain vacuum
  - Material strength lower at cryogenic temperatures

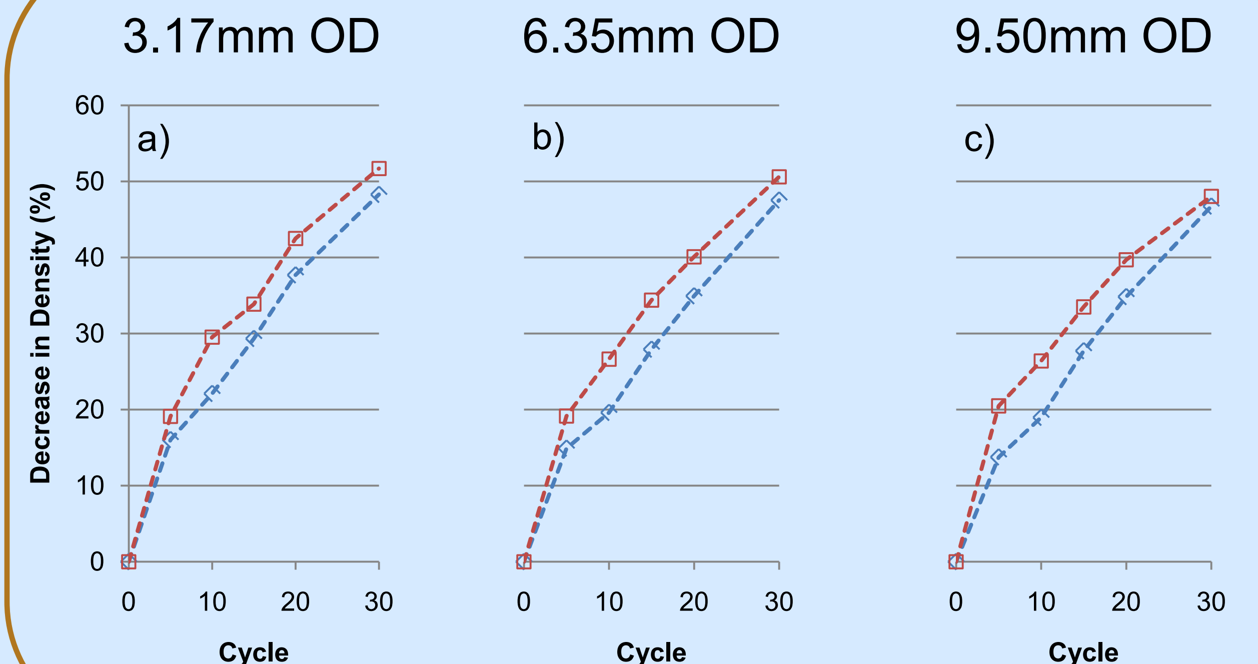
Gravimetric & Volumetric Densities for AX-21 and MOF-5 Systems



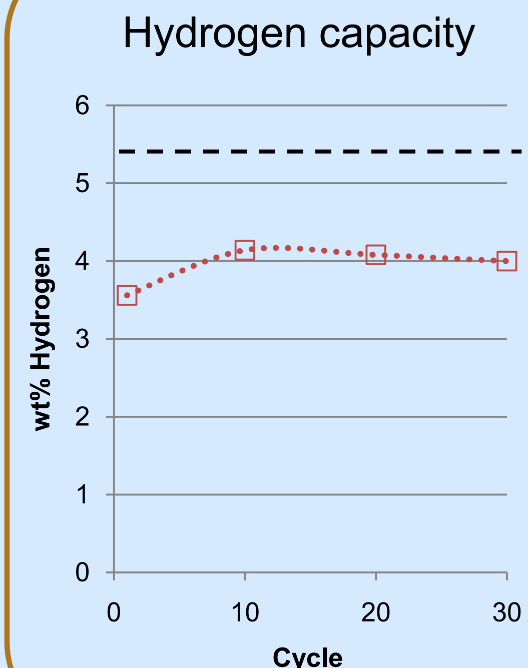


System modeling for 60 bar and 200 bar systems for AX-21 and MOF-5 in collaboration with SRNL. System weights and volumes by PNNL.

NaAlH4 Pellets
Effect of Cycling on Density & Capacity



Blue line: 10kPSI, Red line: 50kPSI

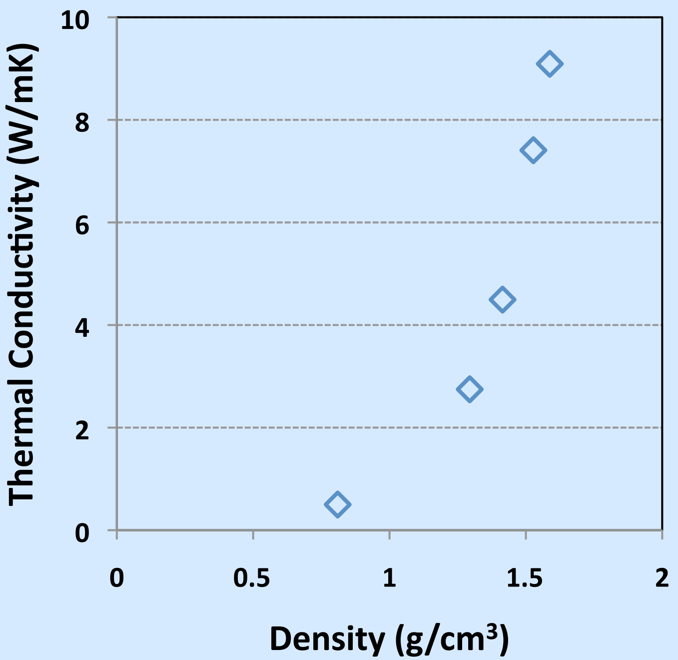


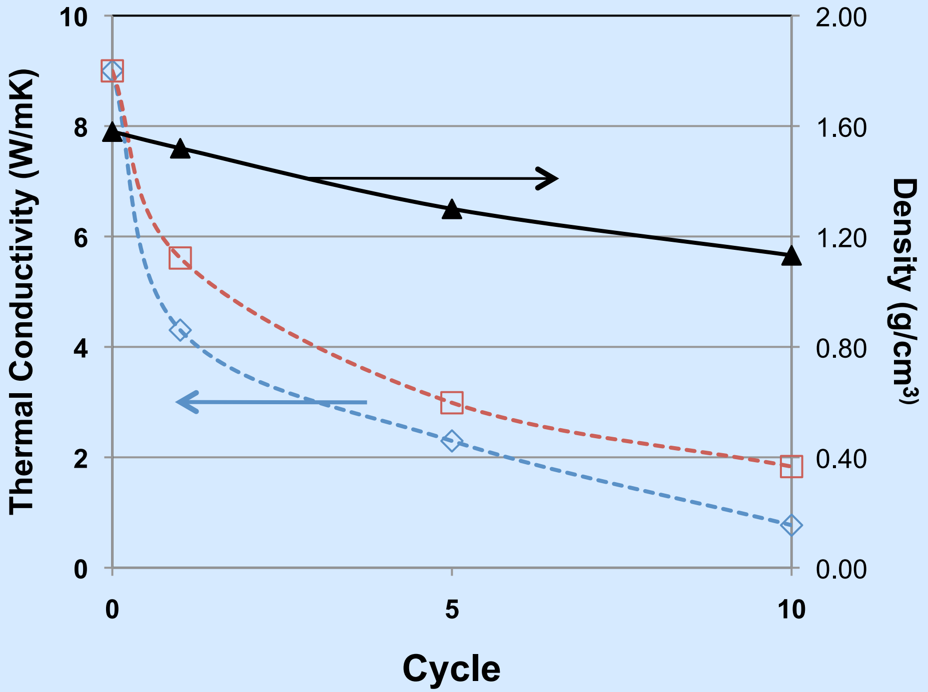
Black line: theoretical

- Significant loss in density of pellets over 30 cycles
- Expansion independent of pellet size and pressure

However, capacity not affected by pellet expansion

NaAlH4 Pellets
Density & Thermal Conductivity

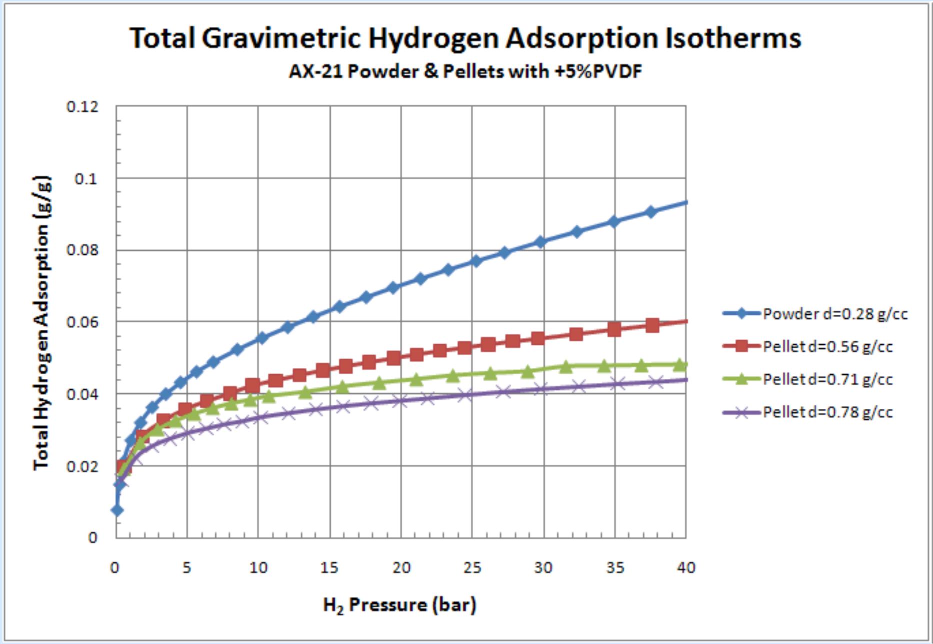


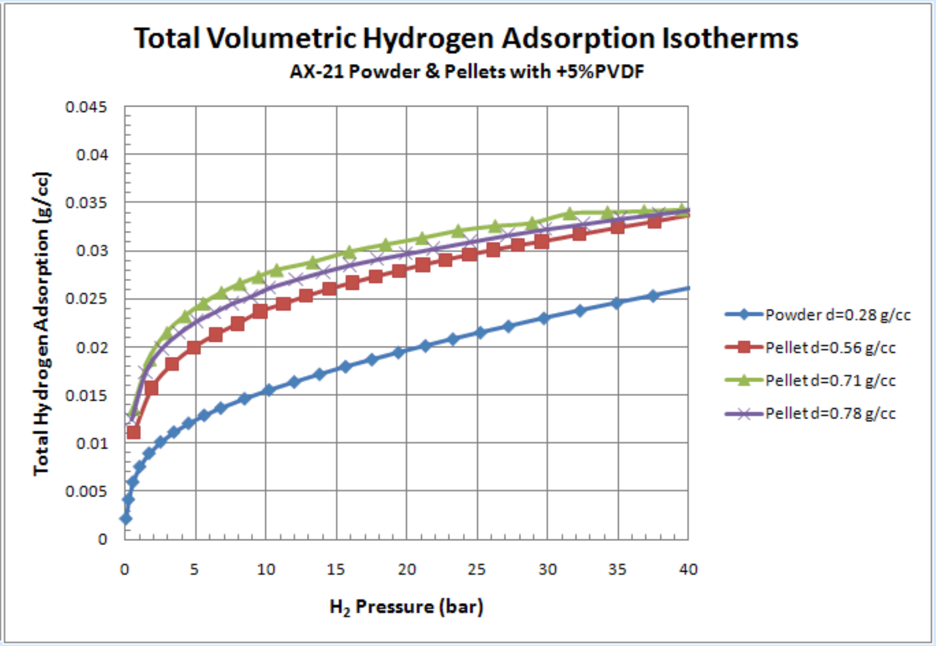


Exponential growth of thermal conductivity for compressed Ti-doped NaH + Al.

Pellet expansion during cycling has significant affect on thermal conductivity

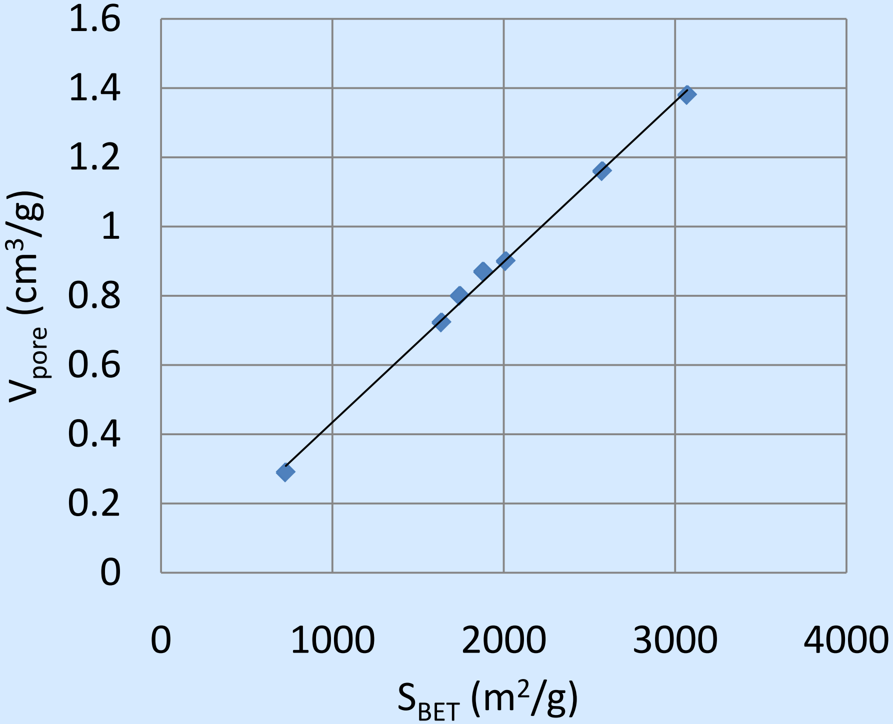
Compacted AX-21 Sorbent
Total gravimetric and volumetric H_2 uptake data

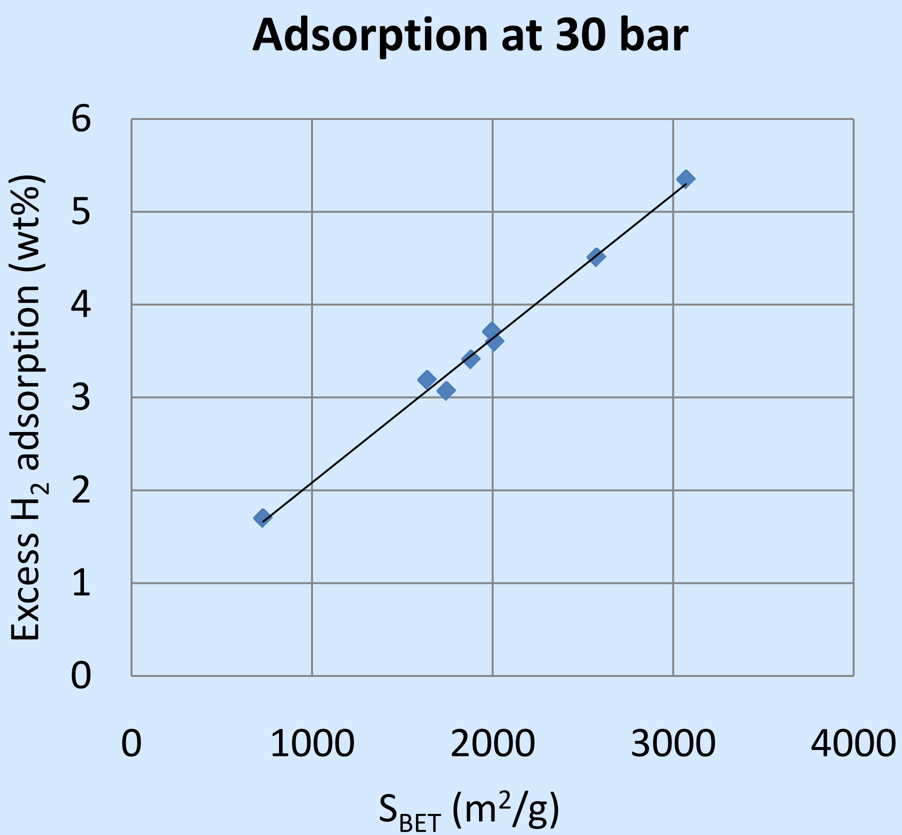




- 2x densification (to 0.56 g/cm^3) resulted in a 33% decrease in total gravimetric capacity
- Total *materials* volumetric capacities for ~ 0.5 g/cm^3 compacts at 60 bar & 77 K: 40 g/L
- 1.5 x improvement in volumetric capacity achieved for AX-21
- Modeling and theoretical studies planned to understand the impact of pellet size on H2 adsorption, heat transfer, and bed packing density

Correlation between hydrogen adsorption and pore structures





Both pore volume and excess gravimetric hydrogen adsorption are linearly correlated with the sample surface area

Collaborations

In general, regular contact with most partners because of participation in system modeling, media compaction, and detailed transport studies

In particular,

- UTRC, NREL, Ford – Integrated Framework Development and system model inclusion in the framework
- Ford – OEM Work on target prioritization, sorbent compaction
- UTRC – sodium alanate pelletization studies, MH system models
- SRNL – Cryoadsorbent system simulation models and detailed transport models
- PNNL – Provided system level schematics and operating conditions data for component sizing and cost

SUMMARY

- System design for sodium alanate developed. The dual bed system has been considered in detail for gravimetric and volumetric densities.
- Three heat exchanger designed optimized and considered in detail.
- Modular helical coil design offers low heat exchanger weight and may offer lower cost than the dual bed system
- All $NaAlH_4$ systems are able to handle the four test drive cycles successfully but require substantial fraction of hydrogen to be used for desorption
- A system model fro cryo-adsorption system has been developed in conjunction with SRNL. System densities considered as a function of pressure
- Design analysis and methodology developed can be adapted to different materials - both MH and adsorption materials. For MH, need higher w (H2 absorption capacity) and bed density ρ, but lower ΔH and lower T operation
- Sodium alanate and AX-21 pelletized and properties – cycling, capacity, thermal conductivity, pellet expansion - studied.

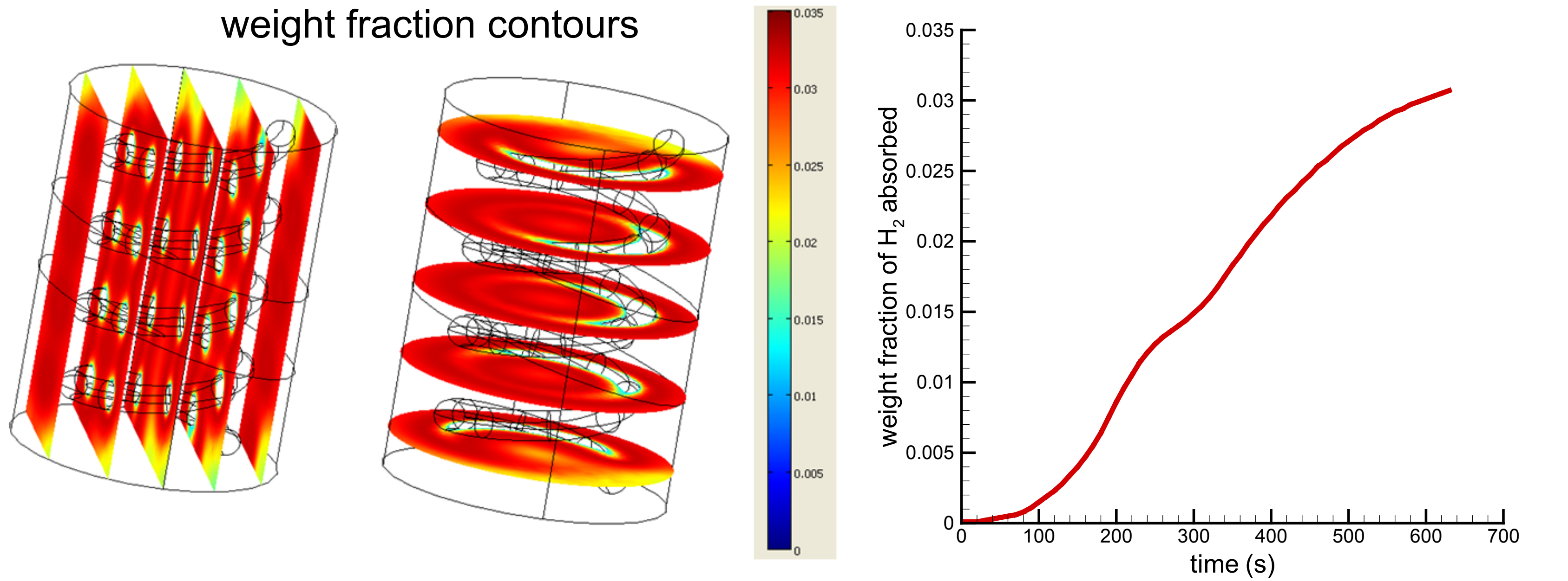
Future Work

- System design and model verification of new and reduced weight HX and other component designs for a better metal hydride chosen by HSECoE
- Include media compaction in system and detailed transport models
- Update system models with novel materials, novel HX designs and component models with goal of developing a suitable metal hydride prototype for Phase 3 testing and evaluation.
- For the cryoadsorption system, build a small vessel to verify critical assumptions and conduct experiments to validate the concept of convection cooling during refueling and validate the detailed transport models.
- Control pellet expansion and thermal conductivity degradation through mechanical confinement
- Cold pelletization of AX-21 and binders to allow for rapid manufacturing and reduce extensive pellet work-up
- Provide input for the design of cryo-adsorption prototype in Phase III.

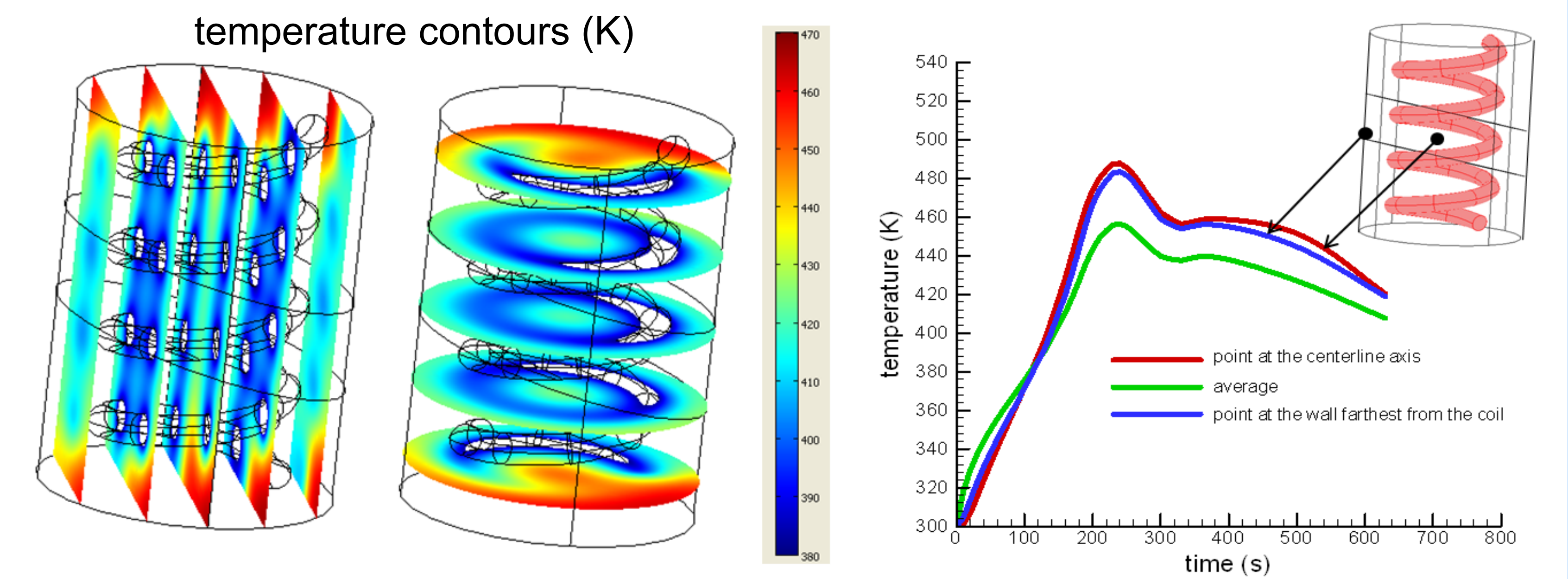
Acknowledgements

- This work was performed under DOE contract DE-FC36-09GO19003 as GM's contribution to the DOE Hydrogen Storage Engineering Center of Excellence (HSECoE)
- Lincoln Composites for providing design estimates for the liner and composite materials
- Ned Stetson and Jesse Adams of DOE for their support
- HSECoE team for many discussions and support
- Mark Verbrugge of General Motors for support and resources

Technical Back-Up Slides

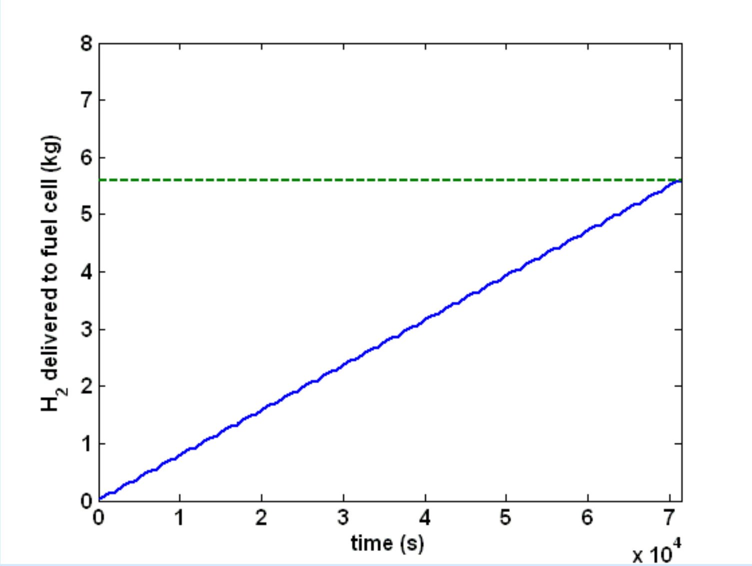


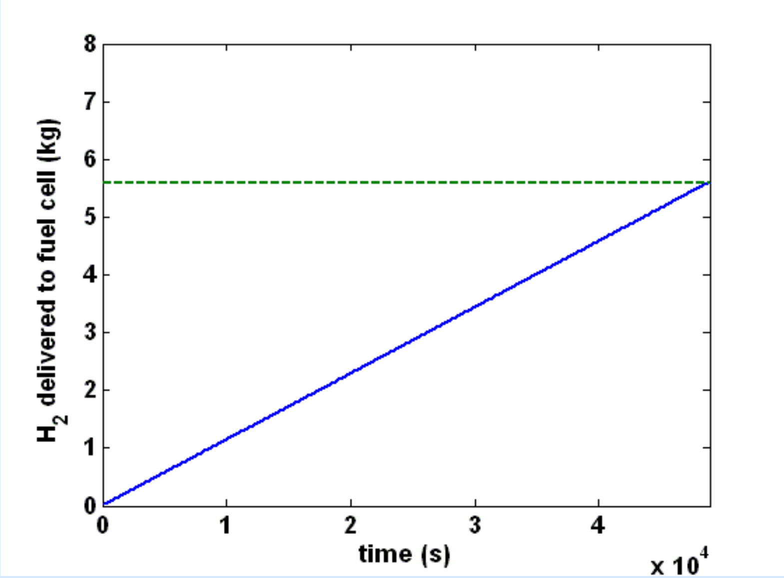
weight fraction contours
0.035
0.03
0.025
0.02
0.015
0.01
0.005
0
weight fraction of H_2 absorbed
time (s)
100
200
300
400
500
600
700

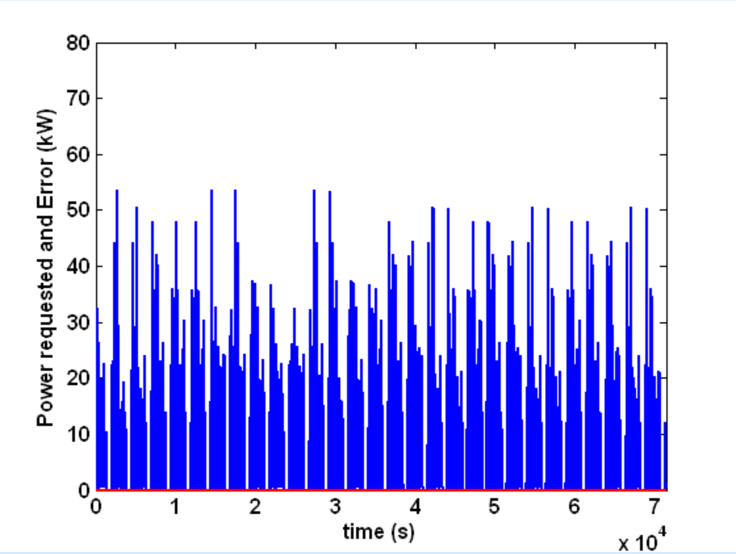


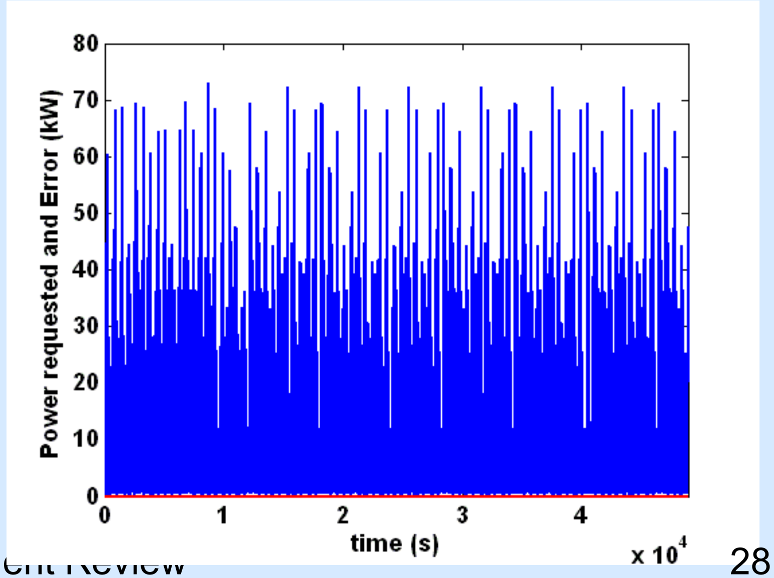
temperature contours (K)
470
460
450
440
430
420
410
400
390
380
temperature (K)
time (s)
540
520
500
480
360
340
320
300
point at the centerline axis
average
point at the wall farthest from the coil
100
200
300
400
500
600
700
800

Cold (DC3) and Hot (DC4) Drive Cycles









Compacted Sorbents
Methods for compaction of AX-21

1. Selection of binders
   - Type of binders (PVDF, PVA, PTFE,…)
   - Same type of binder but with different melt viscosity

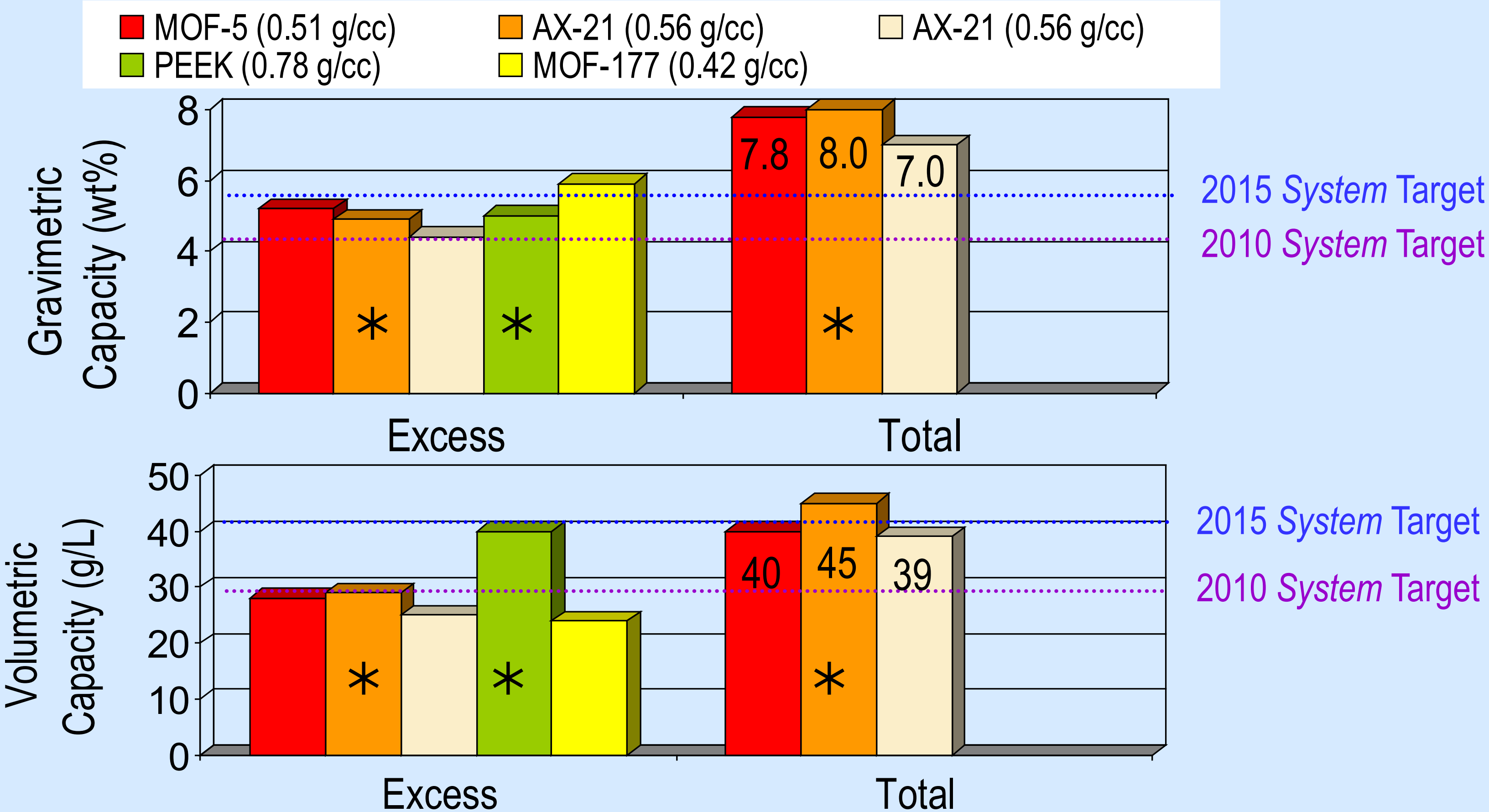
     Kynar® PVDF: HS900 > 301F > 721
   - Binder in the form of powder or solution

     PVDF solution in NMP solvent;

     PTFE solution in water;

     PVA solution in water.
2. Mixing of sorbents with binder (typically 5 wt%)
3. Hydraulic press at 25-300^{o}C (using heating band) and pressure of 40-400 MPa.
4. Post-treatment of the pellets
   - Degassing of the pellets at 155^{o}C for 15 h

Comparative Summary: Materials-based uptake for compacted sorbents at 77 K & 60 bar (Adapted from A. Sudik, Ford Motor Co.)



* = Data based on pellet in press vessel (i.e. freestanding compacts not yet obtained)

MOF-177 data from R. Zacharia et al, *J. Mater. Chem.* 2010, 20, 2145.

Case -1 System level evaluation

	units	Value	Comments
Number of beds		2	
deliverable hydrogen	kg	5.3	
Length (alanate packing)	mm	1000	
Actual length of the bed	mm	1292.0	based on design considerations
Diameter of the bed (inner)	mm	370.0	
Diameter of the bed (outer)	mm	393.3	
Shell material		Composite carbon	
No of cooling tubes		24.0	
Diameter of cooling tubes (inner)	mm	15.0	
Pressure drop for cooling fluid	bar	1.07	pressure drop inside the bed
Temperature rise of the fluid	K	3	between inlet and outlet stream
Weight of alanate	kg	184.42	for 2 beds
weight of shell include liner	kg	65.49	for 2 beds
weight of tubes and fins	kg	69.43	for 2 beds
accessories (manifolds, end plates etc)	kg	25.4	10% of alanate+fins wt
pump/HEX/burner	kg	8.00	rough estimate for 12 kW burner
pump/HEX/burner volume	liters	8.00	rough estimate for 12 kW burner
BOP mass	kg	12.69	5% of alanate+fins wt
Oil mass	kg	6.4	based on 1.5*total tubes volume
Buffer	kg	5.05	0.5 H2+5kg container
Buffer volume	liters	11.30	9.3 H2 + 2 container
Total weight of the bed	kg	319.34	alanate+shell+fins
Total volume of the beds	litres	313.92	2 beds
Total system volume	liters	333.22	bed+HEX+buffer
Total system mass (tubes, plates, shell/insulation, alanate)	kg	376.9	bed+HEX+BOP+buffer
Gravimetric density		**0.014**	
Volumetric density		**0.0159**	