SRNL Technical Work Scope for the Hydrogen Storage Engineering Center of Excellence

Design and Testing of Adsorbent Storage Systems

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Savannah River National Laboratory

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Hydrogen Storage Engineering
CENTER OF EXCELLENCE

Project ID#ST044

This presentation does not contain any proprietary, confidential or otherwise restricted information

Overview

Timeline

- Start: February 1, 2009
- End: June 30, 2014
- 75% Complete (as of 3/1/13)

Barriers

- System Weight and Volume
- H_2 Flow Rate
- Energy Efficiency

Budget

- FY12 Funding: $1,030,000*
- FY13 Funding: $1,030,000*

* Includes $240,000/$240,000 for the University of Quebec Trois Rivieres (UQTR) as a subrecipient for FY12/FY13

Partners

Relevance – Overall Project Objectives

Phase 1: 2009-2011

- Compile all relevant **metal hydride materials data** for candidate storage media and define future data requirements. **Complete**
- Develop engineering and design models to further the understanding of on-board storage **transport phenomena requirements**. **Complete**
- Apply **system architecture approach** to delete specific metal hydride systems not capable of meeting DOE storage targets. **Complete**

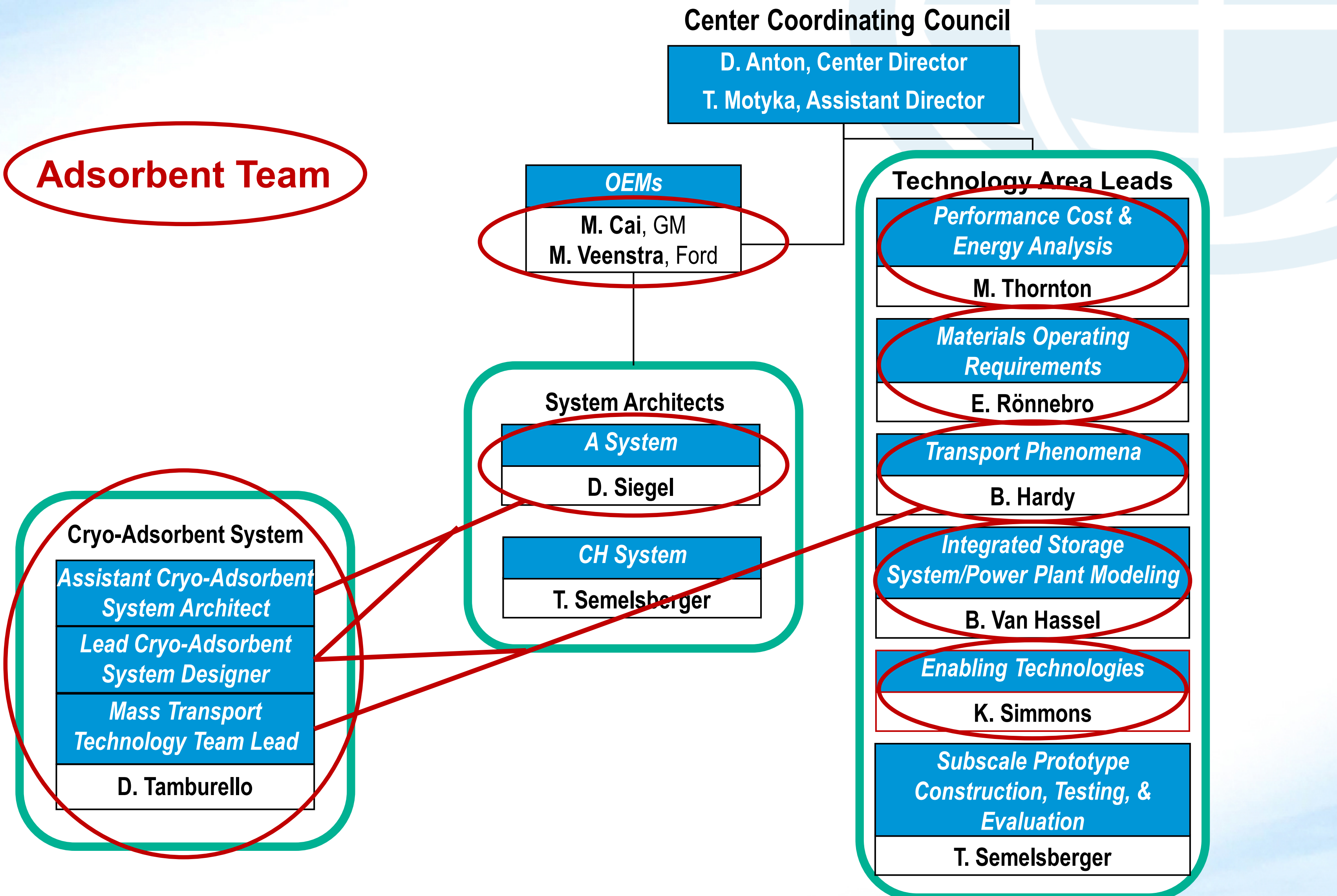
Phase 2: 2011-2013

- Develop and apply **adsorbent acceptability envelope**. **Complete**
- Conduct **component adsorbent experiments**. **Complete**
- Design components and experimental test fixtures to **evaluate the innovative storage devices** and subsystem design concepts, validate model predictions, and improve both component design and predictive capability. **Well Established and in Progress**

Phase 3: 2013-2014

- Design, fabricate, test, and decommission the **subscale prototype systems** for adsorbent storage materials.
- Validate the detailed and system model predictions against the subscale prototype system to **improve model accuracy** and **predictive capabilities**.

Approach - HSECoE Organization



Approach – FY2012 / FY2013 Milestones

SMART Milestone for SRNL/UQTR:

- **Report on the ability to develop a compacted MOF-5 adsorbent media bed having a total H_2 density of 11% g_{H2}/g_{MOF} and 33 g_{H2}/L_{MOF} at P = 60 – 5 bar and T = 80 – 160 K.** – Alternative compaction methods will be pursued with Ford to identify higher volumetric density morphologies meeting the metrics.
- **Report on the ability to develop and demonstrate an internal flow through (FT) heat exchanger (HX) system based on compacted media capable of allowing less than 3 minute scaled refueling time and H_2 release rate of 0.02 g_{H2}/s/kW with a mass less than 6.5 kg and a volume less than 6 L.** – Metric Met.
- **Report on the ability to identify a system design having a mass less than 137 kg and a volume less than 279 L meeting all of the HSECoE drive cycles.** – Metric Exceeded.
- **Report on the ability to develop and demonstrate a non-MATI isolated HX-ing loop capable of allowing less than 3 minute refueling time and a H_2 release rate of 0.02 g_{H2}/s/kW with a mass less than 6.5 kg and a volume less than 6 L.** – Metric suspended as not viable.

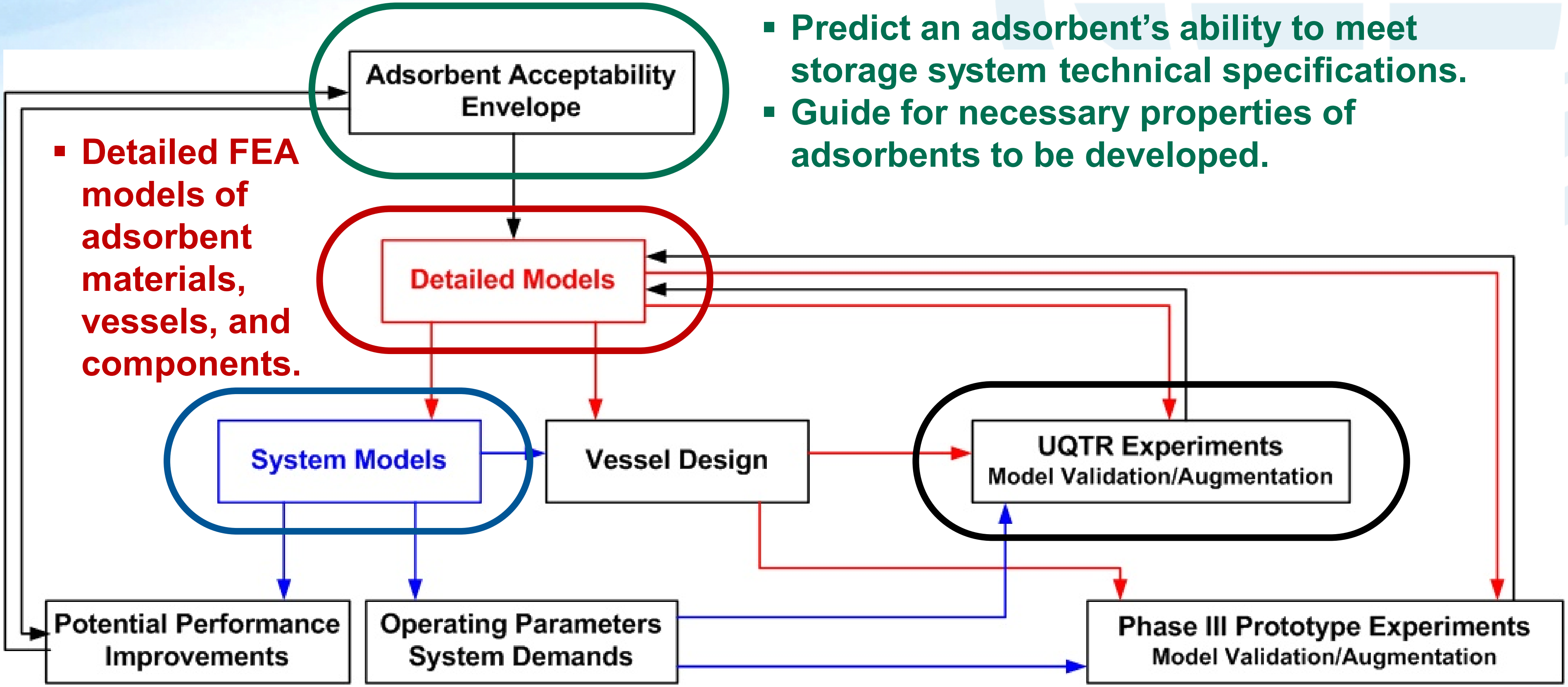
Transport Phenomena Technology Milestones for SRNL/UQTR:

1. **Refine the detailed models for scaled-up and alternative H_2 storage applications.** – In progress.
2. **Continue the FT cooling experiments, investigating MOF-5 powder, pellet, and compacted forms. Employ various HX concepts as applicable.** – In progress.
3. **Optimize the adsorbent system with respect to pressure work, enthalpy of H_2 discharge flow, dormancy conditions, and thermal interaction with the container well.** – Completed.
4. **Develop and apply an Adsorbent Acceptability Envelope (AAE), having a draft publication for refereed journal article by 3/1/2013.** – AAE developed and applied. Draft journal article written.
5. **Select an adsorbent, and form thereof, for use in the Phase 3 prototype.** – In progress.
6. **Begin the prototype design and experimental test matrix development for Phase 3.** – In progress.

Approach – Prototype Selection, Design, and Testing Process

- Predict an adsorbent’s ability to meet storage system technical specifications.
- Guide for necessary properties of adsorbents to be developed.

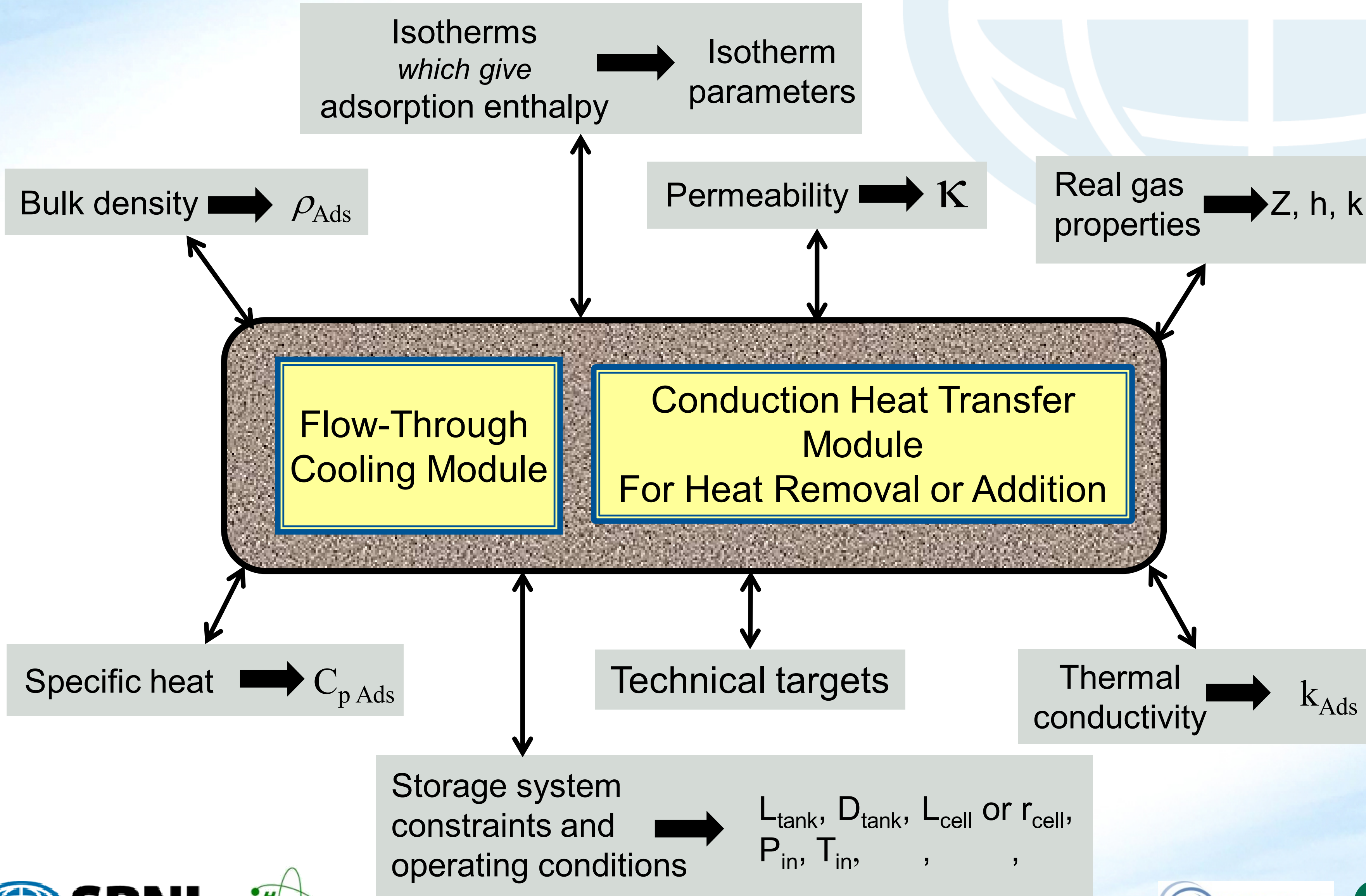
- Detailed FEA models of adsorbent materials, vessels, and components.



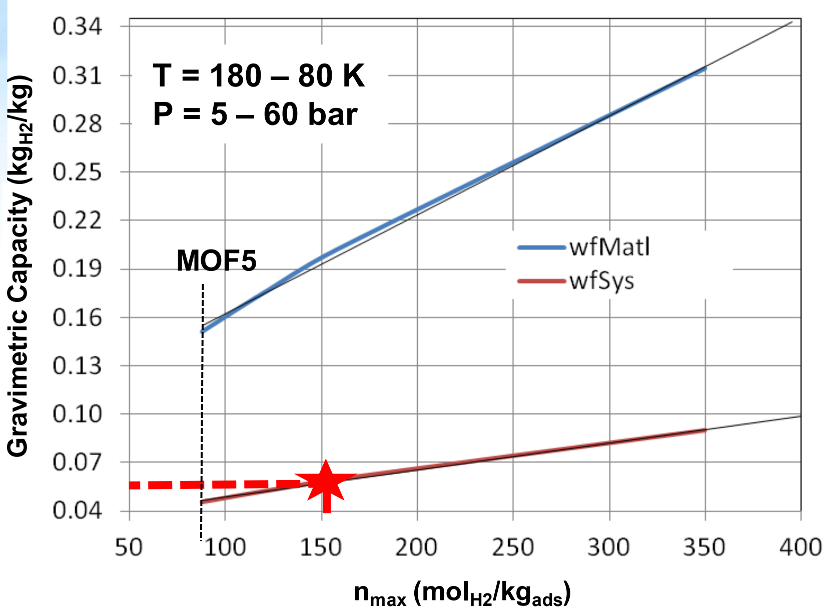
- Lumped capacitance models of the storage system (adsorbent material, vessels, BOP, and other components) to predict the full system performance.

- Continual feedback with the detailed models and system models
- Used to validate, augment, and improve predictive ability of the models

Approach – Adsorbent Acceptability Envelope



Accomplishments and Progress – AAE Analysis: Sensitivity to n_{max} – "Idealized" Material #1

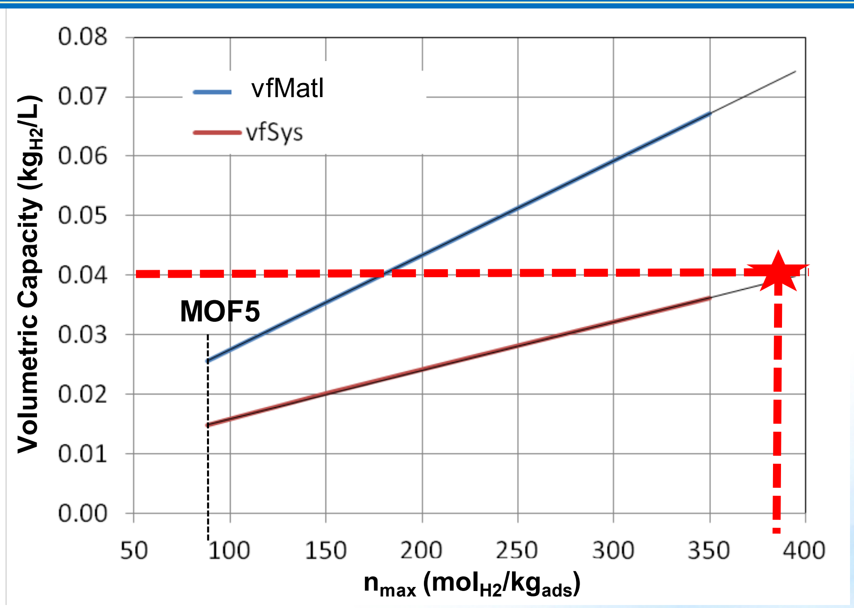


Hydrogen charging:

- Ideal material n_{max}: ~400 mol_{H2}/kg_{ads} to meet the 2017 DOE targets.
  - Grav. cap. target met: n_{max} ~1.8x MOF-5.
  - Vol. cap. target met: n_{max} ~4.6x MOF-5.
- Ideal material m_{inlet} is 42% higher than the corresponding MOF-5 value.

Hydrogen discharging:

- Discharge temperature ~56 K higher than for MOF-5.
- Reduced the internal tank volume by more than 50% of MOF-5.



Need reduction of additional system and BOP weight and volume

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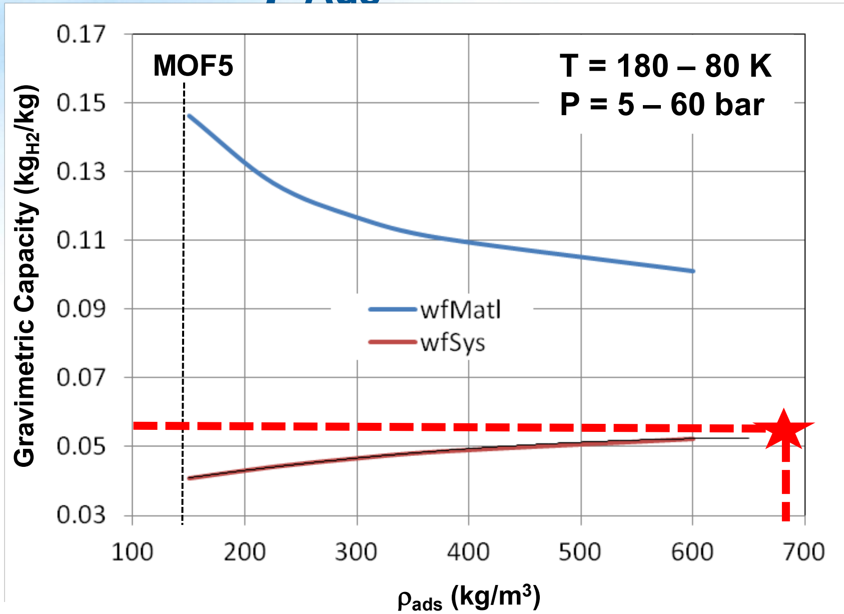
Accomplishments and Progress – AAE Analysis: Sensitivity to ρ_{Ads} – "Idealized" Material #2

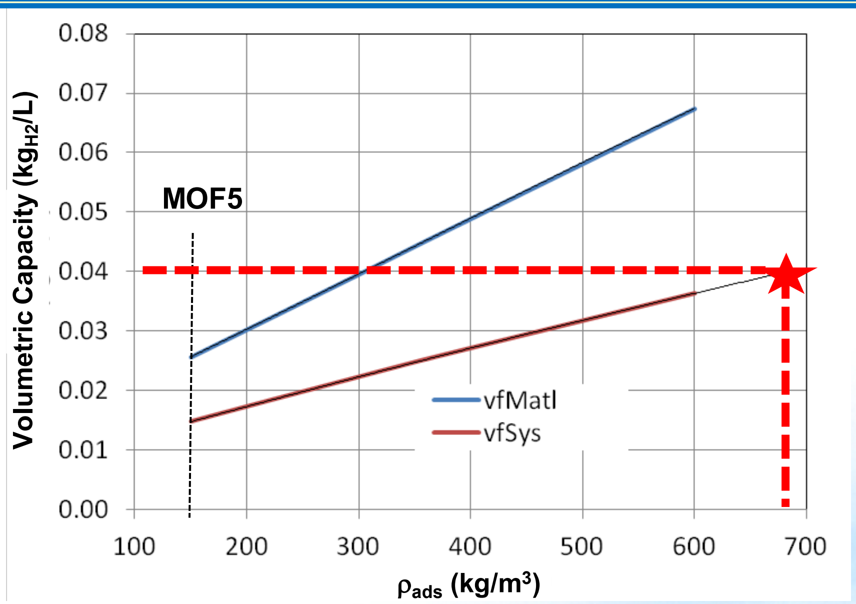


Hydrogen charging:

- Ideal material ρ_{max}: ~690 kg/m^3.
  - Both 2017 DOE Gravimetric & Volumetric capacity targets met at 4.6x MOF-5.
- 4.6x reduction of MOF-5 (V_v-V_a).
- Ideal material m_{inlet} about 55% higher than the corresponding MOF-5 value.

Hydrogen discharging:

- Discharge temperature ~25 K higher than for MOF-5.
- Reduced the internal tank volume by more than 50% of MOF-5.



Need reduction of additional system and BOP weight and volume

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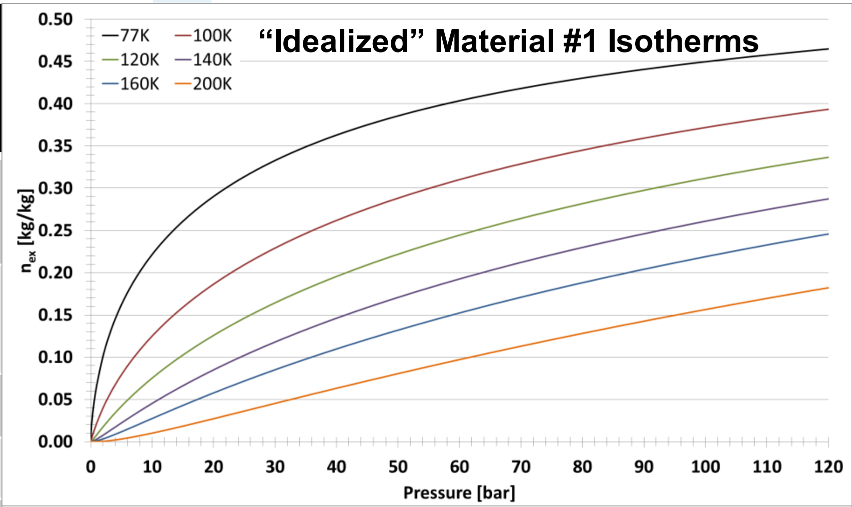
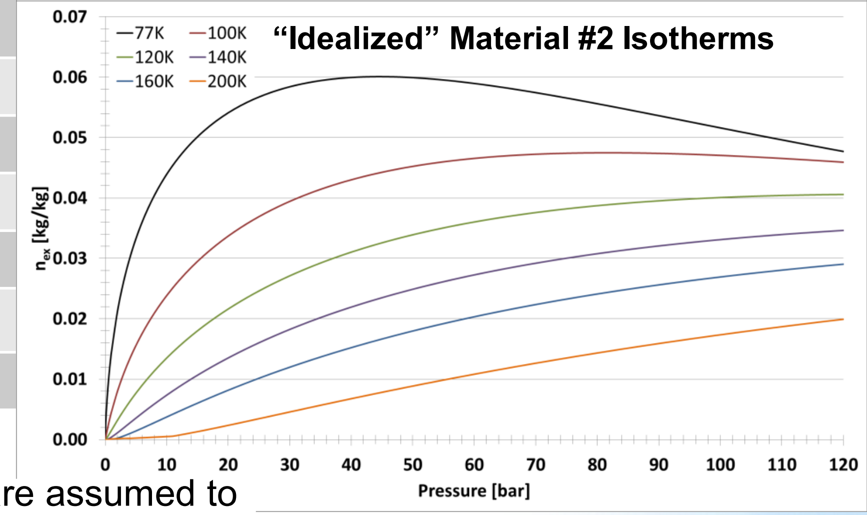
Accomplishments and Progress – Example "Idealized" Adsorbent Materials Determined from the AAE Analysis.

Sensitivity Study Properties	Powder MOF-5	*Idealized* Material #1	*Idealized* Material #2
n_{excess}: gravimetric capacity [kg_{H2}/kg_{ads}]	0.056	0.38	0.056
n_{total}: volumetric capacity [kg_{H2}/L_{ads}]	0.025	0.074	0.074
Bulk density [kg/m^3]	**150**	**150**	**690**
D.-A. Parameters:			
n_{max} [mol_{H2}/kg_{ads}]	**88**	**400**	**88**
P_0 [bar]	3200	3200	3200
alpha [J/mol]	2400	2400	2400
beta [J/mol/K]	11	11	11
V_a [m^3/kg_{ads}]	0.0019	0.0019	0.0019
V_v [m^3/kg_{ads}]	**0.0062**	**0.0062**	**0.0029**
m	2.0	2.0	2.0





- **Bolded values** changed compared to powder MOF-5
- Properties not listed above were not considered (yet) and are assumed to be consistent with existing literature values for powder MOF-5, including:
  - Thermal conductivity, permeability, specific heat, and void fraction.

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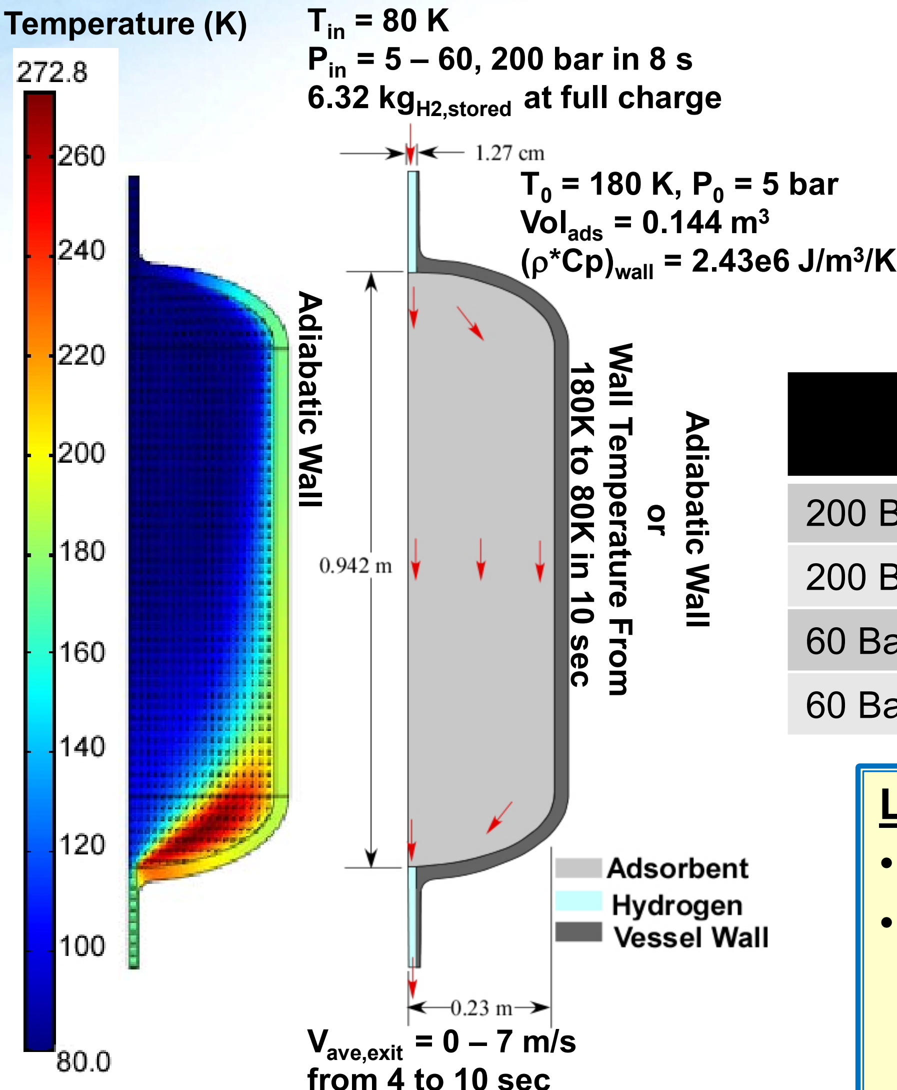
Accomplishments and Progress – Flow-Through Cooling Adiabatic Wall & LN2 Assisted Cooling



Flow-Through Cooling:

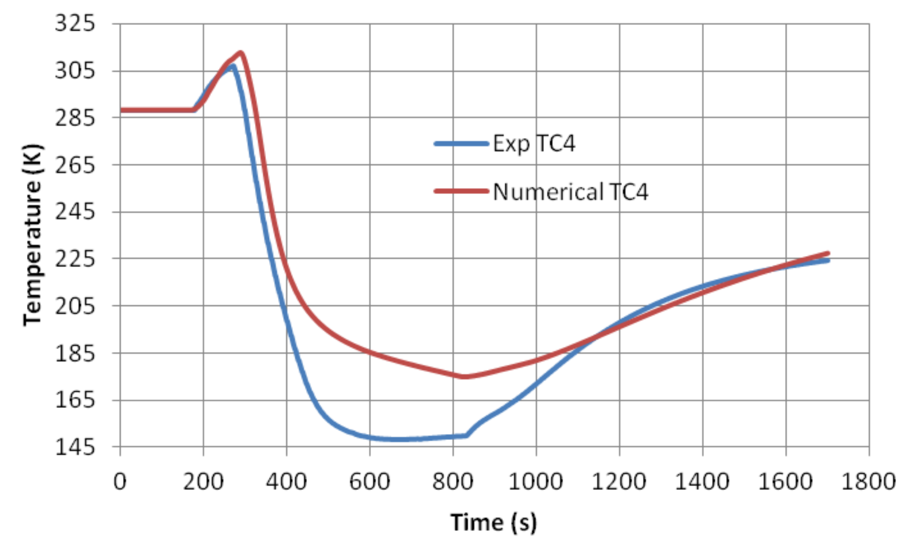
- More efficient heat removal than conduction.
- Requires high adsorbent bed permeability
  - Pelletized adsorbent heat removal by FT cooling is due to convection at the surface of the pellet.
- Can result in high total enthalpy of exhaust H_2.

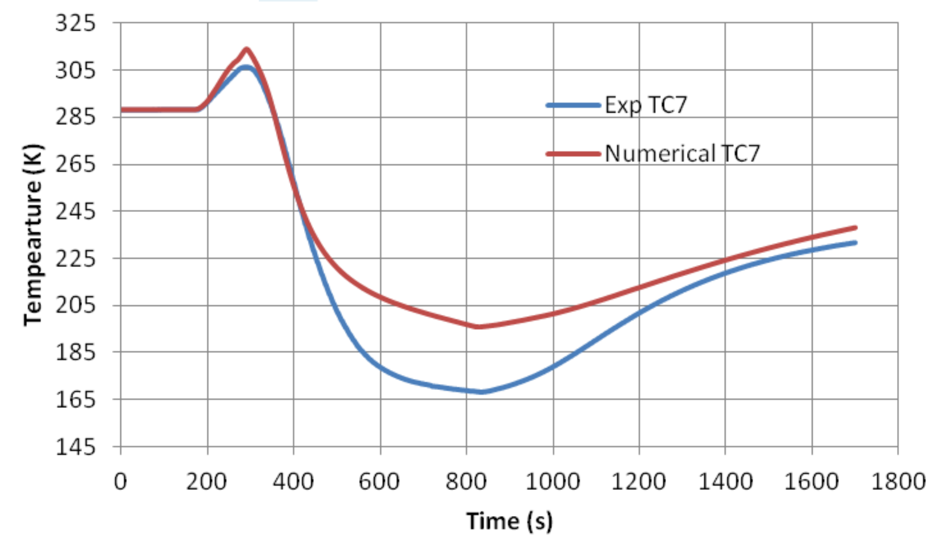
	Time to Charge	Total Mass of Exhaust H_2	Total Exhaust H_2 Enthalpy
200 Bar (LN_2 assist)	25 sec	1.1 kg	3.60×10^6 J
200 Bar (Adiabatic)	101 sec	11.4 kg	1.64×10^7 J
60 Bar (LN_2 assist)	108 sec	2.4 kg	6.48×10^6 J
60 Bar (Adiabatic)	>300 sec	>11.8 kg	$>1.84\times10^7$ J

LN_2 Assisted Flow-Through Cooling:

- Reduced total exhaust H_2 enthalpy.
- A preliminary JPL test indicated that the time required to cool the outer wall is longer than assumed in the model.
  - ~1.5 minutes from 180 K to 80 K.

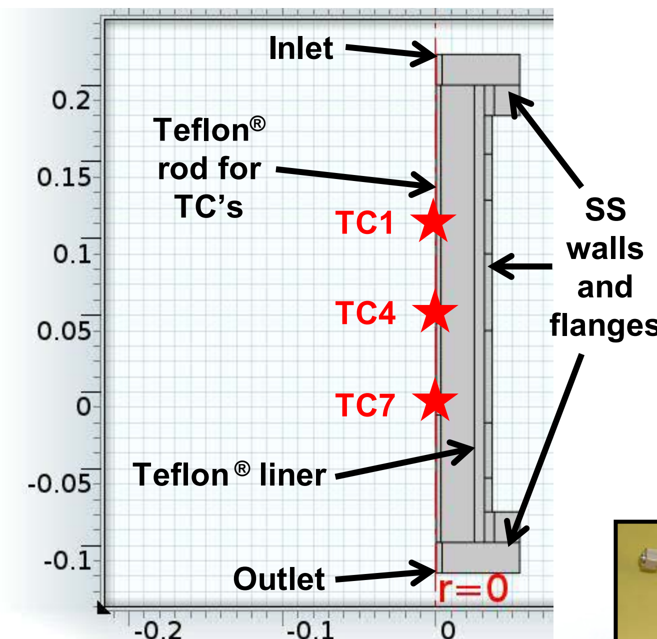
Accomplishments and Progress – MOF-5 Powder with No Internal Heat Exchanger: Data vs. Model





Model Conditions:

- Initial: P = 0.036 MPa,
  T = 288.2 K
- Boundary:
  - Inlet P & T: Exp. data
  - Outlet T: Exp. data
  - Outlet vel.: flow rate
  - Wall BCs: Conv. flow
- NIST reference for SS and Teflon® properties.



- **Paths to improve accuracy:**
  - **Account for H_2 channeling**
  - **Boundary conditions**
  - **Measurement locations**

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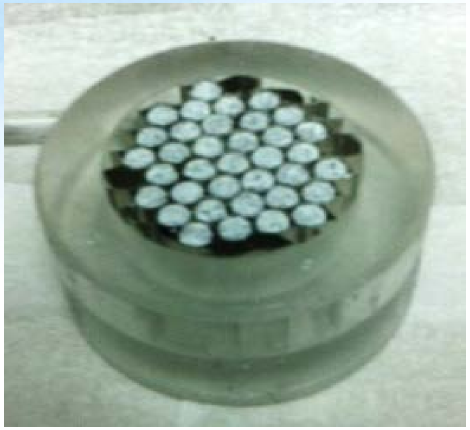
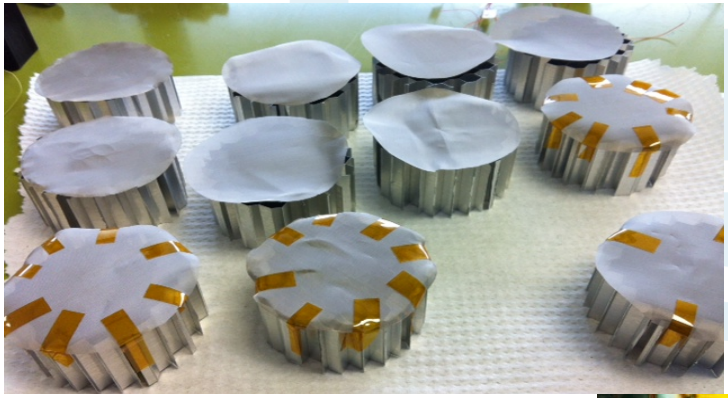
Accomplishments and Progress – MOF-5 Pellets in a HexCell Internal Heat Exchanger: Experimental Data

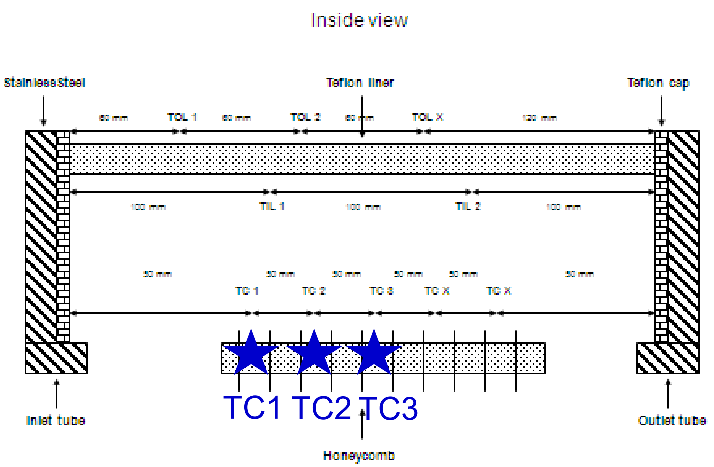


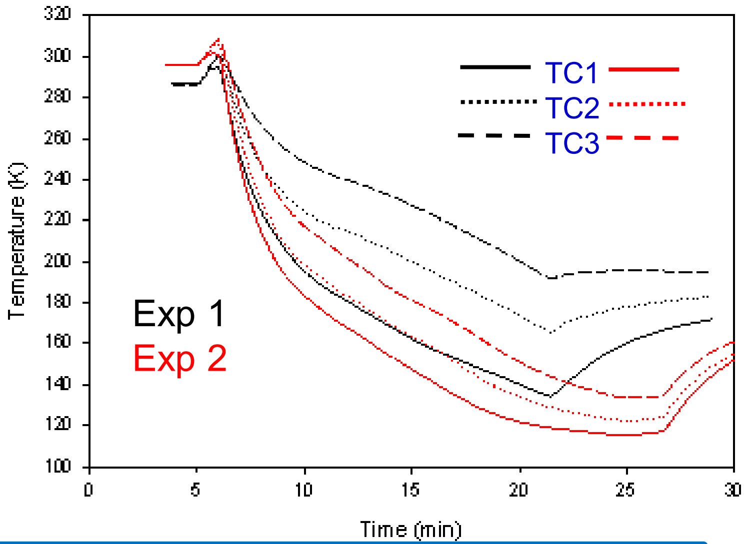
11 structures

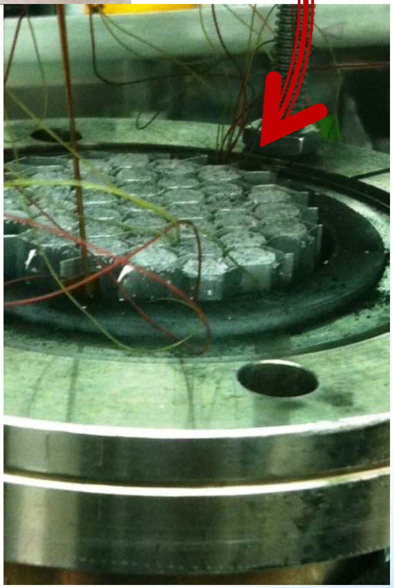
Pelletized MOF-5 + MaxSorb powder filling the void space



Packed in the Teflon® liner







Material weights:

- **Aluminum honeycomb structure: 39.147 g.**
- **MOF-5 pellets: 103.271 g.**
- **MaxSorb activated carbon: 48.674 g.**

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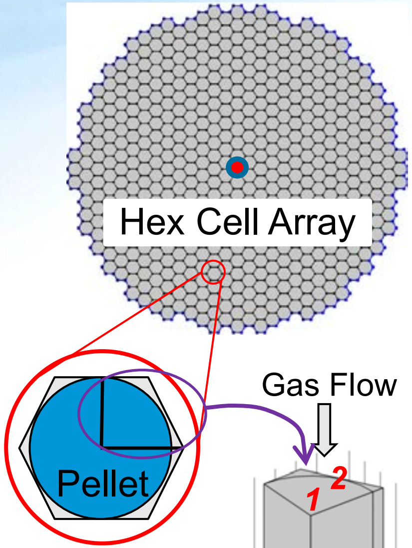
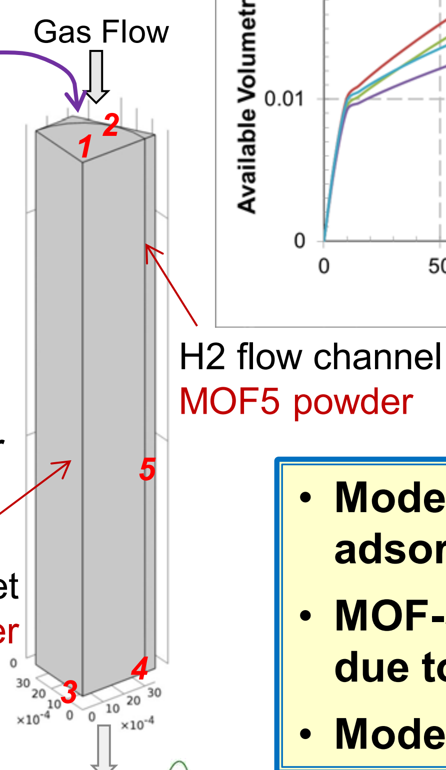
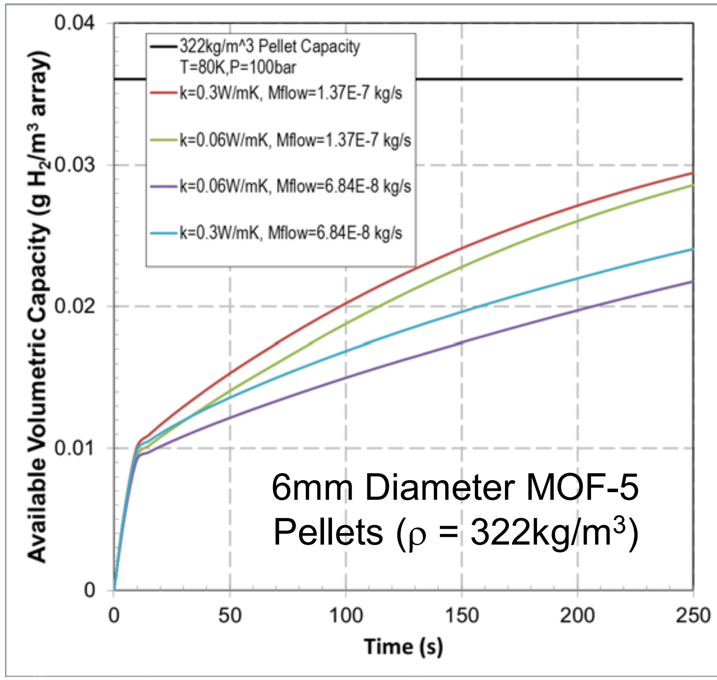
Accomplishments and Progress – Pellet Flow-Over Cooling vs Powder Flow-Through Cooling

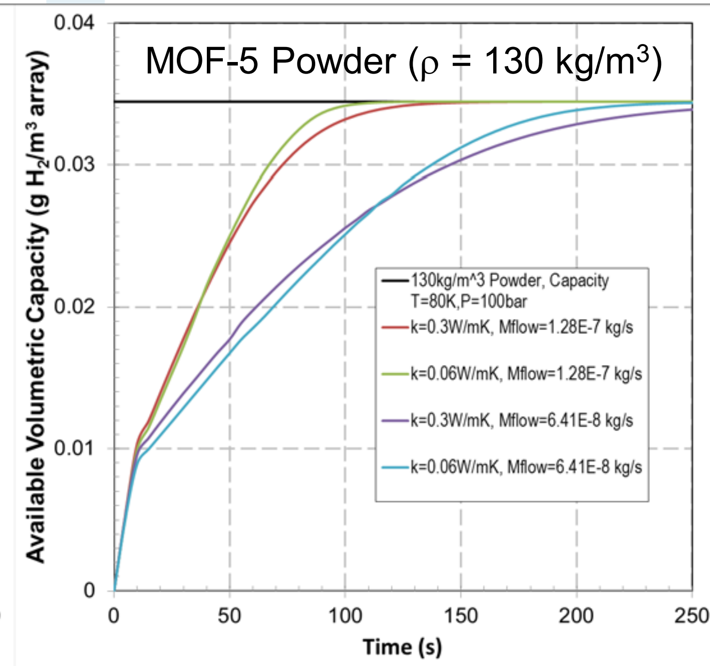




Initial Tank:
$P_{initial}$ = 5 bar
$T_{initial}$ = 180 K

Inlet Gas:
T_{inlet} = 80 K
P_{inlet} = 100 bar (from 5 bar in 10 sec)





The volumetric capacity given in these figures is the deliverable hydrogen divided by the volume bounded by the walls of the hex cell.

- **Models indicate good heat transfer characteristics if the adsorbent and HexCells are in good thermal contact.**
- **MOF-5 Powder charges more rapidly than MOF-5 Pellets due to high permeability.**
- **Model conclusions supported by experimental results.**

Approach – From Over ½ Billion Combinations → Down to Four Phase 2 Systems

Over ½ Billion Possible System Combinations:

- Internal heat exchangers (all options) **(x45)**
- Tank types **(x6)**
- L-to-D ratios **(x3)**
- LN_2 inner wall chiller **(x2)**
- Hemispherical vs. oblate endcaps **(x2)**
- Pressure vessel only vs. full design **(x2)**
- Material types (with volume-% changes) **(x87)**
- Media packing density **(x10)**
- Full tank pressure **(x12)**
- Full tank temperature **(x7)**
- Empty tank temperature **(x4)**

Eliminate unrealizable system options and combinations of options

62 Million Reasonable Systems Combinations:

- Internal heat exchangers (all options) **(x31)**
- Tank types **(x2)**
- L-to-D ratios **(x3)**
- LN_2 inner wall chiller **(x2)**
- Hemispherical vs. oblate endcaps **(x2)**
- Pressure vessel only vs. full design **(x1)**
- Material types (with volume-% changes) **(x29)**
- Media packing density **(x5)**
- Full tank pressure **(x12)**
- Full tank temperature **(x6)**
- Empty tank temperature **(x8)**

Perform a parametric study

Option #1	Option #2	Option #3	…	Option N
1	1	1	…	1
2	1	1	…	1
⋮	⋮	⋮	⋮	⋮
N_1	1	1	…	1
1	2	1	…	1
2	2	1	…	1
⋮	⋮	⋮	⋮	⋮
N_1	N_2	N_3	…	N_N

Filter the Results

Final 4 Systems:

- Three flow-through cooling with resistance HX options:
  1. HexCell with powder MOF-5
  2. HexCell with 0.32 g/cc compacted MOF-5 pellets
  3. Helical coil with powder MOF-5
- One isolated-LN_2 cooling with isolated-H_2 heating option:
  4. MATI with 0.32 g/cc compacted MOF-5 pucks

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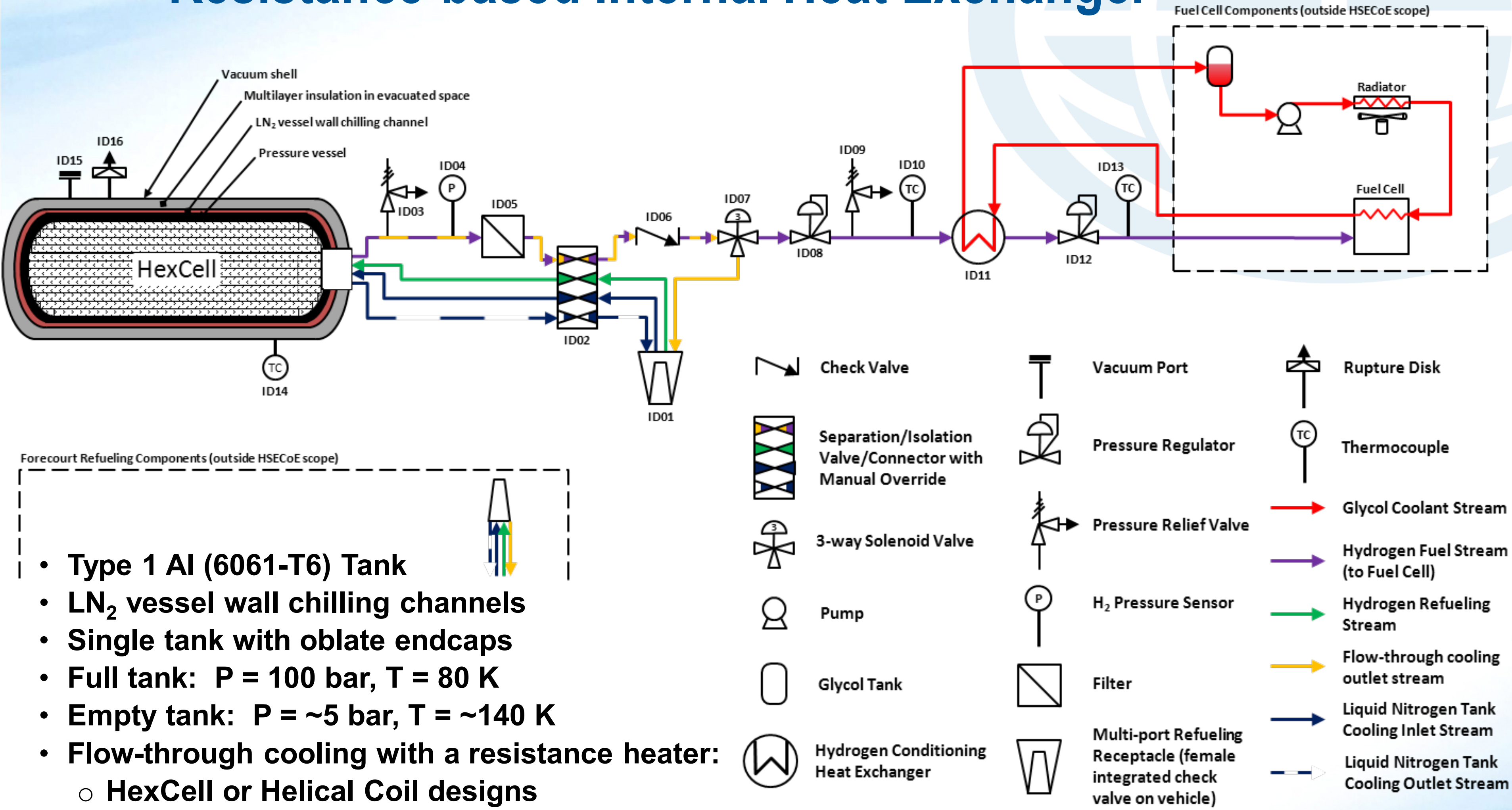
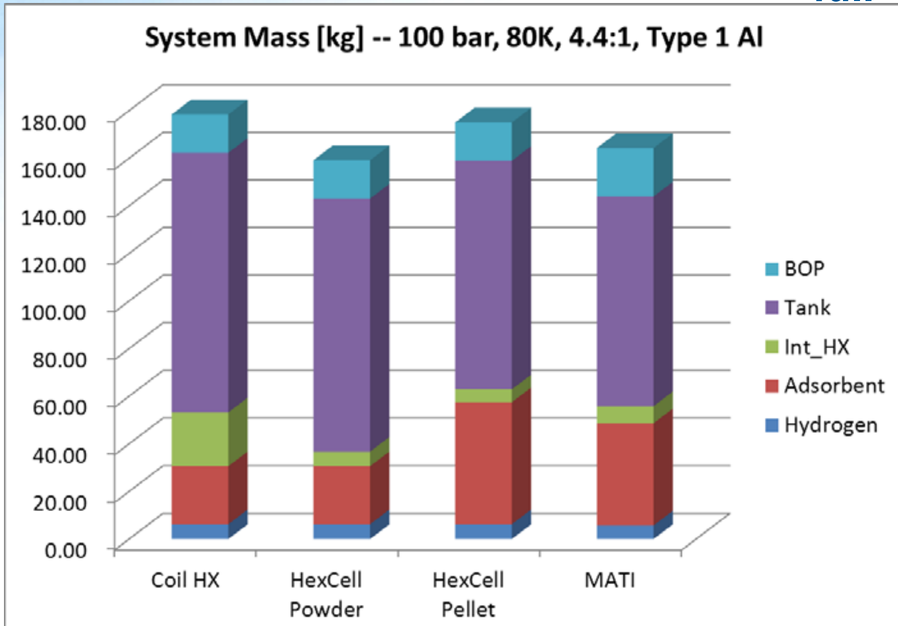
Approach – System Designs: Flow-Through Cooling with a Resistance-based Internal Heat Exchanger

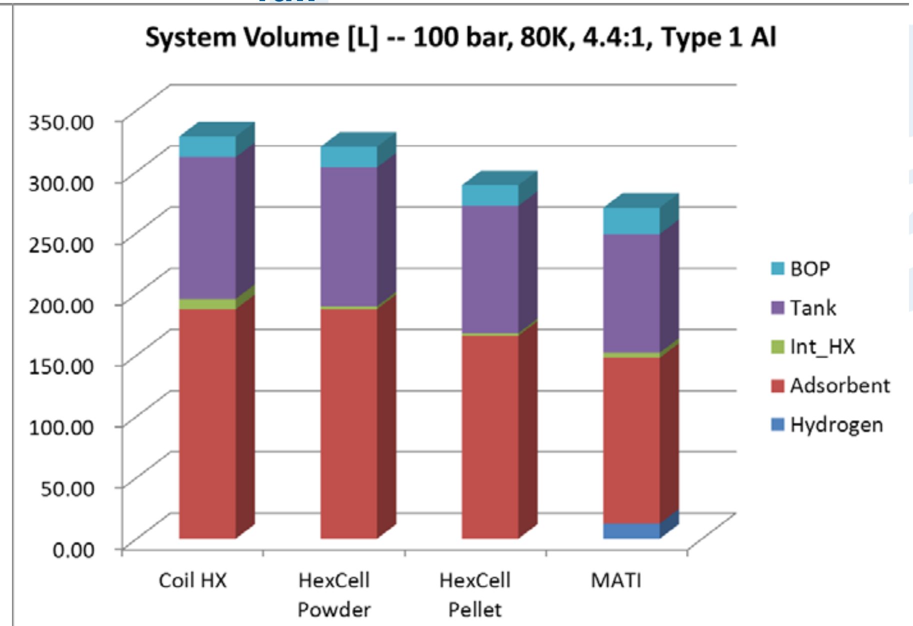


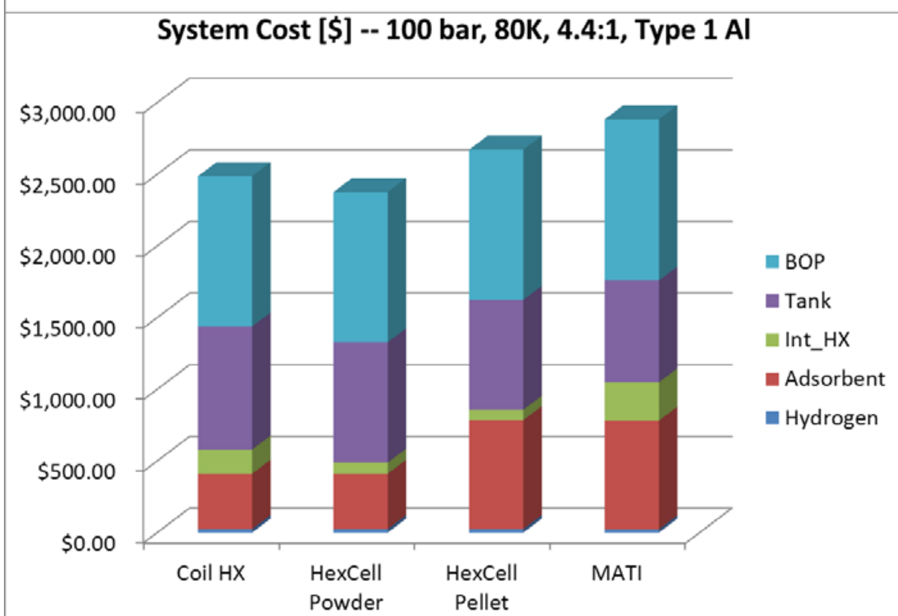
- Type 1 Al (6061-T6) Tank
- LN_2 vessel wall chilling channels
- Single tank with oblate endcaps
- Full tank: P = 100 bar, T = 80 K
- Empty tank: P = ~5 bar, T = ~140 K
- Flow-through cooling with a resistance heater:
  - HexCell or Helical Coil designs
- 0.13 g/cc powder MOF-5, with 100% packing density

NOTE: System design for an isolated heating/cooling fluid internal heat exchanger (MATI) is not shown.

Accomplishments and Progress – System Comparisons: 4.4:1 Type 1 Al Tank, T_{full} = 80 K, P_{full} = 100 bar.







- **The largest contribution to the total system mass is the storage tank:**
  - **53% – 67% of total system mass**
- **Two large system volume contributors:**
  - **Adsorbent: 50% – 59% of sys. volume**
  - **Storage vessel: ~36% of sys. volume**
- **System cost drivers:**
  - **BOP: 38% – 44% of system cost**
  - **Storage vessel: 24% – 36% of sys cost**
  - **Adsorbent: 15% – 29% of system cost**

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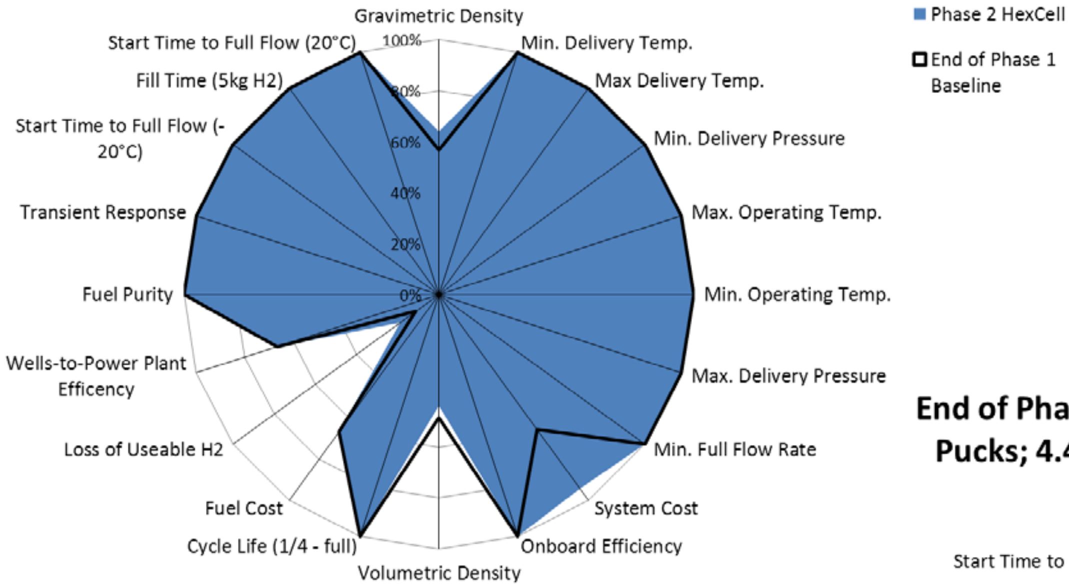
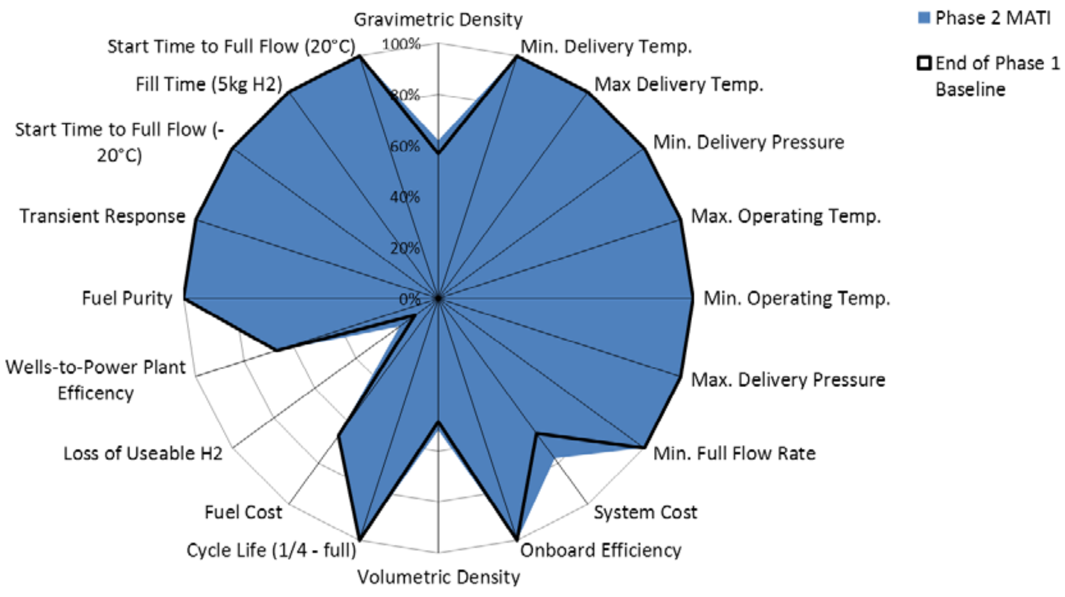
Accomplishments and Progress – System Spider Chart Comparisons: Phase 1 Baseline vs. HexCell vs. MATI

End of Phase 2 HexCell (projected) vs. 2017 Targets: MOF-5 Powder; 4.4:1 Type 1 Al Tank w/ LN_2; HexCell HX; 100 bar, 80 K (full)



	Gravimetric Capacity (g_{H2}/g_{sys})	Estimate System Cost ($/$kWh_{net}$)	Volumetric Capacity (g_{H2}/L_{sys})	Loss of Usable H_2 ($g/hr/kg_{H2}$)
End of Phase 1 Baseline	0.0312	$18.30	0.0194	0.445
HexCell with Powder MOF-5	0.0352	$12.73	0.0175	0.267
MATI with Comp. 0.32 g/cc MOF-5	0.0341	$15.45	0.0207	0.267

End of Phase 2 MATI (projected) vs. 2017 Targets: 0.32 g/cc MOF-5 Pucks; 4.4:1 Type 1 Al Tank w/ LN_2; MATI HX; 100 bar, 80 K (full)



- **Tank**:
  Type 3 Al+CF vs. Type 1 Al
- **Adsorbent Material**:
  AX-21 vs. MOF-5
- **Full Tank Pressure**:
  200 bar vs. 100 bar
- **Internal HX**:
  "generic" vs. HexCell vs. MATI

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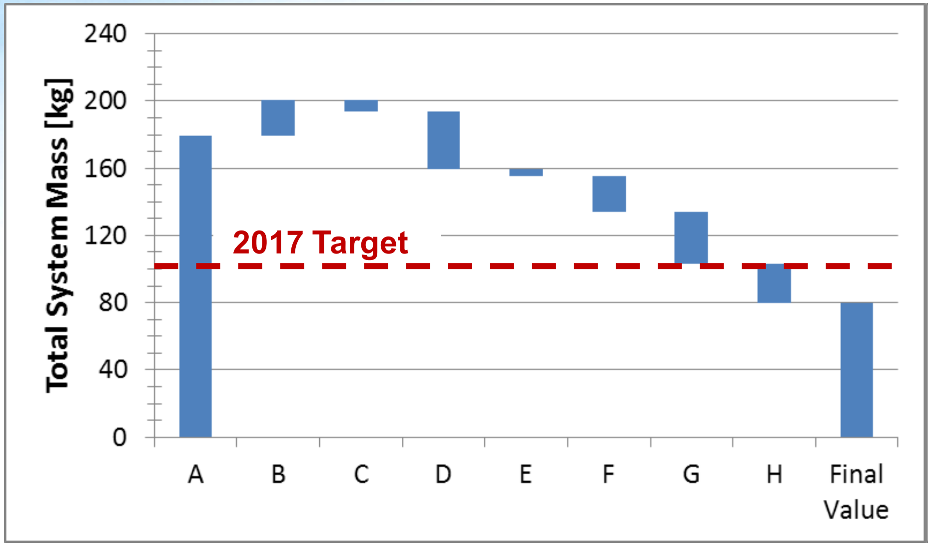
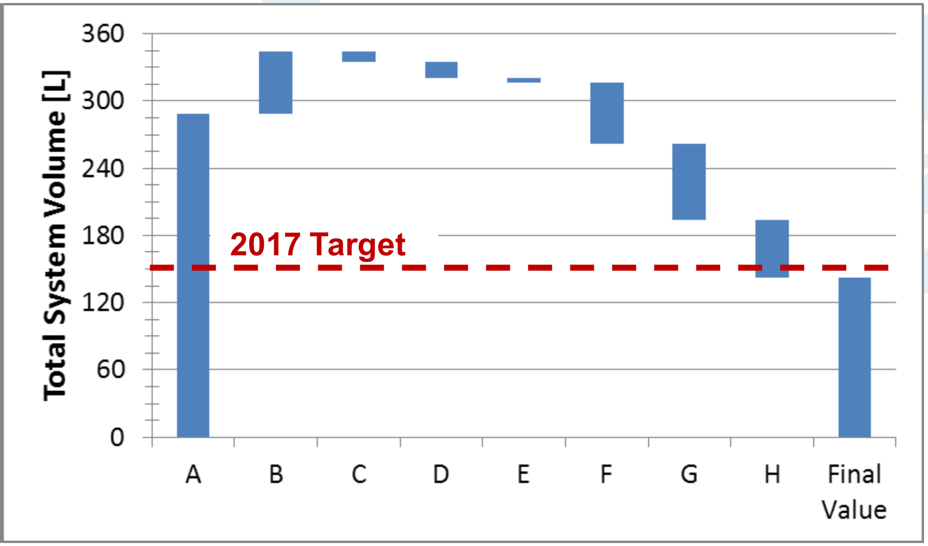
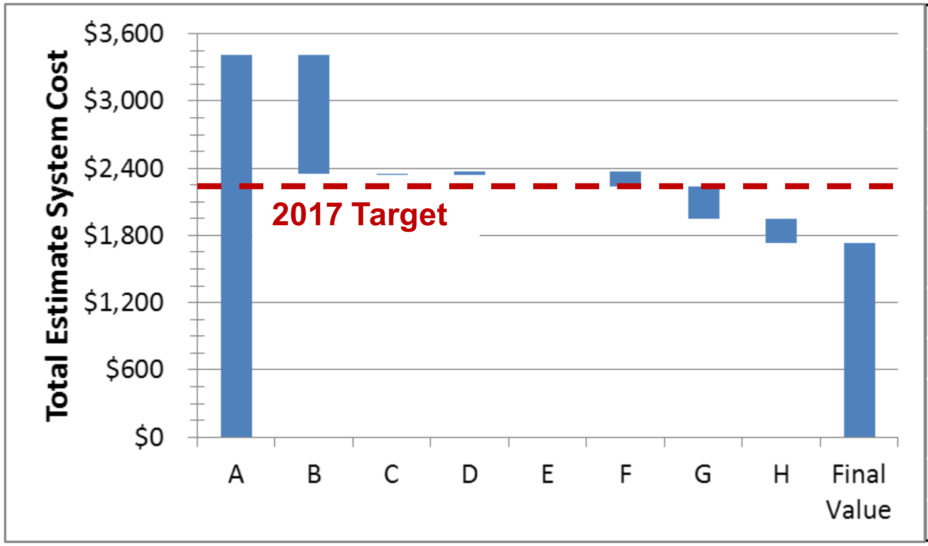
Future Work – Possible Changes/Improvements: Waterfall Charts for an 80 K, 100 bar HexCell Storage System





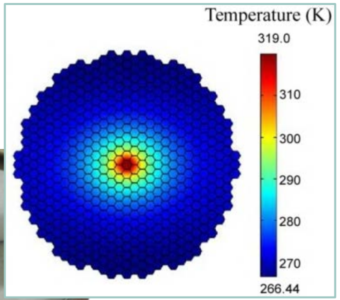


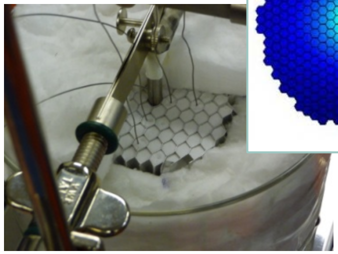
Step	Description
A	Phase 1 Baseline – Activated Carbon; Type 3 tank; Full at 80K, 200 bar; FT Cooling + Generic Resistance Heater
B	Set Operating Conditions to 80 K, 100 bar and Type 1 Al Tank
C	Identify Internal Heat Exchanger Design: HexCell w/ Resistance Heater
D	Change Material from Activated Carbon to Powder MOF-5
E	Improve BOP Components (reduce mass & volume by 25%)
F	Maintain Capacity with increased Operating Temperature (reduce MLVI by 50%; remove LN_2)
G	Increase Material Capacity to 140% of Powdered MOF-5
H	Increase Material Capacity to 200% of Powdered MOF-5

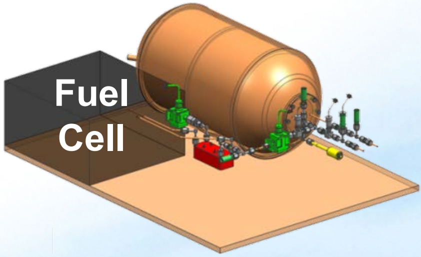
Future Work – Phase III Prototype Design

- **Finalize selection of the cooling and heating methods for the Phase III Prototype.**
- **Subscale component/concept testing.**
  - Continue experiments at UQTR, GM, and OSU.
    - **Component/concept validation.**
    - **Preliminary testing with MOF-5.**
  - Validate detailed models with experimental results.
    - **Perform specifically designed experiments to aid in understanding the physical behavior.**
    - **Improve model accuracy for full system scale-up and/or future material predictions.**
  - Subscale testing of internal heat exchanger components.
  - Identify design modifications as necessary.
- **Full system scale-up and future system predictions**
  - Finalize the system-level Balance of Plant (BOP).
    - **Component selection and selected mass, volume, cost, etc.**
    - **Identify possible automotive-scale component combinations/reductions.**
  - System-level modifications based on subscale and prototype results.
- **Additional detailed model development (as required).**
- **Additional system model development (as required).**

UQTR's new testing facilities for Phase 3 experiments



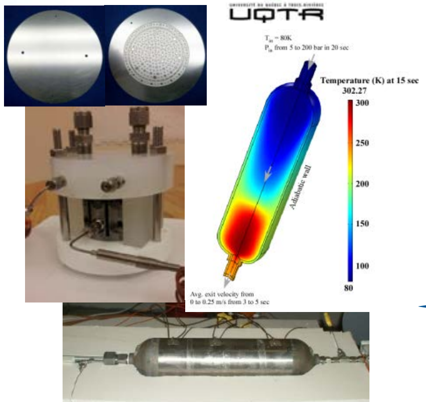




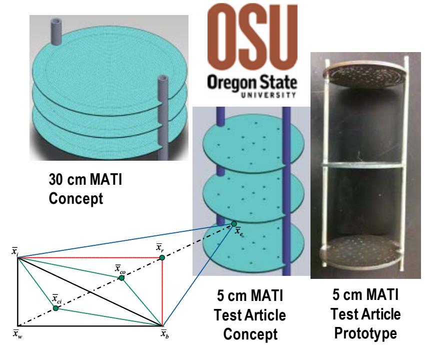
All Planned Activities Will Automatically Support the Phase III SMART Milestones.

Collaborations

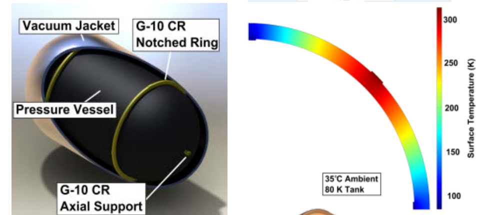
Adsorbent Prototypes: Design, Testing and Model Validation

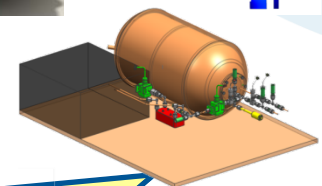


Modular Tank Insert: Optimization

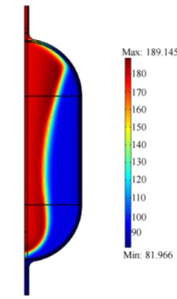


H_2 Flow and Heat Exchanger: Modeling and Analysis

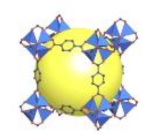




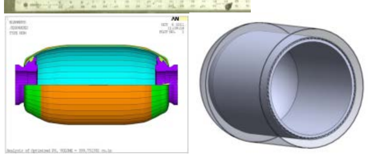
Flow-Through Heat Transfer Modeling



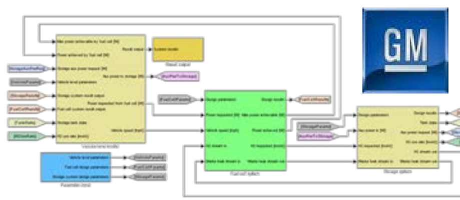
Compacted Media: Properties and Behavior

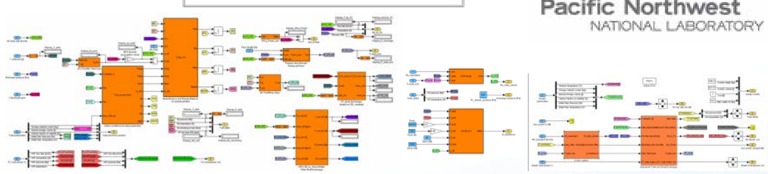


Pressure Vessels: Properties, Thicknesses, and "Thermos Design"



Adsorbent System Models





Project Summary

Relevance

As both the overall lead and a major technical contributor to the HSECoE project, SRNL is using its extensive expertise in thermodynamics, hydrogen materials compatibility, transport phenomena modeling & analysis, and hydrogen storage system & component design & fabrication to evaluate solid-state hydrogen storage systems for vehicle application that meet or exceed DOE's 2017 goals.

SRNL, through a subcontract grant, is also utilizing the expertise of the UQTR, which has been internationally recognized for its work in hydrogen adsorbent material and system development and testing.

Approach

- Provided analyses for the Phase III Prototype Design and Go/No-Go decisions.
- Developed, validated, and applied detailed models of several adsorbent media options.
- Investigated the viability of the flow-through cooling concept for adsorbent systems, from both modeling and experimental perspectives.
- Developed and applied full system models that determined hydrogen storage requirements for combinations of media, vessel, and components.

Technical Accomplishments and Progress (as of 03/2013)

- Developed an Adsorbent Acceptability Envelope (AAE) that identifies coupled material properties and system dimension that affect gravimetric capacity, volumetric capacity, charging rates, and discharging rates.
- Detailed model results and experimental results (through UQTR, the subrecipient of SRNL) suggest:
  - Charging is best achieved using LN_2 assisted flow through cooling.
  - While pelletized MOF-5 offers some improved volumetric capacity, the time for charging is significantly increased.
    - Mass and enthalpy of exhaust H_2 increases as well.
  - The HexCell insert with an electrical resistance heater can be used to discharge hydrogen, while still permitting effective flow-through cooling.
- Developed fully customizable adsorbent system models to compare possible full-scale systems.
  - Parametric study: reduced over ½ Billion systems down to four leading adsorbent systems designs.
  - Projected future system designs assuming possible system, component, and/or material improvements.
- Developed external, publically accessible, web site and disseminated the metal hydride acceptability envelope and heat transfer models.

Collaborations

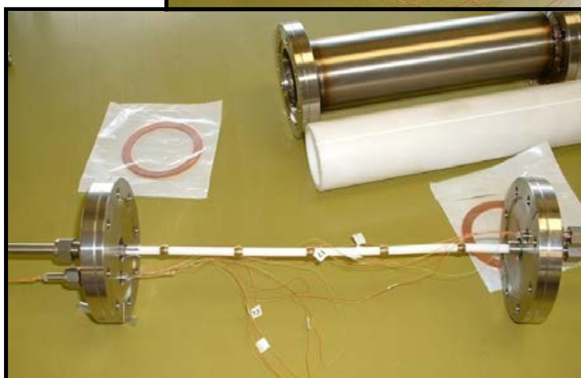
HSECoE partners, Materials Centers, SSAWG, IPHE, IEA ; Griffith University, Brisbane, Australia

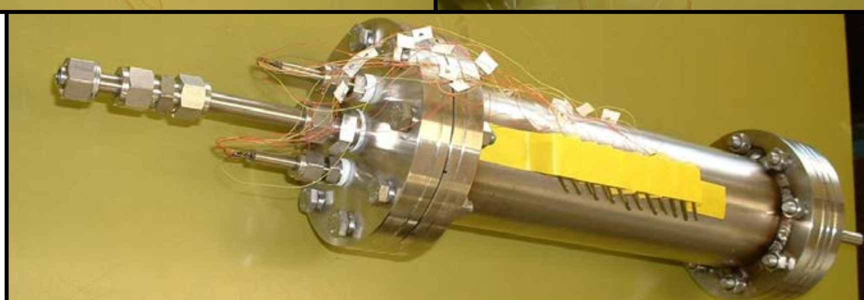
Proposed Future Work – Phase III Prototype Development

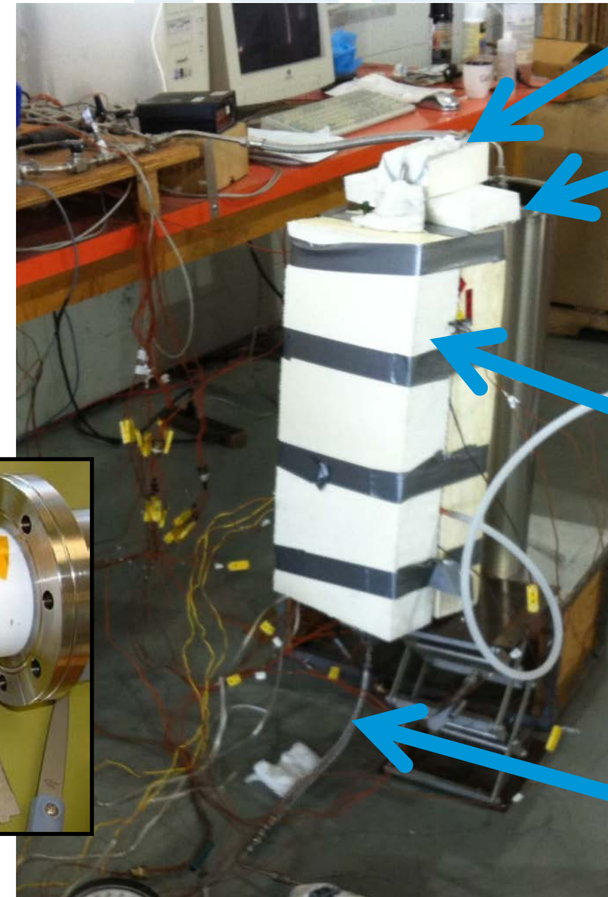
- Finalize selection of the cooling and heating methods for the Phase III Prototype.
- Subscale component / concept testing:
  - Continue experiments at UQTR, GM, and OSU for further component/concept validation with MOF-5.
  - Validate detailed models with experimental results, with specifically designed experiments to aid in understanding the physical behavior and improve model accuracy.
  - Subscale testing of internal heat exchanger components.
- Full system scale-up and future system predictions:
  - Finalize the system-level Balance of Plant component selection (mass, volume, cost, etc.), identifying possible automotive-scale component combinations/reductions.
  - System-level modifications based on subscale and prototype results.

Technical Back-up Slides

Accomplishments and Progress – Flow-Through Cooling Validation Experiments

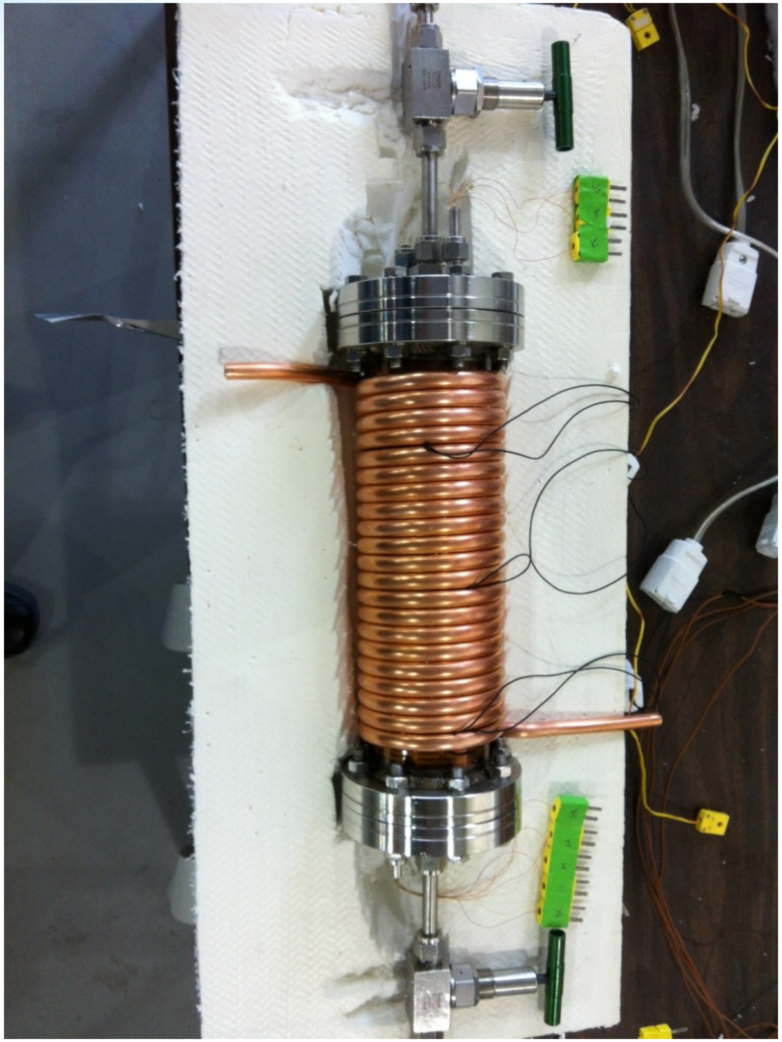






• Accessible Internal Volume	0.56 L
• Vessel Mass	8.0 kg
• Pressure Rating	10.0 MPa
• Pressure tested	8.0 MPa

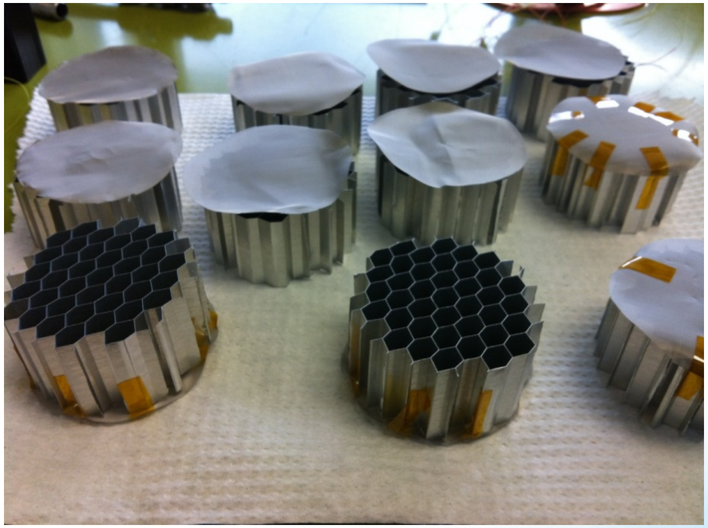
Approach – MOF-5 Powder With HexCell Lattice: Assembly of Apparatus with LN_2 coil



Al HexCell weight = 39.0 g
Al HexCell volume = 15 ml
MOF-5 Powder: 88.6 g (ρ = 160 kg/m^3)

Planned experiments:

1. **Powder w/ hex cell**
2. **Powder w/ hex cell w/ LN2 coil**



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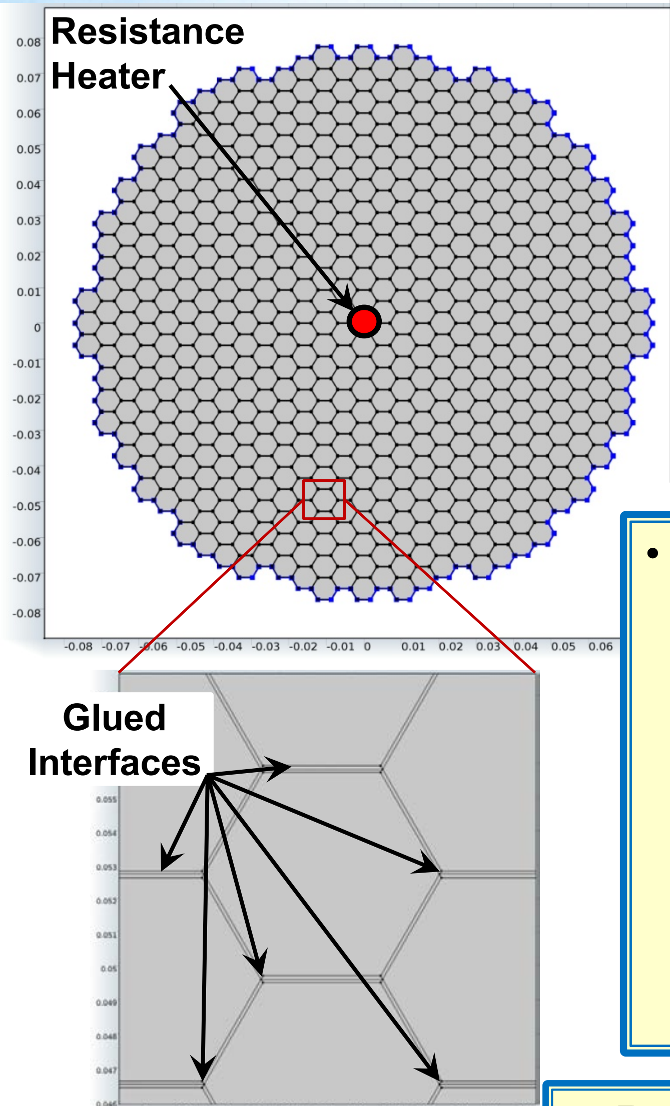
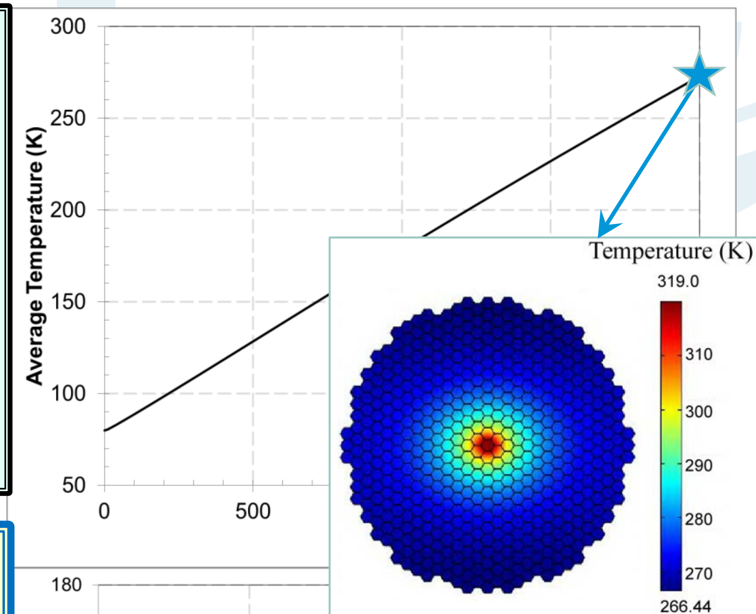
Accomplishments and Progress – Model Results for HexCell HX with Resistive Heating

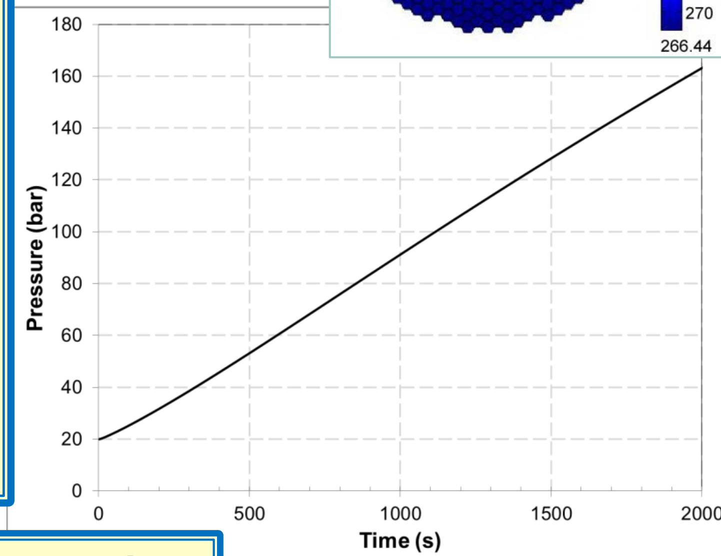


Conditions:

- Initial: 20 bar, 80 K
- Heather power: 550 W
- HexCell size: 6 mm
- Wall thickness: 0.10 mm
- Includes glued interfaces
- Overall diameter: 15.41 cm
- HexCell thermal properties (assume 6063-T83 Al):
  - k = 201 W/m/K
  - ρ = 2700 kg/m^3
  - C_p = 900 J/kg/K

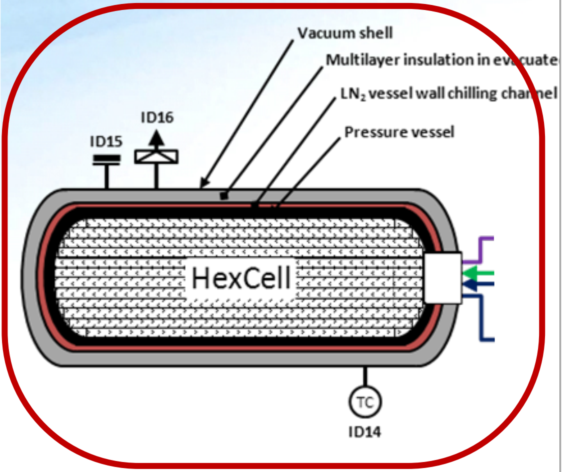


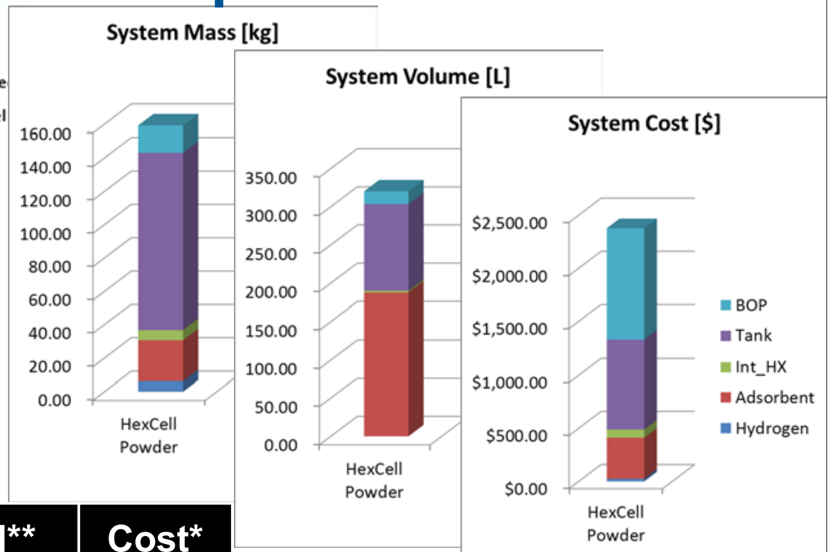
- **3D Model for HexCell Heat Exchanger:**
  - **Structures contain powder or pellets.**
  - **Charging – flow-through cooling.**
  - **Discharging – heating by an electric resistance heater.**

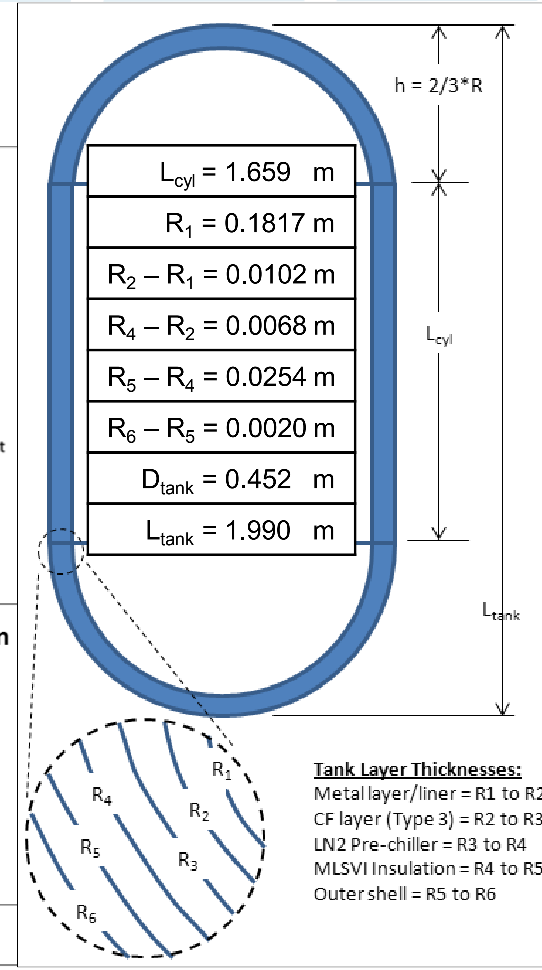


Resistive heater in HexCell mesh provides adequate H_2 discharge rate.

Accomplishments and Progress – Powder MOF-5 HexCell System: Tank Components Breakdown



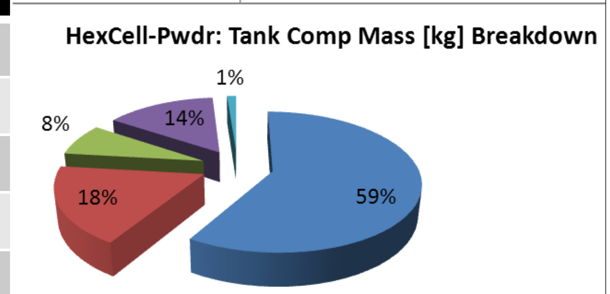


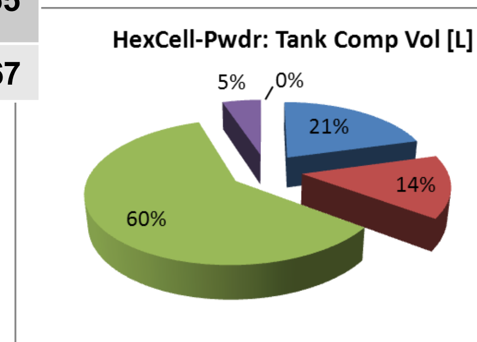


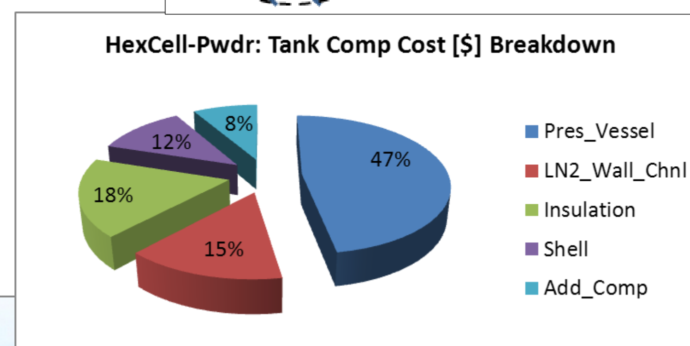
Component	Mass	Vol**	Cost*
Pressure Vessel	62.45 kg	23.45 L	$397.47
LN_2 Channel	19.24 kg	16.42 L	$122.45
Insulation	8.01 kg	67.84 L	$151.51
Outer Shell	15.35 kg	5.77 L	$97.70
Boss, Plug, & Support Rings	1.28 kg	0.00 L	$70.55
Tank-only Totals	106.33 kg	303.36 L	$839.67

* Tank costs include manufacturing cost (34% multiplier on Al mass).

**Tank volume total is the tank outer volume (outside of the shell).







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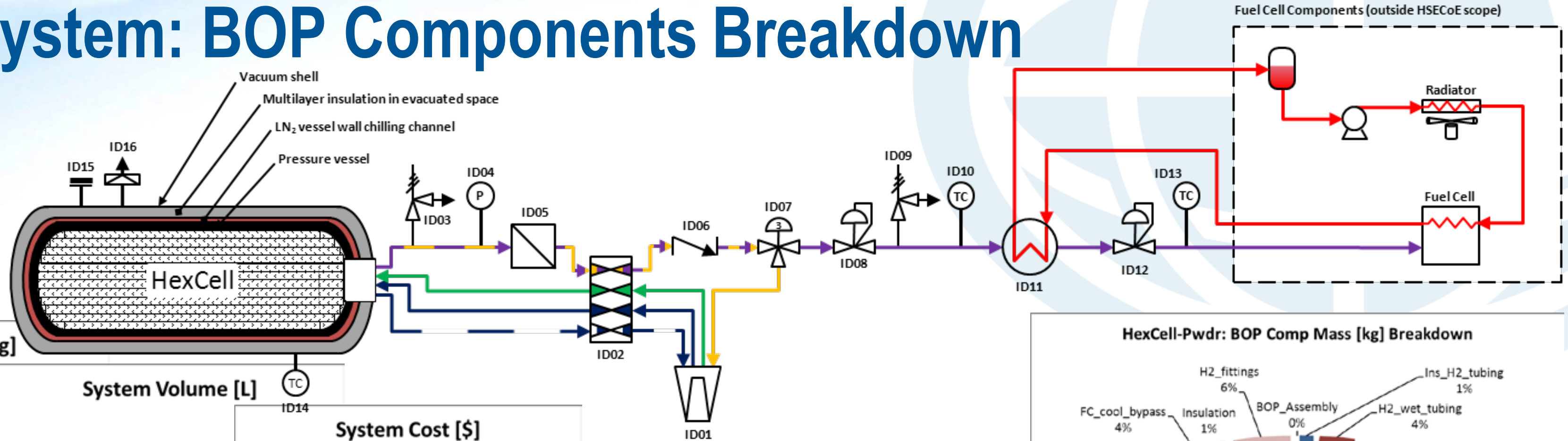
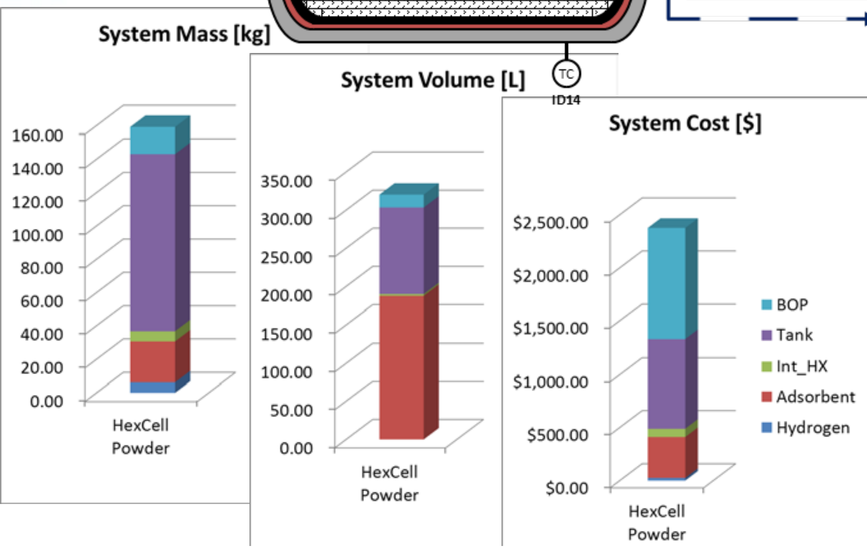
Accomplishments and Progress – Powder MOF-5 HexCell System: BOP Components Breakdown





- BOP accounts for ~44% of system cost.
- H_2 conditioning heat exchanger and (2x) pressure regulators account for ~50% of BOP cost.