Hydrogen Storage Engineering
CENTER OF EXCELLENCE

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Project ID# ST004

SRNL
SAVANNAH RIVER NATIONAL LABORATORY

Overview

Timeline

- Start: February 1, 2009
- End: June 30, 2014
- 70% Complete (as of 3/31/13)

Budget

- Total Center Funding:
  - DOE Share: $ 36,232,765
  - Contractor Share: $ 3,591,709
  - FY '12 Funding: $ 5,930,000
  - FY '13 Funding: $ 5,150,000
- Prog. Mgmt. Funding
  - FY '12: $ 400,000
  - FY '13: $ 300,000

Barriers

A. System Weight and Volume
B. System Cost
C. Efficiency
D. Durability
E. Charging/Discharging Rates
G. Materials of Construction
H. Balance of Plant (BOP) Components
J. Thermal Management
K. System Life-Cycle Assessment
O. Hydrogen Boil-Off
P. Understanding Physi/Chemi-sorption
S. By-Product/Spent Material Removal

Partners

SRNL Savannah River National Laboratory
Pacific Northwest National Laboratory
Los Alamos National Laboratory
JPL Jet Propulsion Laboratory California Institute of Technology
NREL National Renewable Energy Laboratory
Michigan
OSU Oregon State University
HRI UQTR
Ford
GM
United Technologies Research Center
BASF The Chemical Company
Hexagon Lincoln

HSECoE

HSECoE Technical Objectives

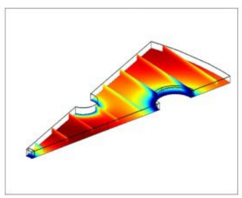
Using systems engineering concepts, design innovative material-based hydrogen storage system architectures with the potential to meet DOE performance and cost targets.

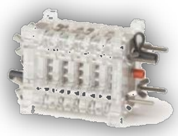
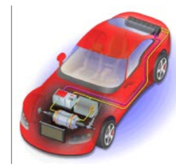
- **Develop and validate system, engineering and design models** that lend insight into overall fuel cycle efficiency.
- Compile all relevant materials data for candidate storage media and **define required materials properties to meet the technical targets**.
- **Design, build and evaluate subscale prototype systems** to assess the innovative storage devices and subsystem design concepts, validate models, and improve both component design and predictive capability.

Why Perform Materials Development and System Engineering in Parallel?

continuous feedback with system design

identifying materials requirements

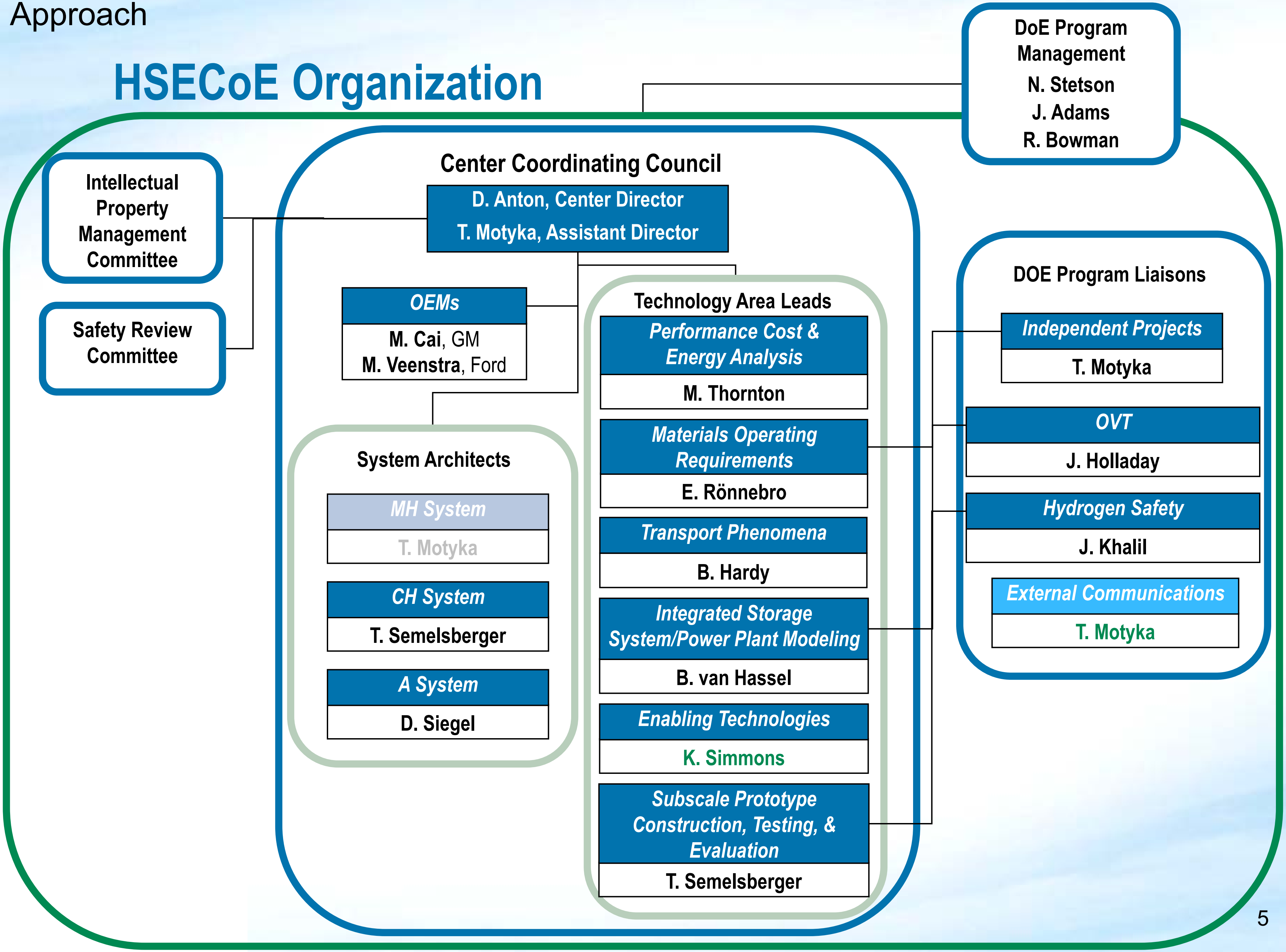




Materials → Thermal Management → H_2 Storage BoP → Fuel Cell → Vehicle → Wheels

- Materials ↓ Engineered Materials Properties
- Thermal Management ↓ Heat Transfer Designs
- H_2 Storage BoP ↓ BoP Component Requirements
- Fuel Cell, Vehicle, Wheels ↓ What is Needed of the Hydrogen Storage Media & System

HSECoE Organization



Technical Matrix

Technology Areas		System Architects: Adsorbent System *Siegel*	System Architects: Chemical Hydride System *Semelsberger*
	Performance Modeling & Cost Analysis *Thornton*	Thornton Weimar	Thornton Weimar
	Integrated Power Plant & Storage System Modeling *van Hassel*	Tamburello	Brooks
	Transport Phenomena *Hardy*	Hardy Corgnali, Sulic Ortman, Drost	Brooks Semelsberger
	Materials Operating Requirements *Rönnebro*	Veenstra Chahine Simpson	Rönnebro Semelsberger
	Enabling Technologies *Simmons*	Simmons Newhouse Reiter	van Hassel Holladay Simmons Semelsberger
	Subscale Prototype Demonstrations *Semelsberger*	Chahine Hardy	Semelsberger

Phased Approach

Phase I: System Requirements & Novel Concepts

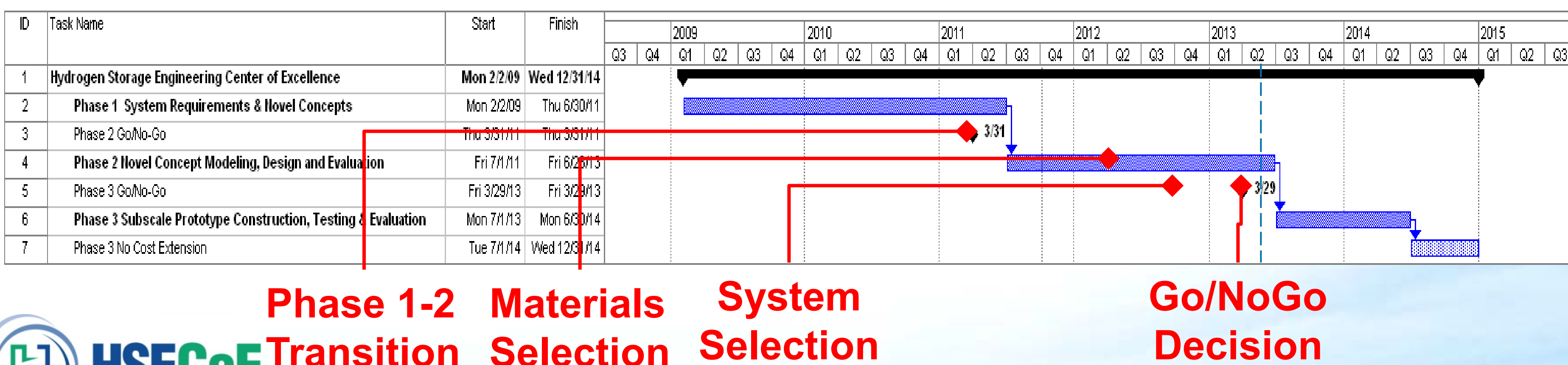
Phase II: Novel Concept Modeling Design & Evaluation

Phase III: Sub-Scale Prototype Construction, Test and Evaluation

- **Where are we and where can we get to?**
  - Model development
  - Benchmarking
  - Gap Identification
  - Projecting advances
- **How do we get there (closing the gaps) and how much further can we go?**
  - Component development
  - Concept validation
  - Integration testing
  - System design
  - **Materials requirements**
- **Put it all together and confirm claims.**
  - **System integration**
  - **System assessments**
  - **Model validation**
  - Gap analysis
  - Performance projections

Important Dates Phase 2

- Duration: 5.5 years
  - Phase 1 Start: Feb. 1, 2009
  - Phase 1-2 Transition: March 31, 2011
  - Phase 1 End: June 30, 2011
  - Phase 2 Start: **July 1, 2011**
  - Phase 3 Go/No-Go Determination: **March 31,2013**
  - *Phase 2 End:* **June 30, 2013**
  - Phase 3 Start: **July 1, 2013**
  - Completion Date: June 30, 2014 ⇨ *3/31/15?*

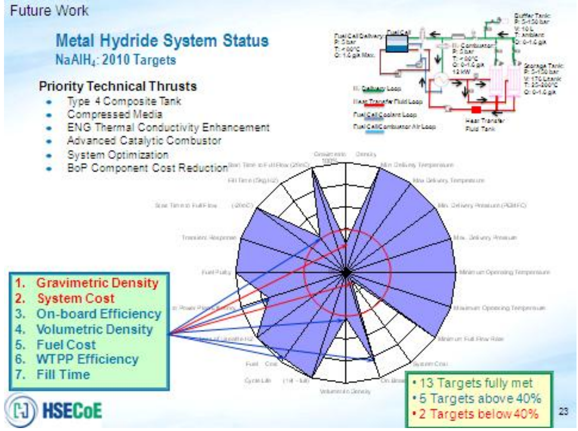


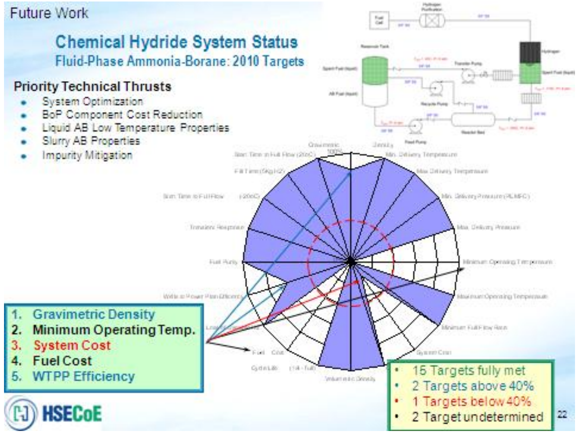
HSECoE

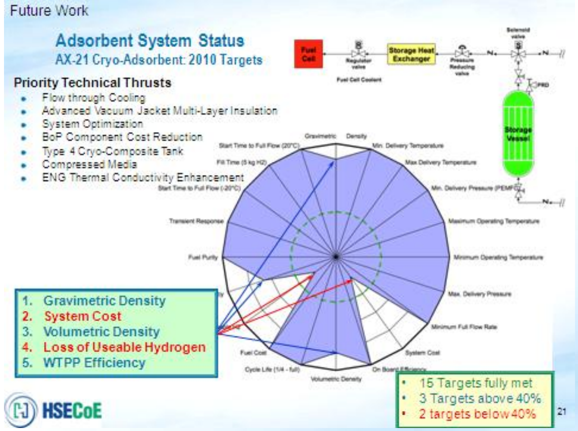
Phase 1-2 State-of-the-Art

State-of-the-Art Identified for Chemical and Adsorbent Hydrogen Storage Systems

- Current status vs targets
- Identification of critical technical barriers
- Identification of potential solutions to barriers
- Summary of projected system performance vs targets







HSECoE Phase 2 Go/NoGo Milestones

Chemical Hydrides			3/31/2011			3/31/2013		
			Phase 1 HSECoE Baseline (System)			**Phase 2 HSECoE Go/No-Go *Targets* *(full scale)***		
Target	Units	2015 DOE Goal (System)	Phase 1 HSECoE Baseline (Material)	Phase 1 HSECoE Basline (BOP only)	Phase 1 HSECoE Baseline (System)	Phase 2 HSECoE Actuals (Material)	Phase 2 HSECoE Actuals (BOP only)	Phase 2 HSECoE Actuals (System)
Gravametric Capacity	kg H2/kg system	0.055	0.076	0.092	0.042	0.076	0.109	0.045
mass	*liters*	*102*			*133*			*124*
Volumetric Capacity	kg H2/L system	0.04	0.074	0.077	0.039	0.074	0.102	0.043
volume	*kg*	*140*			*144*			*130*
System Cost *	$/kWh net	6		25.6	25.6		25.6	25.6
	$	*480*						
Fuel Cost	$/gge at pump	2-6						
Min Operating Temp	°C	-40			?			0
Max Operating Temp	°C	60			50			50
Min Delivery Temp	°C	-40			-40			-40
Max Delivery Temp	°C	85			85			85
Cycle Life	cycles	1500			1000			1000
Min Delivery Pressure	bar	5			5			5
Max Delivery Pressure	bar	12			12			12
Onboard Efficiency	%	90			97			97
Well to Power Plant Efficiency	%	60			37			37
System Fill Time	min	3.3			2.7			2.7
Min Full Flow Rate	(g/s/kW)	0.02			0.02			0.02
	g/s	*1.6*			*1.6*			*1.6*
Start Time to Full Flow (20°C)	sec	5			1			1
Start Time to Full Flow (-20°C)	sec	15			1			1
Transient Response	sec	0.75			0.49			0.49
Fuel Purity	%H2	99.97			99.97			99.99
Permeation, Toxicity, Safety	Scc/h	Meets or Exceeds Standards			s			s
Loss of Useable Hydrogen	(g/h)/kg H2 stored	0.05			0.1			0.1

Responsible Organization	**Component**	**3/31/2011**	**3/31/2013**
LANL, PNNL	Media	Fluid AB at 50wt%	Fluid AB at 65wt%
PNNL	Tank	Bladder Tank	Bladder Tank
LANL	Reactor	Flow Through Reactor	Flow Through Reactor
PNNL	System Design		
	BoP		
PNNL	Pumps	Feed/Recycle/Transfer Pumps	Feed/Recycle/Transfer Pumps
UTRC	Heat Exchanger		Heat Exchanger mass and volume cut
UTRC	GLS	Gas\Liquid Seperator	Gas\Liquid Seperator
UTRC	Purification	Purification	Hydrogen Purification mass and volume

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Volumetric Capacity	kg H2/L system	0.04	0.074	0.077	0.039	0.074	0.102	0.043
volume	*kg*	*140*			*144*			*130*
System Cost *	$/kWh net	6		25.6	25.6		25.6	25.6
	$	*480*						
Fuel Cost	$/gge at pump	2-6						
Min Operating Temp	°C	-40			?			0
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Min Delivery Temp	°C	-40			-40			-40
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Cycle Life	cycles	1500			1000			1000
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Onboard Efficiency	%	90			97			97
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System Fill Time	min	3.3			2.7			2.7
Min Full Flow Rate	(g/s/kW)	0.02			0.02			0.02
	g/s	*1.6*			*1.6*			*1.6*
Start Time to Full Flow (20°C)	sec	5			1			1
Start Time to Full Flow (-20°C)	sec	15			1			1
Transient Response	sec	0.75			0.49			0.49
Fuel Purity	%H2	99.97			99.97			99.99
Permeation, Toxicity, Safety	Scc/h	Meets or Exceeds Standards			s			s
Loss of Useable Hydrogen	(g/h)/kg H2 stored	0.05			0.1			0.1

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HSECoE

HSECoE Phase 2 Go/NoGo Milestones

Chemical Hydrides

Target	Units	2015 DOE Goal (System)	3/31/2011 Phase 1 HSECoE Baseline (System): Phase 1 HSECoE Baseline (Material)	Phase 1 HSECoE Basline (BOP only)	Phase 1 HSECoE Baseline (System)	3/31/2013 Phase 2 HSECoE Go/No-Go *Targets (full scale)*: Phase 2 HSECoE Actuals (Material)	Phase 2 HSECoE Actuals (BOP only)	Phase 2 HSECoE Actuals (System)
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Max Delivery Temp	°C	85			85			85

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UTRC	Purification	Purification	Hydrogen Purification mass and volume

Approach

Phase 2 Adsorbent System Milestones

Adsorbent System Component	Partner	S*M*A*R*T Milestone	Status 10/1/12	Projected Outcome
Materials Development	Ford	Report on ability to develop compacted MOF-5 adsorbent media having a total hydrogen material density of greater than or equal to 0.3 g/L, H2 density of 11 wt. % and 33 g/liter and thermal conductivity of 0.5 W/m-K at P = 60-5 bar and T = 80-160K.	H2 grav. density of the MOF-5 material >11% **is possible** with .3 g/cc (w/o ENG) at P = 60-5 bar and T = 80-160K with 60% packing efficiency. H2 vol. density of the MOF-5 material >33 g/l **is possible** with .5 g/cc (+5% ENG) at P = 60-5 bar and T = 80-160K with 100% packing efficiency. Thermal conductivity of .5 W/m-K **is possible** with .3 g/cc to .5 g/cc + 10% ENG with temperatures > 100-120 K.	The capability of achieving specific metrics with a given configuration is possible, investigations will be continue to devise a media morphology which will **meet all of the metrics**.
Materials Development	Ford/UM/ BASF	Report on ability to demonstrate a composite MOF-5 adsorbent monoliths having H2 effective kinetics equivalent to 5.6 kg usable H2 over 3 minutes and permeation in packed and powder particle beds with flow rate of 1 m/s superficial velocity and pressure drop of 5 bar.	H2 effective kinetics have been conducted and proven over 240 cycles for MOF-5 powder. The monolith testing for kinetics is planned. Permeation testing has been conducted for various temperatures and densities. Based on the extrapolation of permiation test data at 0.12 m/s, the 5bar pressure drop milestone is possible (initial assessment of uncompressed darcy) at a media density of 0.3 g/cc but will be a signficant challenge beyond this density, **meeting the metric**.	**Met Metric** The kinetic response of the MOF-5 material will achieve the desired response while the permeation will continue to be a challenge with densities greater than 0.3 g/cc.
Materials Development	SRNL/ UQTR	Report on ability to develop a compacted MOF-5 adsorbent media bed having a total hydrogen density of: 11 % g H2/(g MOF) and 33 g H2/(liter MOF) at P = 60 - 5 bar and T = 80 - 160 K	Evaluation of isotherms provided by Ford for initial & final states gives: 180kg/m^3 (uncompacted) GC=0.15 VC=26.5 **missing the VC metric** 322kg/m^3 GC=0.10 VC=33.0 **missing the GC metric** 520g/m^3 GC=0.07 VC=36.7 **missing the GC metric**	Alternative compaction methods will be pursued with Ford to identify higher volumetric density morphologies **meeting the metrics**.
Structured Bed	GM	Report on ability to develop MOF-5 powder bed having a total hydrogen density of: 15 wt. % g H2/(g MOF) and 20 g H2/(liter MOF) at P = 60 - 5 bar and T = 80 - 160 K.	Based on the modified Dubinin-Asthakov adsorption model, at 60 - 5 bar and 80 - 160 K the 3 liter test vessel contains 18.6% total deliverable g H2/(g MOF) and 30.5% g H2/(liter MOF) **surpassing the metric**.	**Exceeded metric** These results will be validated with lab experiments.
Composite Tank	JPL	Report on ability to develop testing capability to burst test Type 4 composite and Type 1 (metal) tanks at 40K and demonstrate tanks meeting minimally 2.5x nominal operating burst pressure.	Design and fabrication of a cryogenic pressure test/burst system capable of testing at 77K has been completed. Safety oversight and documentation is currently 75% complete. *Operating this system at 40 K is not feasible.* The capability to perform cryogenic cycling has also been implimented.	Safety documentation will be completed and burst testing of Type 4 COPVs, pressure testing of Type 1 tanks will be performed at 77K and adding the capability of cryogenic cycoic testing capability **exceeding the metrics** at his temperature.
Composite Tank	Lincoln	Report on ability to develop Type 4 (composite) and Type 1 (metal) tanks capable of use between 40 and 160K meeting ASME pressure vessel code for use at 60 bar having a mass less than 10 kg and a volume less than 120 liters.	Type 1 tanks have been designed and manufactured having a mass of 2.44 kg and a volume of 2.0 liters. These tanks were designed to operate at 100 bar with a minimum burst ratio of 2.25 (225 bar). The actual burst achieved during RT testing was 686 bar. Type 4 tanks have been designed and manufactured having a mass of 3.7 kg and a volume of 5.68 liters. These tanks were designed to operate at 100 bar with a minimum burst ratio of 2.25 (225 bar). The actual burst achieved during RT testing was 370 bar. anks have been suppied to JPL for burst testing at 77K to verify low temperature burst pressures. These tanks were appropriately designed having safety factors equivalent to current **DOT NHTSA standards** for compressed gas fuel containers.	Based on these resutls single piece 120 liter Type 1 and Type 4 tanks will be designed and and masses calculated. It is anticipated that the Type 1 tank will not meet hte mass target while the **Type 4 tank will meet the mass metric**.
Composite Tank	PNNL	Report on ability to identify Type IV tank liner materials suitable for 40K operation having a mass less than 8 kg and a volume less than 3 liters (2.55 mm thickness).	After evaluating 8 different materials it was concluded that the liner separates from the shell when the pressure is decreased below 35bar with a liner thickness of 2.55mm. With current materials this **metric is not feasible** and either a Type 1 or 3 tank design is necessary.	**Metric not achievable**
MLVI	JPL	Report on ability to develop a thermal insulation design having less than a 5 W heat leak at 40K having a mass less than 11 kg and volume less than 35 liters.	Detailed modeling and coupon-scale validation experiments have been completed showing that the thermal isolation system composed of a 60-layer MLI blanket composed of VDA mylar and dacron separators within a vacuum of at least 1e-4 Torr, reduces parasitic heat load to 2 W **far exceeding the metric.**	25% scale experimental verification has been started, and preliminary results are being analyzed which should prove **exceeding of metric**.
Internal MATI HX	OSU	Report on ability to develop and demonstrate a Modular Adsorption Tank Insert capable of allowing less than 3 min. refueling time and H2 release rate of 0.02 g H2/(sec. kW) with a mass less than 9.4 kg and a volume less than 4.2 liters.	Current MATI designs **exceed the metric** for weight and volume, simlulation demonstrates that these designs can provide the required discharge performance.	**Exceeded metric** Laboratory testing is being used to confirm simulations and manufacturing studies have confirmed that aluminum can be used for this component.
Internal non-MATI HX	~~UTRC~~ SRNL	Report on ability to develop and demonstrate an isolated heat-exchanging loop capable of allowing less than 3 min. refueling time and H2 release rate of 0.02 g H2/(sec. kW) with a mass less than 6.5 kg and a volume less than 6 liters.	The efficacy of an isolated-loop internal heat exchanger was examined. Computational analyses showed that flowing externally heated hydrogen (fuel cell radiator heated) through isolated heating channels of a fin-and-tube HX within the adsorbent would NOT provide enough heat for the minimum drive cycle requirements. An H2 combustor should be able to raise the H2 temperature high enough, however the fin-and-tube HX has higher mass and volume than a comparable MATI.	This **metric was suspended** as not viable.
Internal flow through HX	SRNL/ UQTR	Report on ability to develop and demonstrate an internal flow through HX system based on compacted media capable of allowing less than 3 min. scaled refueling time and H2 release rate of 0.02 g H2/(sec. kW) with a mass less than 6.5 kg and a volume less than 6 liters.	Models for 6mm 322kg/m3 pellets indicate that, relative to 130kg/m3 powder, flow through cooling requires a significantly larger mass of exhaust hydrogen and a longer time to cool. **Compacted MOF will not meet the metric.** It appears that <u>180kg/m3 MOF-5 powder in an aluminum honeycomb</u> **will meet the metric.**	**Met metric** Experiments to validate the models and demonstrate the concept are in progress at UQTR. Pellets have been loaded into hex mesh.
Internal flow through HX	GM	Report on ability to develop and demonstrate an internal flow through cooling system based on powder media capable of allowing less than 3 min. scaled refueling time, and an internal heating system for scaled H2 release rate of 0.02 g H2/(sec. kW) with a mass less than 6.5 kg and a volume less than 6 liters.	Model of charging process predicts that for a 60bar system, a 10.3 liter, 27.7 kg heat exchanger is required to successfully discharges 5.6 kg H2 at full-scale. For a 200 bar system, a 5.5 liter 15 kg aluminum helical coil HX is capable of meeting discharge target. The current experimental stainless steel sheathed coils have higher density. **Neither HX meets the mass metric.**	**It is not anticipated that the mass metric can be achieved.** Bypass line and pressure transducer will be added to the test system in order to control the inlet H2 and initial bed temperature at conditions needed for flow-through cooling experiment.The model predictions will be determined experimentally
External HX	JPL	Report on ability to develop and demonstrate FC radiator capable of heating 80K hydrogen stream to 233K flowing at 1.6g/sec with no icing at 50%RH with a mass increase of less than 2.5 kg and a volume less than 1.5 liters.	System and detailed segmented models suggest that a small Downstream H2 HX (1.1 kg, 1.0 L) will meet the performance metrics at all but -40°C ambient conditions. An auxiliary heater may be required for such conditions. Results also indicate that a "cold start" heater will be necessary for conditions of T < -10°C. The performance of this HX predicted by modeling **meets the metrics.**	**Met metrics.** Changes in funding and scope have exluded demonstration, and no experimental validation will be conducted.
Catalytic Combustor	OSU	Report on ability to develop and demonstrate a 1 kW catalytic combustor to augment partial H2 preconditioning by an existing FC radiator with >85% efficiency having a mass less than 0.6 kg and volume less than 0.5 liters.	Validated simulation results demonstrate that the microchannel combustor has an efficency >95% **meeting the metric.**	**Metric exceeded** A small prototype with 7 to 10 unit cells will be tested to validate models and estimate the mass and volume.
BoP	PNNL	Report on ability to identify BoP materials (excluding internal HX, external HX, and combustor) suitable for 60 bar cryogenic adsorbent system having mass less than 17 kg and a volume less than 18.5 liters.	The BOP mass is significantly reduced with the lower pressure from 200bar to 69bar. The mass of the 69 bar solenoid operated valves are 1/10th the weight of the 200 bar valves with an overall mass and volume of 0.81kg and 0.63L respectively. The final BoP mass and volume without the internal tank heat exchanger, the fuel cell, H2 gas warm up loop, and the tank is 6.7kg and 8.5L **far exceeding the metric.**	**Metric exceeded**
System Design	SRNL	Report on ability to identify a system design having a mass less than 137 kg and a volume less than 279 liters meeting the all of the HSECoE drive cycles	Several system designs **exceeding metricss**: -- 200 bar, 80 K, Powder MOF-5, FT Cooling + HexCell HX, Type 3 Tank (System mass = 110 kg, System volume = 219 L) -- 100 bar, 70 K, Powder MOF-5, FT Cooling + HexCell HX, Type 1 Al Tank (System mass = 127 kg, System volume = 258 L) -- 80 bar, 80 K, 80% MPD 0.322 g/cc Compacted MOF-5, MATI, Type 3 Tank (System mass = 120 kg, System volume = 259 L)	**Metric exceeded**
Efficiency Analysis	NREL	Calculate and model the well-to-powerplant (WTPP) efficiency for two adsorbent storage system designs and compare results relative to the 60% technical target.	In progress	Will complete by 12/31/12

HSECoE

Exceeded Met Continuing Suspended Not Met

Phase 2 Adsorbent System Milestones

Adsorbent System

Component	Partner	S*M*A*R*T Milestone	Status 10/1/12	Projected Outcome
Materials Development	Ford	Report on ability to develop compacted MOF-5 adsorbent media having a total hydrogen material density of greater than or equal to 0.3 g/L, H2 density of 11 wt. % and 33 g/liter and thermal conductivity of 0.5 W/m-K at P = 60-5 bar and T = 80-160K.	H2 grav. density of the MOF-5 material >11% **is possible** with .3 g/cc (w/o ENG) at P = 60-5 bar and T = 80-160K with 60% packing efficiency. H2 vol. density of the MOF-5 material >33 g/l **is possible** with .5 g/cc (+5% ENG) at P = 60-5 bar and T = 80-160K with 100% packing efficiency. Thermal conductivity of .5 W/m-K **is possible** with .3 g/cc to .5 g/cc + 10% ENG with temperatures > 100-120 K.	The capability of achieving specific metrics with a given configuration is possible, investigations will be continue to devise a media morphology which will **meet all of the metrics**.
Materials Development	Ford/UM/ BASF	Report on ability to demonstrate a composite MOF-5 adsorbent monoliths having H2 effective kinetics equivalent to 5.6 kg usable H2 over 3 minutes and permeation in packed and powder particle beds with flow rate of 1 m/s superficial velocity and pressure drop of 5 bar.	H2 effective kinetics have been conducted and proven over 240 cycles for MOF-5 powder. The monolith testing for kinetics is planned. Permeation testing has been conducted for various temperatures and densities. Based on the extrapolation of permiation test data at 0.12 m/s, the 5bar pressure drop milestone is possible (initial assessment of uncompressed darcy) at a media density of 0.3 g/cc but will be a signficant challenge beyond this density, **meeting the metric**.	**Met Metric** The kinetic response of the MOF-5 material will achieve the desired response while the permeation will continue to be a challenge with densities greater than 0.3 g/cc.
Materials Development	SRNL/ UQTR	Report on ability to develop a compacted MOF-5 adsorbent media bed having a total hydrogen density of: 11 % g H2/(g MOF) and 33 g H2/(liter MOF) at P = 60 - 5 bar and T = 80 - 160 K	Evaluation of isotherms provided by Ford for initial & final states gives: 180kg/m^3 (uncompacted) GC=0.15 VC=26.5 **missing the VC metric** 322kg/m^3 GC=0.10 VC=33.0 **missing the GC metric** 520g/m^3 GC=0.07 VC=36.7 **missing the GC metric**	Alternative compaction methods will be pursued with Ford to identify higher volumetric density morphologies **meeting the metrics**.
Structured Bed	GM	Report on ability to develop MOF-5 powder bed having a total hydrogen density of: 15 wt. % g H2/(g MOF) and 20 g H2/(liter MOF) at P = 60 - 5 bar and T = 80 - 160 K.	Based on the modified Dubinin-Asthakov adsorption model, at 60 - 5 bar and 80 - 160 K the 3 liter test vessel contains 18.6% total deliverable g H2/(g MOF) and 30.5% g H2/(liter MOF) **surpassing the metric**.	**Exceeded metric** These results will be validated with lab experiments.
Composite Tank	JPL	Report on ability to develop testing capability to burst test Type 4 composite and Type 1 (metal) tanks at 40K and demonstrate tanks meeting minimally 2.5x nominal operating burst pressure ...	Design and fabrication of a cryogenic pressure test/burst system capable of testing at 77K has been completed. Safety oversight and documentation is currently 75% complete. *Operating this system at 40 K is not feasible.* The capability to perform cryogenic cycling has also been implimented ...	Safety documentation will be completed and burst testing of Type 4 COPVs, pressure testing of Type 1 tanks will be performed at 77K and adding the capability of cryogenic cycoic testing capability **exceeding the** ...
Internal MATI HX	OSU	Report on ability to develop and demonstrate a Modular Adsorption Tank Insert capable of allowing less than 3 min. refueling time and H2 release rate of 0.02 g H2/(sec. kW) with a mass less than 9.4 kg and a volume less than 4.2 liters.	Current MATI designs **exceed the metric** for weight and volume, simlulation demonstrates that these designs can provide the required discharge performance.	**Exceeded metric** Laboratory testing is being used to confirm simulations and manufacturing studies have confirmed that aluminum can be used for this component.
Internal non-MATI HX	~~UTRC~~ SRNL	Report on ability to develop and demonstrate an isolated heat-exchanging loop capable of allowing less than 3 min. refueling time and H2 release rate of 0.02 g H2/(sec. kW) with a mass less than 6.5 kg and a volume less than 6 liters.	The efficacy of an isolated-loop internal heat exchanger was examined. Computational analyses showed that flowing externally heated hydrogen (fuel cell radiator heated) through isolated heating channels of a fin-and-tube HX within the adsorbent would NOT provide enough heat for the minimum drive cycle requirements. An H2 combustor should be able to raise the H2 temperature high enough, however the fin-and-tube HX has higher mass and volume than a comparable MATI.	This **metric was suspended** as not viable.
Internal flow through HX	SRNL/ UQTR	Report on ability to develop and demonstrate an internal flow through HX system based on compacted media capable of allowing less than 3 min. scaled refueling time and H2 release rate of 0.02 g H2/(sec. kW) with a mass less than 6.5 kg and a volume less than 6 liters.	Models for 6mm 322kg/m3 pellets indicate that, relative to 130kg/m3 powder, flow through cooling requires a significantly larger mass of exhaust hydrogen and a longer time to cool. **Compacted MOF will not meet the metric**. It appears that <u>180kg/m3 MOF-5 powder in an aluminum honeycomb</u> **will meet the metric**.	**Met metric** Experiments to validate the models and demonstrate the concept are in progress at UQTR. Pellets have been loaded into hex mesh.
Internal flow through HX	GM	Report on ability to develop and demonstrate an internal flow through cooling system based on powder media capable of allowing less than 3 min. scaled refueling time, and an internal heating system for scaled H2 release rate of 0.02 g H2/(sec. kW) with a mass less than 6.5 kg and a volume less than 6 liters.	Model of charging process predicts that for a 60bar system, a 10.3 liter, 27.7 kg heat exchanger is required to successfully discharges 5.6 kg H2 at full-scale. For a 200 bar system, a 5.5 liter 15 kg aluminum helical coil HX is capable of meeting discharge target. The current experimental stainless steel sheathed coils have higher density. **Neither HX meets the mass metric.**	**It is not anticipated that the mass metric can be achieved.** Bypass line and pressure transducer will be added to the test system in order to control the inlet H2 and initial bed temperature at conditions needed for flow-through cooling experiment.The model predictions will be determined experimentally.
External HX	JPL	Report on ability to develop and demonstrate FC radiator capable of heating 80K hydrogen stream to 233K flowing at 1.6g/sec with no icing at 50%RH with a mass increase of less than 2.5 kg and a volume less than 1.5 liters.	System and detailed segmented models suggest that a small Downstream H2 HX (1.1 kg, 1.0 L) will meet the performance metrics at all but -40°C ambient conditions. An auxiliary heater may be required for such conditions. Results also indicate that a "cold start" heater will be necessary for conditions of T < -10°C. The performance of this HX predicted by modeling **meets the metrics.**	**Met metrics.** Changes in funding and scope have exluded demonstration, and no experimental validation will be conducted.
Catalytic Combustor	OSU	Report on ability to develop and demonstrate a 1 kW catalytic combustor to augment partial H2 preconditioning by an existing FC radiator with >85% efficiency having a mass less than 0.6 kg and volume less than 0.5 liters.	Validated simulation results demonstrate that the microchannel combustor has an efficency >95% **meeting the metric**.	**Metric exceeded** A small prototype with 7 to 10 unit cells will be tested to validate models and estimate the mass and volume.
BoP	PNNL	Report on ability to identify BoP materials (excluding internal HX, external HX, and combustor) suitable for 60 bar cryogenic adsorbent system having mass less than 17 kg and a volume less than 18.5 liters.	The BOP mass is significantly reduced with the lower pressure from 200bar to 69bar. The mass of the 69 bar solenoid operated valves are 1/10th the weight of the 200 bar valves with an overall mass and volume of 0.81kg and 0.63L respectively. The final BoP mass and volume without the internal tank heat exchanger, the fuel cell, H2 gas warm up loop, and the tank is 6.7kg and 8.5L **far exceeding the metric**.	**Metric exceeded**
System Design	SRNL	Report on ability to identify a system design having a mass less than 137 kg and a volume less than 279 liters meeting the all of the HSECoE drive cycles	Several system designs **exceeding metricss**: -- 200 bar, 80 K, Powder MOF-5, FT Cooling + HexCell HX, Type 3 Tank (System mass = 110 kg, System volume = 219 L) -- 100 bar, 70 K, Powder MOF-5, FT Cooling + HexCell HX, Type 1 Al Tank (System mass = 127 kg, System volume = 258 L) -- 80 bar, 80 K, 80% MPD 0.322 g/cc Compacted MOF-5, MATI, Type 3 Tank (System mass = 120 kg, System volume = 259 L)	**Metric exceeded**
Efficiency Analysis	NREL	Calculate and model the well-to-powerplant (WTPP) efficiency for two adsorbent storage system designs and compare results relative to the 60% technical target.	In progress	Will complete by 12/31/12

Report on ability to identify Type IV tank liner materials suitable for 40K operation having a mass less than 8 kg and a volume less than 3 liters (2.55 mm thickness).	After evaluating 8 different materials it was concluded that the liner separates from the shell when the pressure is decreased below 35bar with a liner thickness of 2.55mm. With current materials this **metric is not feasible** and either a Type 1 or 3 tank design is necessary.	**Metric not achievable**

HSECoE

Exceeded Met Continuing Suspended Not Met

Phase 2 Adsorbent System Milestones

Adsorbent System

Component	Partner	S*M*A*R*T Milestone	Status 10/1/12	Projected Outcome
Materials Development	Ford	Report on ability to develop compacted MOF-5 adsorbent media having a total hydrogen material density of greater than or equal to 0.3 g/L, H2 density of 11 wt. % and 33 g/liter and thermal conductivity of 0.5 W/m-K at P = 60-5 bar and T = 80-160K.	H2 grav. density of the MOF-5 material >11% **is possible** with .3 g/cc (w/o ENG) at P = 60-5 bar and T = 80-160K with 60% packing efficiency. H2 vol. density of the MOF-5 material >33 g/l **is possible** with .5 g/cc (+5% ENG) at P = 60-5 bar and T = 80-160K with 100% packing efficiency. Thermal conductivity of .5 W/m-K **is possible** with .3 g/cc to .5 g/cc + 10% ENG with temperatures > 100-120 K.	The capability of achieving specific metrics with a given configuration is possible, investigations will be continue to devise a media morphology which will **meet all of the metrics**.
Materials Development	Ford/UM/ BASF	Report on ability to demonstrate a composite MOF-5 adsorbent monoliths having H2 effective kinetics equivalent to 5.6 kg usable H2 over 3 minutes and permeation in packed and powder particle beds with flow rate of 1 m/s superficial velocity and pressure drop of 5 bar.	H2 effective kinetics have been conducted and proven over 240 cycles for MOF-5 powder. The monolith testing for kinetics is planned. Permeation testing has been conducted for various temperatures and densities. Based on the extrapolation of permiation test data at 0.12 m/s, the 5bar pressure drop milestone is possible (initial assessment of uncompressed darcy) at a media density of 0.3 g/cc but will be a signficant challenge beyond this density, **meeting the metric**.	**Met Metric** The kinetic response of the MOF-5 material will achieve the desired response while the permeation will continue to be a challenge with densities greater than 0.3 g/cc.
Materials Development	SRNL/ UQTR	Report on ability to develop a compacted MOF-5 adsorbent media bed having a total hydrogen density of: 11 % g H2/(g MOF) and 33 g H2/(liter MOF) at P = 60 - 5 bar and T = 80 - 160 K	Evaluation of isotherms provided by Ford for initial & final states gives: 180kg/m^3 (uncompacted) GC=0.15 VC=26.5 **missing the VC metric** 322kg/m^3 GC=0.10 VC=33.0 **missing the GC metric** 520g/m^3 GC=0.07 VC=36.7 **missing the GC metric**	Alternative compaction methods will be pursued with Ford to identify higher volumetric density morphologies **meeting the metrics**.
Structured Bed	GM	Report on ability to develop MOF-5 powder bed having a total hydrogen density of: 15 wt. % g H2/(g MOF) and 20 g H2/(liter MOF) at P = 60 - 5 bar and T = 80 - 160 K.	Based on the modified Dubinin-Asthakov adsorption model, at 60 - 5 bar and 80 - 160 K the 3 liter test vessel contains 18.6% total deliverable g H2/(g MOF) and 30.5% g H2/(liter MOF) **surpassing the metric**.	**Exceeded metric** These results will be validated with lab experiments.
Composite Tank	JPL	Report on ability to develop testing capability to burst test Type 4 composite and Type 1 (metal) tanks at 40K and demonstrate tanks meeting minimally 2.5x nominal operating burst pressure	Design and fabrication of a cryogenic pressure test/burst system capable of testing at 77K has been completed. Safety oversight and documentation is currently 75% complete. *Operating this system at 40 K is not feasible.* The capability to perform cryogenic cycling has also been implimented	Safety documentation will be completed and burst testing of Type 4 COPVs, pressure testing of Type 1 tanks will be performed at 77K and adding the capability of cryogenic cycoic testing capability **exceeding the**
		Report on ability to identify Type IV tank liner materials suitable for 40K operation having a mass less than 8 kg and a volume less than 3 liters (2.55 mm thickness).	After evaluating 8 different materials it was concluded that the liner separates from the shell when the pressure is decreased below 35bar with a liner thickness of 2.55mm. With current materials this **metric is not feasible** and either a Type 1 or 3 tank design is necessary.	**Metric not achievable**
Internal MATI HX	OSU	Report on ability to develop and demonstrate a Modular Adsorption Tank Insert capable of allowing less than 3 min. refueling time and H2 release rate of 0.02 g H2/(sec. kW) with a mass less than 9.4 kg and a volume less than 4.2 liters.	Current MATI designs **exceed the metric** for weight and volume, simlulation demonstrates that these designs can provide the required discharge performance.	**Exceeded metric** Laboratory testing is being used to confirm simulations and manufacturing studies have confirmed that aluminum can be used for this component.
Internal non-MATI HX	~~UTRC~~ SRNL	Report on ability to develop and demonstrate an isolated heat-exchanging loop capable of allowing less than 3 min. refueling time and H2 release rate of 0.02 g H2/(sec. kW) with a mass less than 6.5 kg and a volume less than 6 liters.	The efficacy of an isolated-loop internal heat exchanger was examined. Computational analyses showed that flowing externally heated hydrogen (fuel cell radiator heated) through isolated heating channels of a fin-and-tube HX within the adsorbent would NOT provide enough heat for the minimum drive cycle requirements. An H2 combustor should be able to raise the H2 temperature high enough, however the fin-and-tube HX has higher mass and volume than a comparable MATI.	This **metric was suspended** as not viable.
Internal flow through HX	SRNL/ UQTR	Report on ability to develop and demonstrate an internal flow through HX system based on compacted media capable of allowing less than 3 min. scaled refueling time and H2 release rate of 0.02 g H2/(sec. kW) with a mass less than 6.5 kg and a volume less than 6 liters.	Models for 6mm 322kg/m3 pellets indicate that, relative to 130kg/m3 powder, flow through cooling requires a significantly larger mass of exhaust hydrogen and a longer time to cool. **Compacted MOF will not meet the metric**. It appears that 180kg/m3 MOF-5 powder in an aluminum honeycomb **will meet the metric**.	**Met metric** Experiments to validate the models and demonstrate the concept are in progress at UQTR. Pellets have been loaded into hex mesh.
		Report on ability to develop a thermal insulation design having less than a 5 W heat leak at 40K having a mass less than 11 kg and volume less than 35 liters.	Detailed modeling and coupon-scale validation experiments have been completed showing that the thermal isolation system composed of a 60-layer MLI blanket composed of VDA mylar and dacron separators within a vacuum of at least 1e-4 Torr, reduces parasitic heat load to 2 W **far exceeding the metric.**	25% scale experimental verification has been started, and preliminary results are being analyzed which should prove **exceeding of metric**.
System Design	SRNL	Report on ability to identify a system design having a mass less than 137 kg and a volume less than 279 liters meeting the all of the HSECoE drive cycles	Several system designs **exceeding metricss**: -- 200 bar, 80 K, Powder MOF-5, FT Cooling + HexCell HX, Type 3 Tank (System mass = 110 kg, System volume = 219 L) -- 100 bar, 70 K, Powder MOF-5, FT Cooling + HexCell HX, Type 1 Al Tank (System mass = 127 kg, System volume = 258 L) -- 80 bar, 80 K, 80% MPD 0.322 g/cc Compacted MOF-5, MATI, Type 3 Tank (System mass = 120 kg, System volume = 259 L)	**Metric exceeded**
Efficiency Analysis	NREL	Calculate and model the well-to-powerplant (WTPP) efficiency for two adsorbent storage system designs and compare results relative to the 60% technical target.	In progress	Will complete by 12/31/12

HSECoE

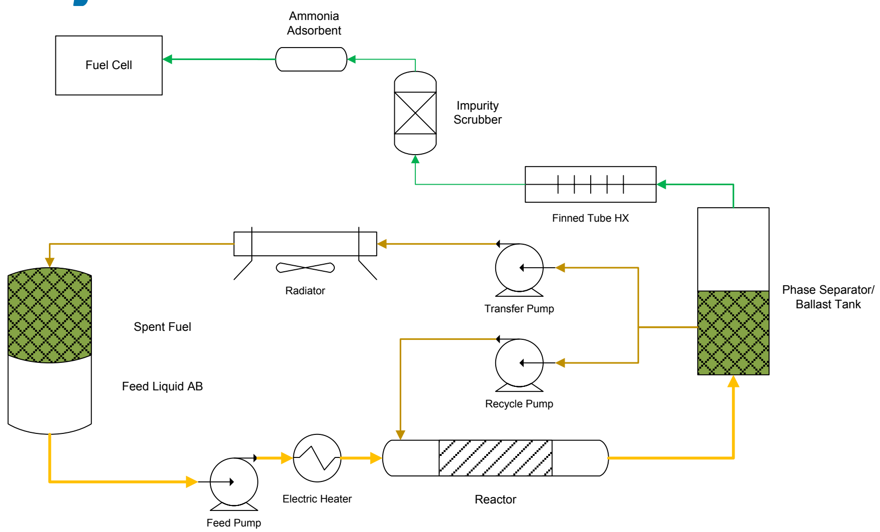
Exceeded Met Continuing Suspended Not Met

Accomplishment

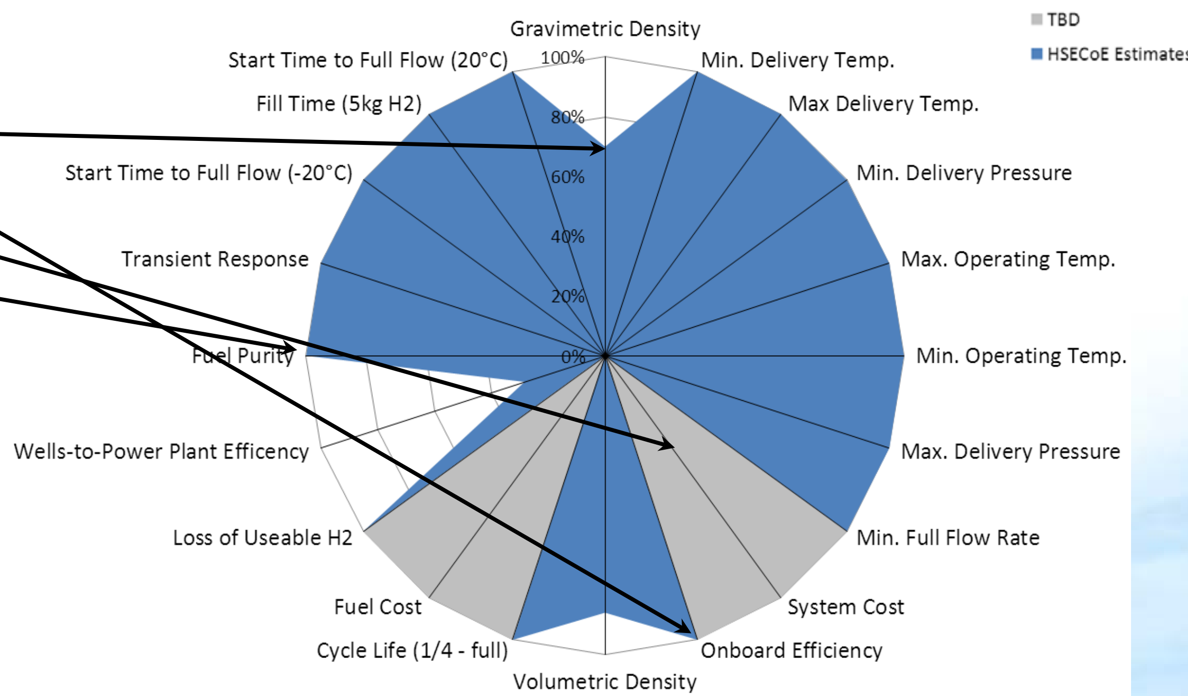
Chemical Hydride System Projection End of Phase 1

2017 Targets

- **Media: Fluid Phase Ammonia Borane: 50wt.% AB in BMIMCl (1-n-butyl-3-methylimidazolium chloride)**
- **12 Components:**
  - **Bladder Tank**
  - **Flow Through Reactor**
  - **Gas Liquid Separator/Ballast Tank**
  - **Radiator**
  - **Hydrogen Purification**



1. Gravimetric Density
2. On-Board Efficiency
3. System Cost
4. H_2 Purity



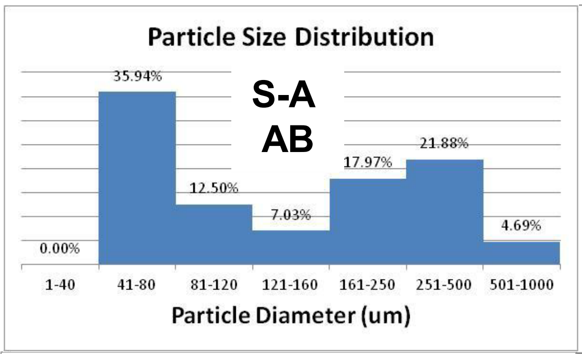
HSECoE

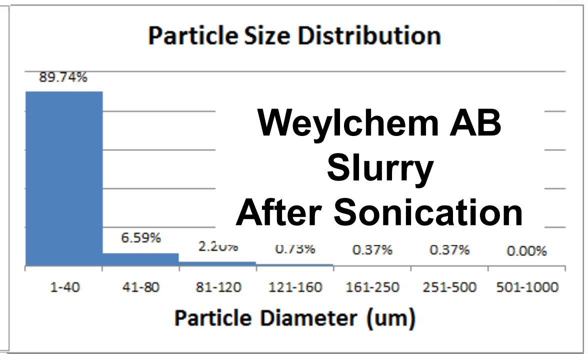
Pacific Northwest NATIONAL LABORATORY

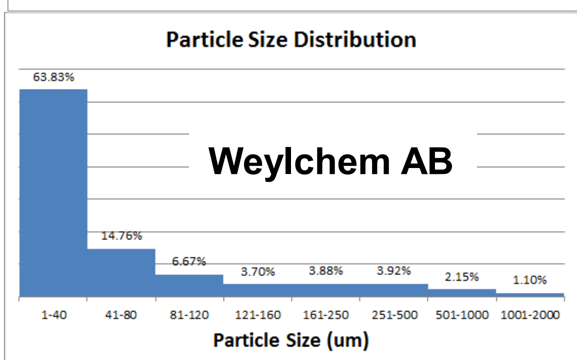
Chemical Hydride: Slurry Development

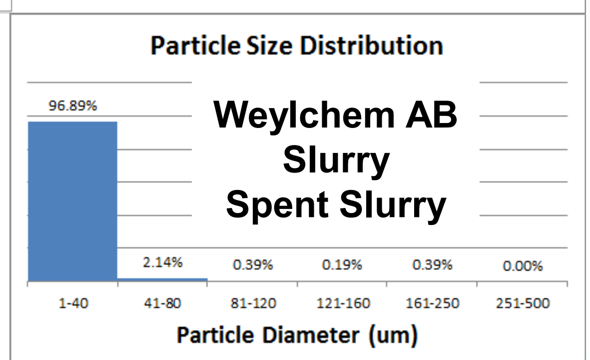
Milestone	Metric Outcome
Report on ability to **develop a 40 wt% slurry AB** material having viscosity less than 1500cP pre- and post-dehydrogenation and kinetics comparable to the neat.	**Exceeded metrics**

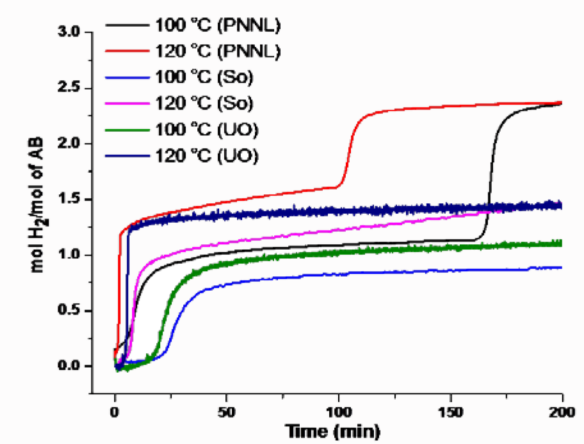
Ammonia Borane Slurry Development



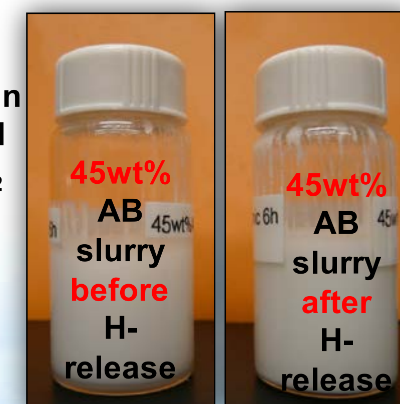








45w/o AB in silicon oil ~7 w/o H_2



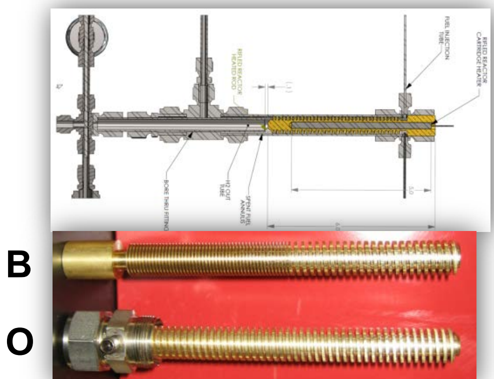
HSECoE

Chemical Hydride: Reactor

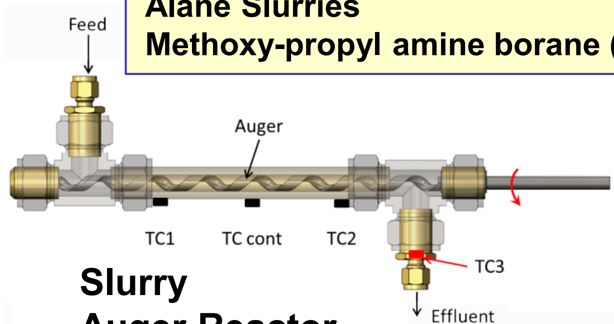
Milestone	Metric Outcome
Report on ability to **develop a flow through reactor** capable of discharging 0.8 g/s H2 from a 40 wt.% AB fluid-phase composition having a mass of no more than 2 kg and a volume of no more than 1 liter.	Reactor performance tests with kinetics will be performed on • 35-40 wt% AB slurries • 40-60 wt.% Alane slurries with the anticipation of meeting the target

Flow-Through Reactor

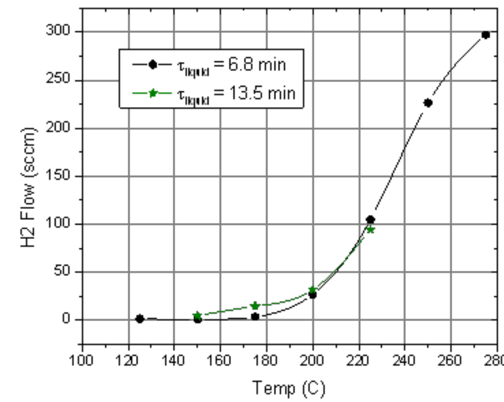
Media
Ammonia Borane Slurries
Alane Slurries
Methoxy-propyl amine borane (MPAB)



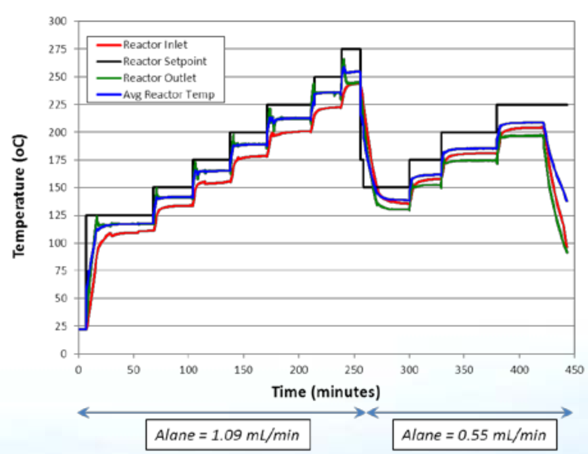
Liquid Helical Reactors

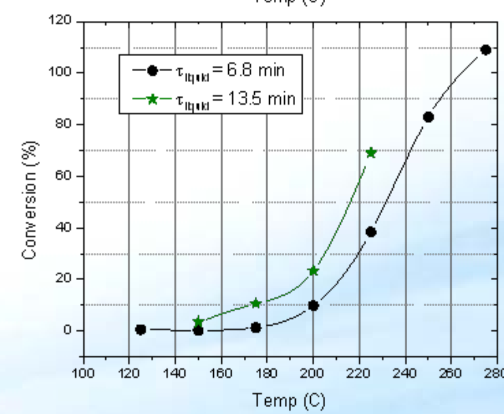


Slurry Auger Reactor



Alane Auger Reactor Results



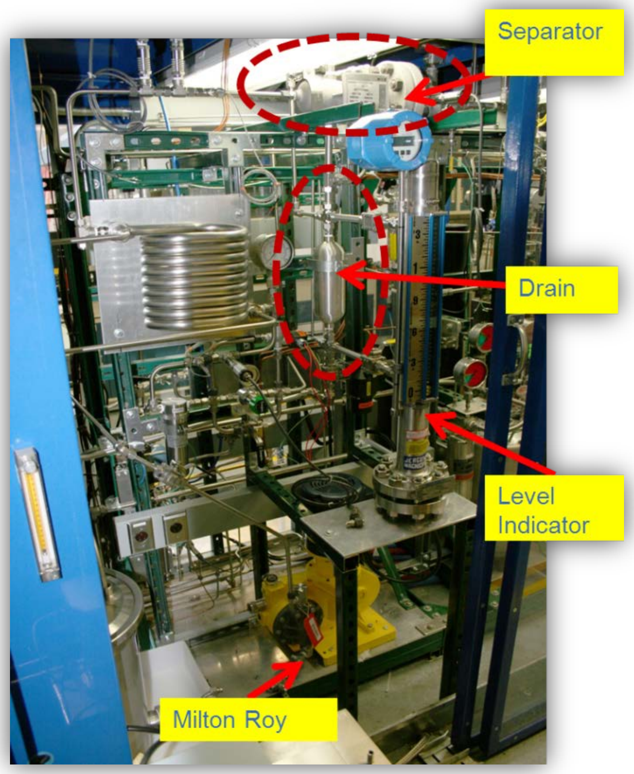


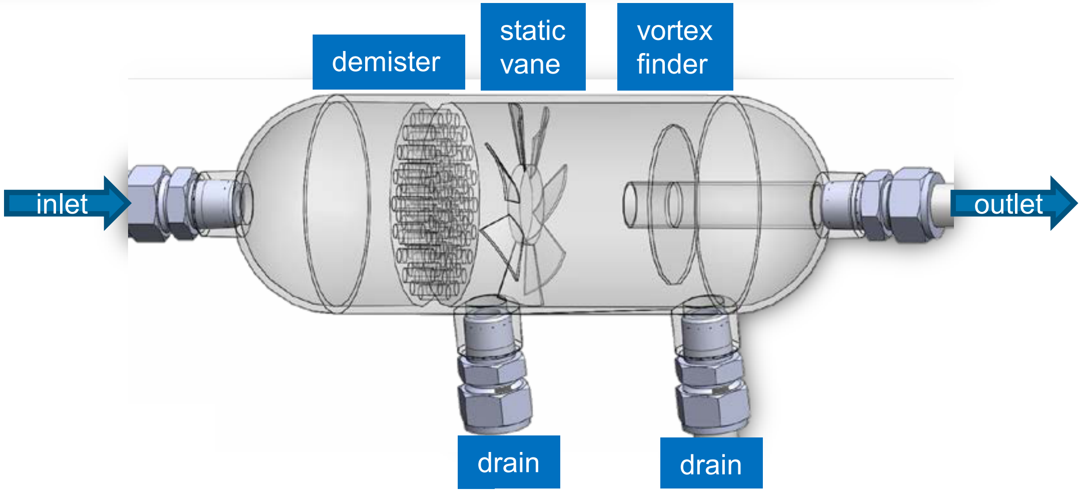
HSECoE

United Technologies Research Center

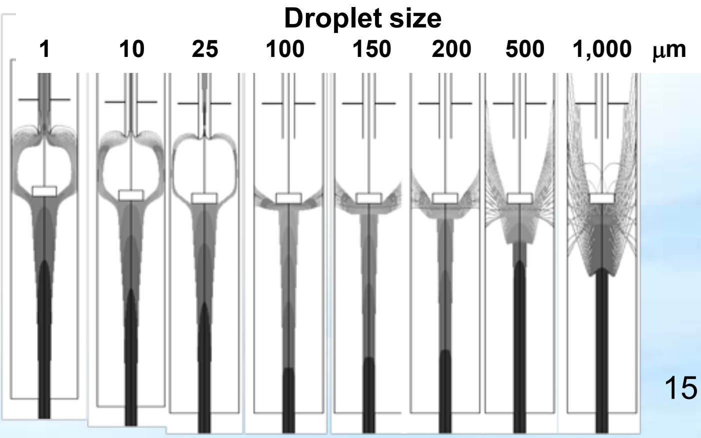
Chemical Hydride: BoP-Gas/Liquid Separator

Milestone	Metric Outcome
Report on ability to **develop a GLS** capable of handeling 720 mL/min liquid phase and 600 L/min of H2 @ STP (40 wt% AB @ 2.35 Eq H2 and max H2 flow of 0.8 g/s H2) fluid having a viscosity less than 1500cp with resulting in a gas with less than 100ppm aerosol having a mass less than 5.4 kg and volume less than 19 liters.	**Could not meet mass but far exceeded volume metric** Demonstrated operation meeting metrics utilizing spent fuel simulant.





Gas-Liquid Separator Efficiency Modeling

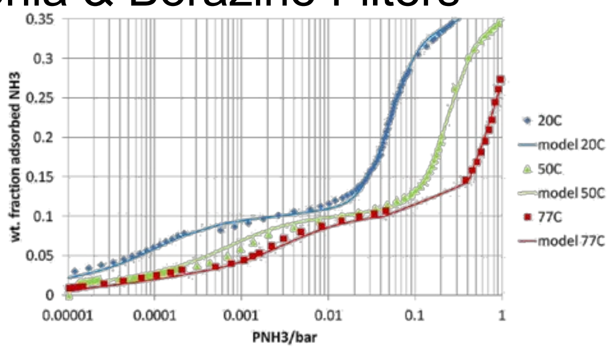


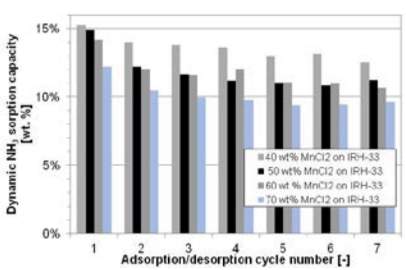
HSECoE

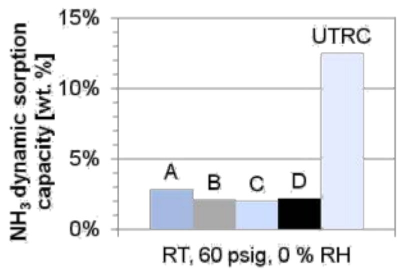
Chemical Hydride: BoP-Gas Purification

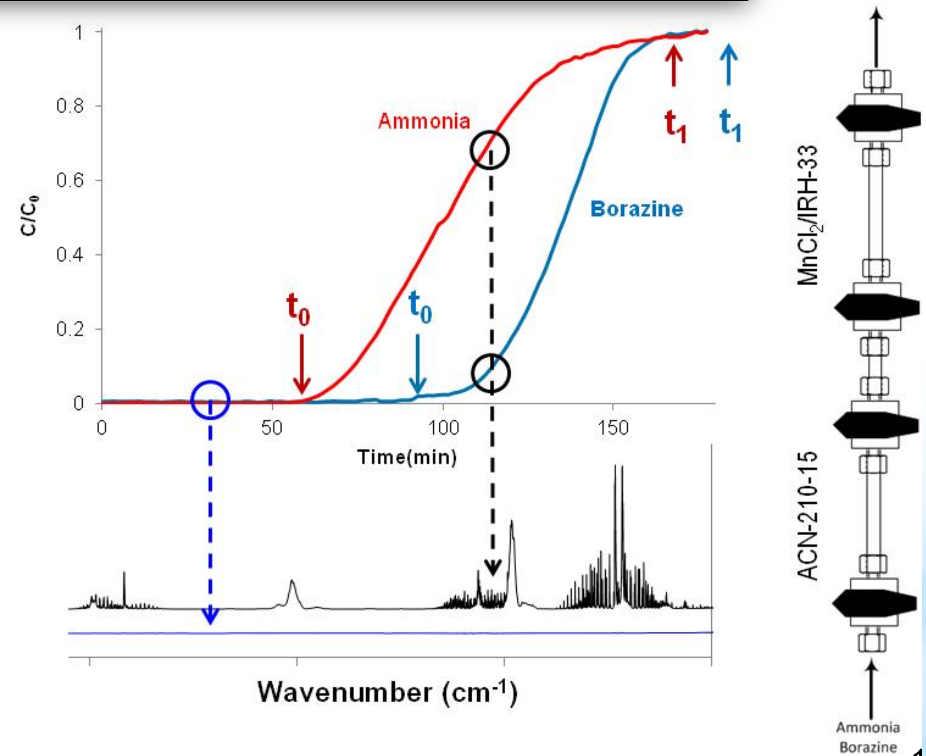
Milestone	Metric Outcome
Report on ability to **develop a borazine scrubber** with a minimum replacment interval of 1800 miles of driving resulting in a minimum outlet borazine concentration of 0.1 ppm (inlet concentration = 4,000 ppm) having a maximum mass of 3.95 kg and maximum volume less of 3.6 liters.	**Mass metric achieved but volume metric missed.** Compaction of adsorbent media could be conducted to meet the volume metric but emphasis will be placed on reactor testing.
Report on ability to **develop an ammonia scrubber** with a minimum replacment interval of 1800 miles of driving resulting in a minimum ammonia outlet concentration of 0.1 ppm (inlet concentration = 500 ppm)having a maximum mass of 1.2 kg and a maximum volume of 1.6 liters.	**Met Metric**

Ammonia & Borazine Filters



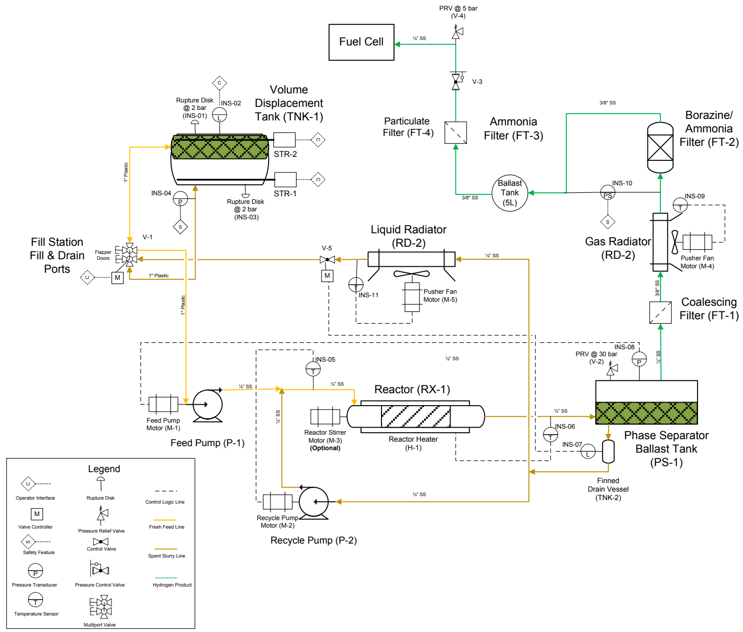


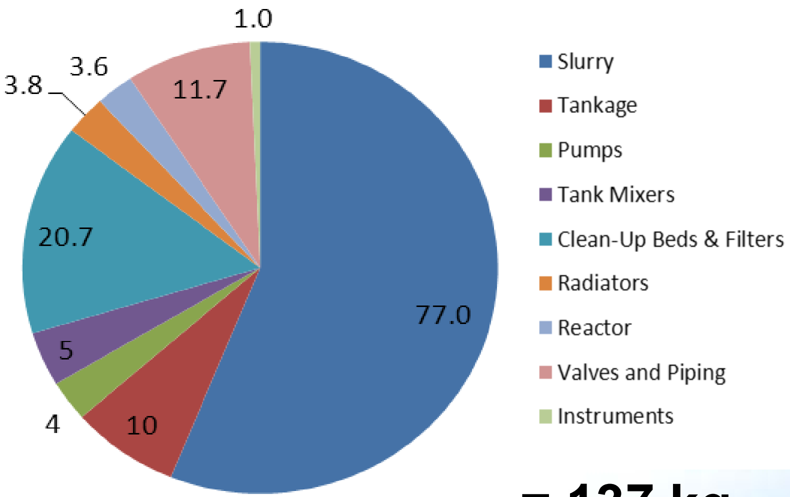




Chemical Hydride: System Design

Milestone	Metric Outcome
Report on ability to **identify BoP materials** suitable for the Chemical Hydrogen system having a system mass no more than 41 kg and a system volume no more than 57 liters.	**Volumetric metric met.** **Gravimetric metric not met.** The requirements for the Hydrogen purification system increased from 4.3kg to 19.1 kg.
Report on ability to **identify a system design** having a mass less than 97 kg and a volume less than 118 liters meeting the all of the HSECoE drive cycles.	**Metric not met.** A path to minimize the mass and volume of the system to meet the targets has been identified, but higher slurry concentration (64w% AB) or a slurry with a higher hydrogen loading (9.8 wt%) will be required to meet the metric.





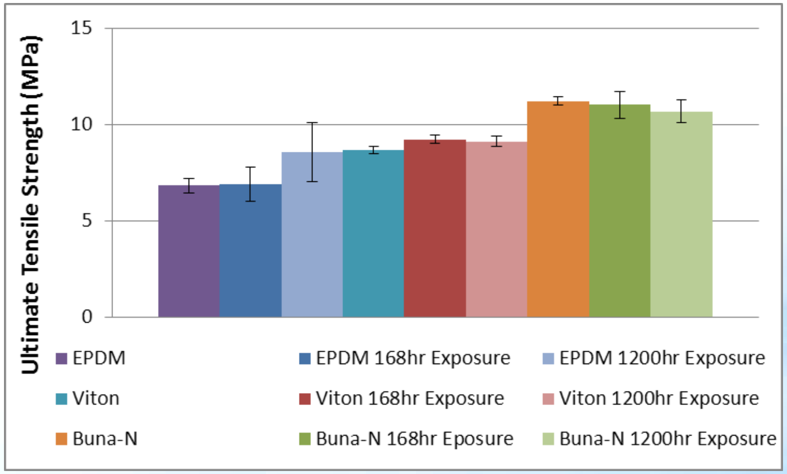
= 137 kg

Chemical Hydride: BoP-Displacement Tank

One liter volume displacement tank designed/built/tested

Pleated membrane design validated to minimize strain and allow flexibility in membrane materials

Exposure testing of membrane materials to AB and silicon oil before and after dehydrogenation



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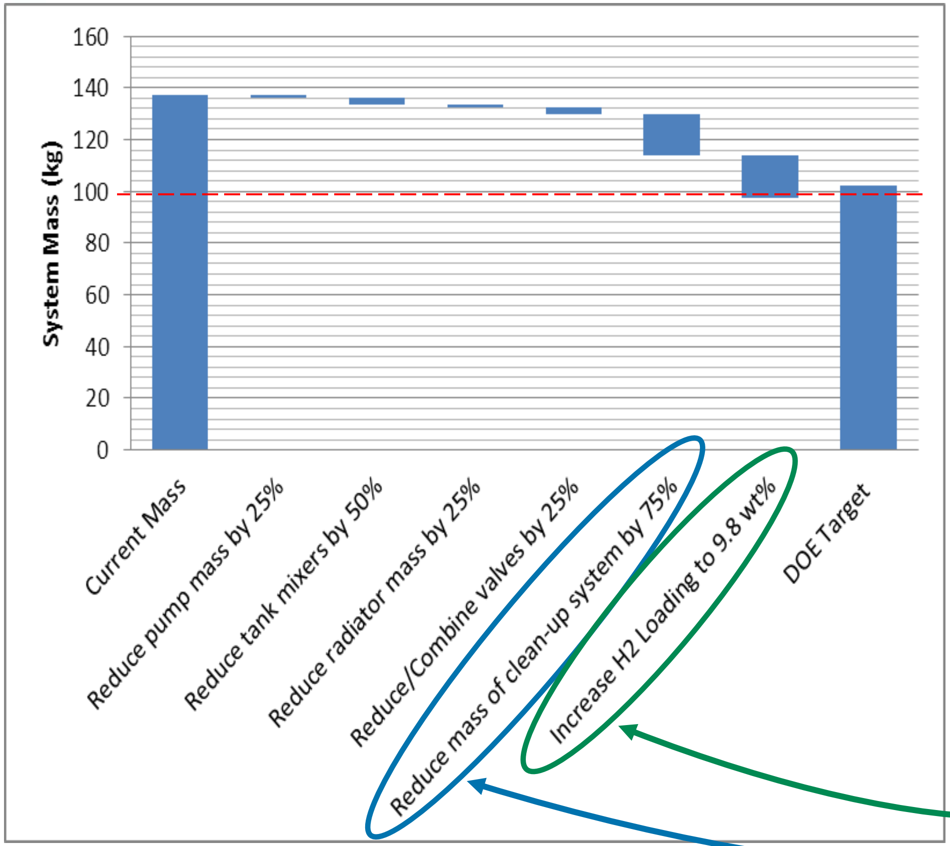
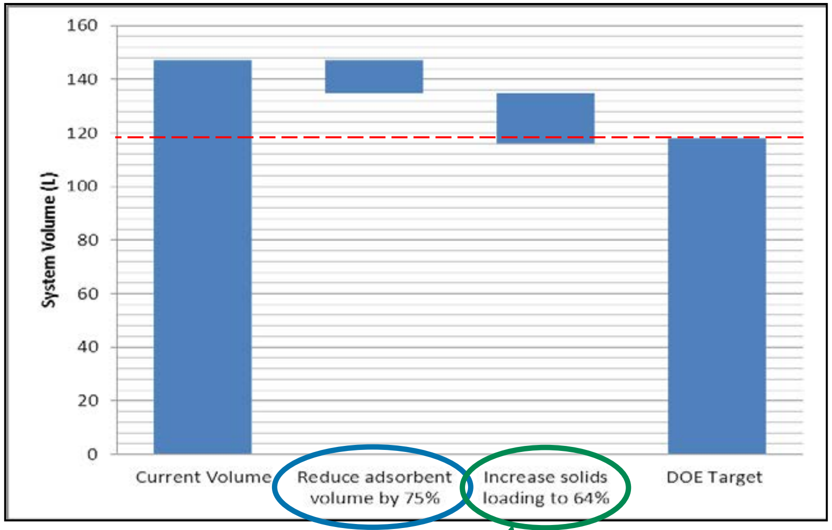
Chemical Hydride System Waterfall Charts

Mass Target



Volume Target



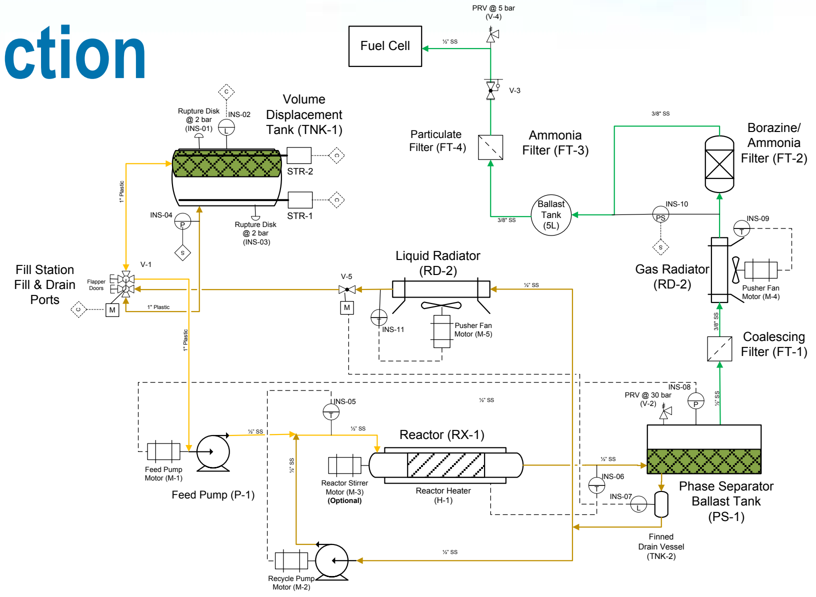
Achieving Mass target through increased fluid loading and reduced clean-up system will result in achievement of volume target.

HSECoE

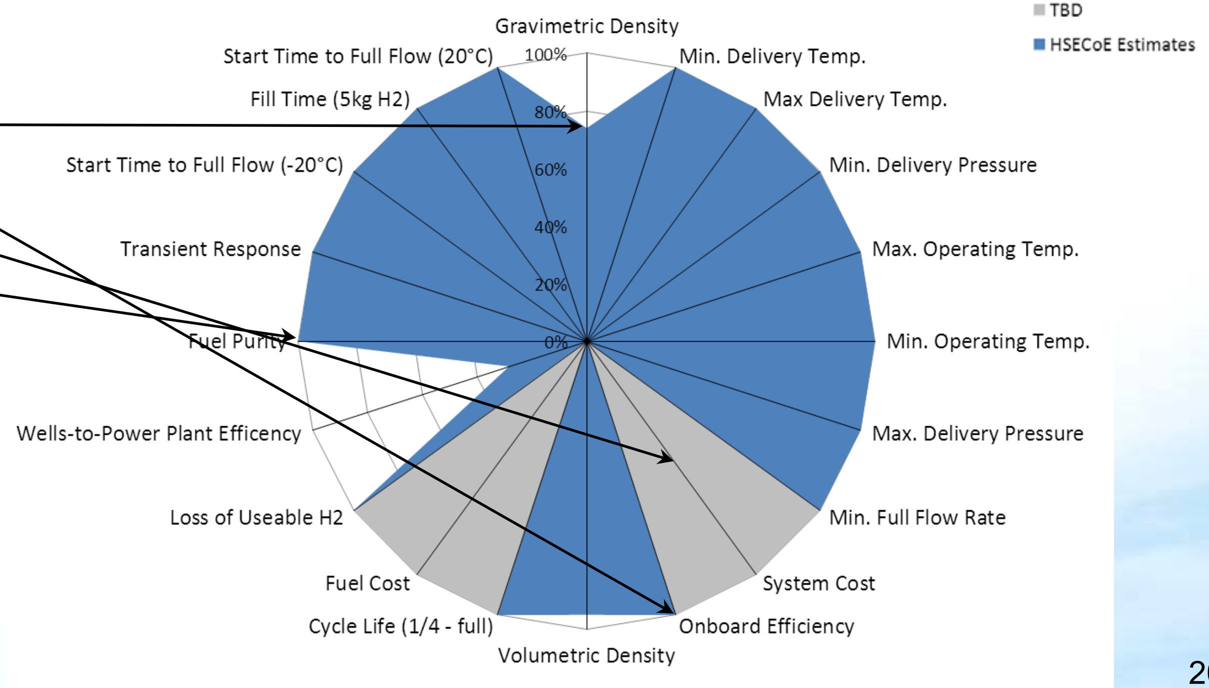
Chemical Hydride System Projection End of Phase 2

2017 Targets

- **Media Type: 50wt% Slurry Ammonia Borane in silicon oil**
- **Primary Components:**
  - **Bladder Tank**
  - **Flow Through Reactor**
  - **Gas Liquid Separator/Ballast Tank**
  - **Radiator**
  - **Purification**



1. **Gravimetric Density**
2. **On-Board Efficiency**
3. **System Cost**
4. **H_2 Purity**



HSECoE

Accomplishment

Chemical Hydride System Projection End of Phase 2

2017 Targets

- **Media Type: 50wt% Slurry Ammonia Borane in silicon oil**
- **Primary Components:**
  - **Bladder Tank**
  - **Flow Through Reactor**
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  - **Radiator**
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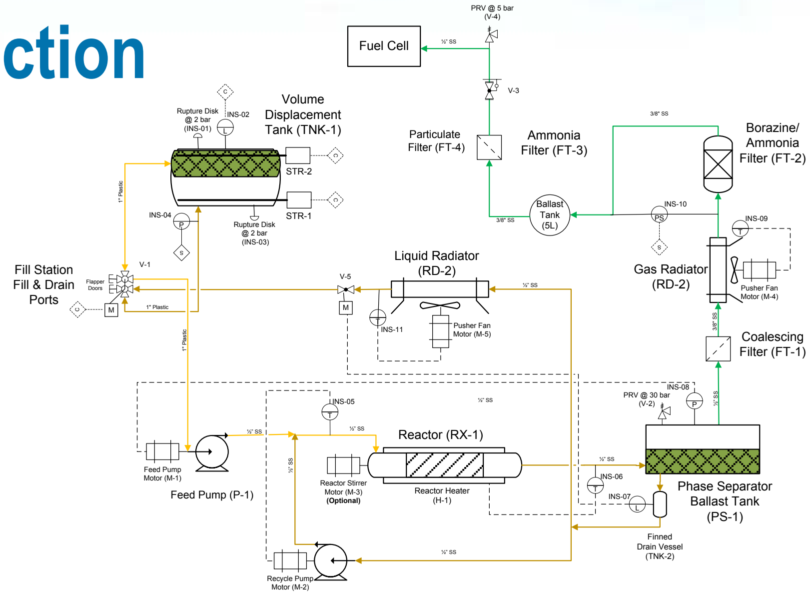

1. Gravimetric Density
2. On-Board Efficiency
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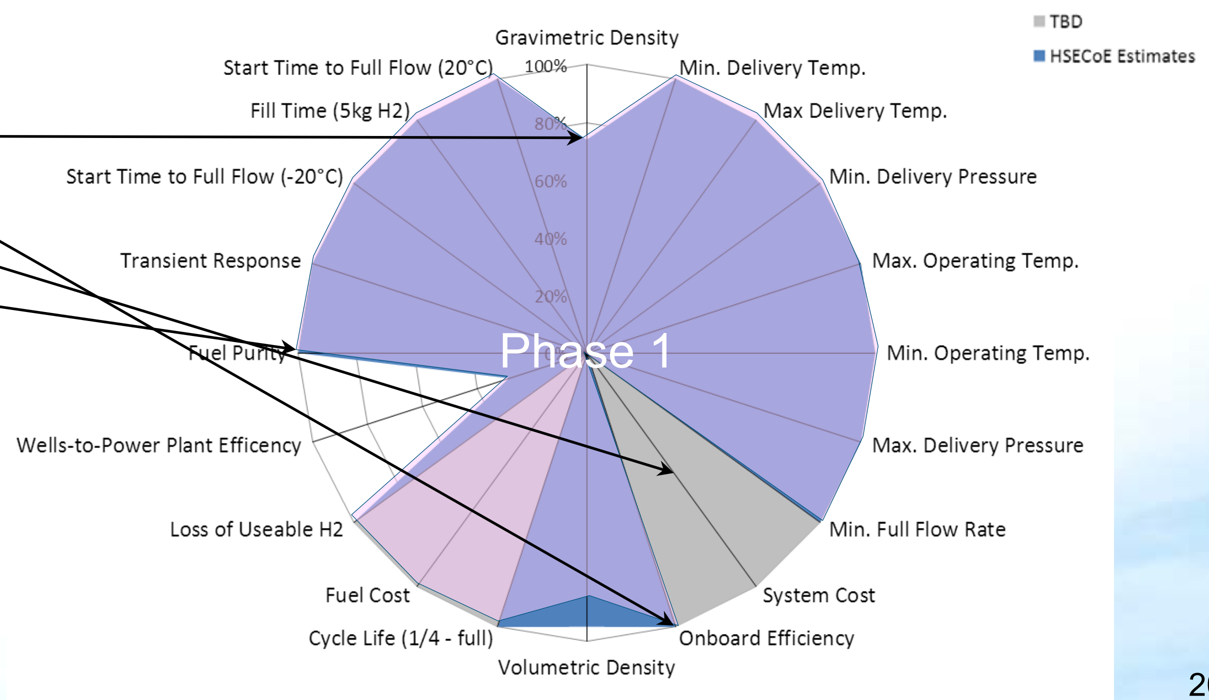
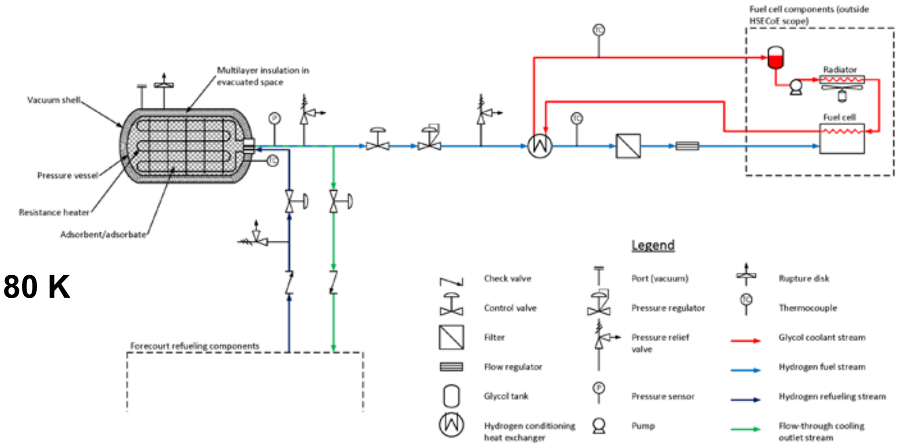


HSECoE

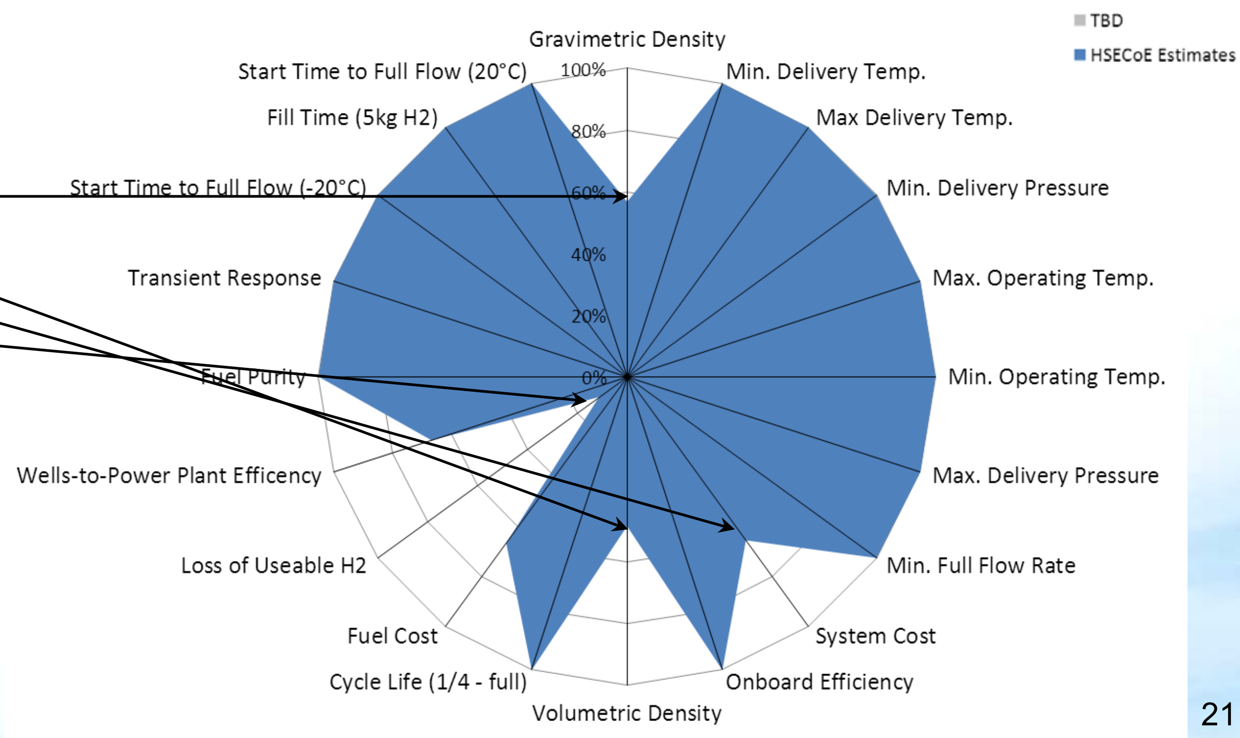
Adsorbent System Projection End of Phase 1

2017 Targets

- **AX-21, no thermal enhancement, 80 K initial fill**
- **Type 3 CF/Al lined pressure vessel, 6 mm liner, 200 bar**
- **Double-wall 60-layer MLVI jacket design, 5W heat leak @ 80 K**
- **Porous-bed “flow-through” cooling/fueling design for adsorption**
- **Desorption heat via tank-integral electrical resistance elements/HX**



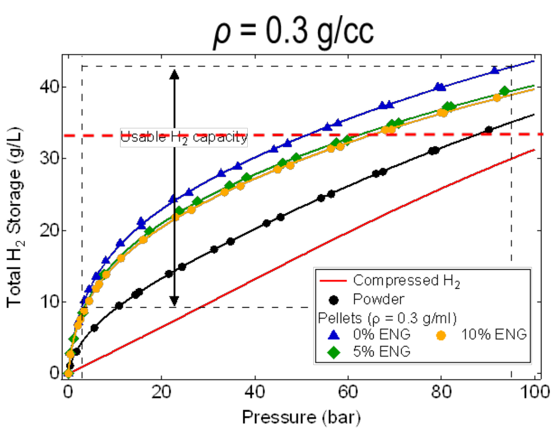
1. Gravimetric Density
2. Volumetric Density
3. System Cost
4. Loss of Usable H_2

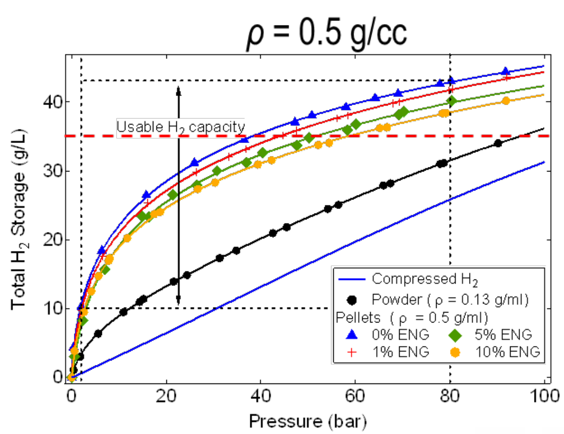


Adsorbent System: Media Engineering

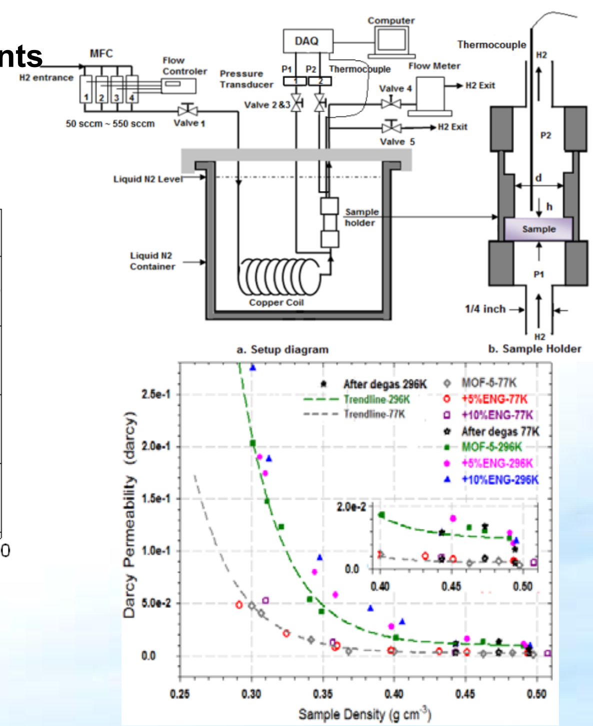
Milestone	Metric Outcome
Report on ability to **develop compacted MOF-5 adsorbent media** having a total hydrogen material density of greater than or equal to 0.3 g/L, H2 density of 11 wt. % and 33 g/liter and thermal conductivity of 0.5 W/m-K at P = 60-5 bar and T = 80-160K.	The capability of achieving individual metrics with a given configuration has been demonstrated. **No one structure has been identified achieving all of the metrics.**
Report on ability to **demonstrate a composite MOF-5 adsorbent monoliths** having H2 effective kinetics equivalent to 5.6 kg usable H2 over 3 minutes and permeation in packed and powder particle beds with flow rate of 1 m/s superficial velocity and pressure drop of 5 bar.	**Met Metric** The kinetic response of the MOF-5 material will achieve the desired response while the permeation will continue to be a challenge with densities greater than 0.3 g/cc.

Volumetric Density





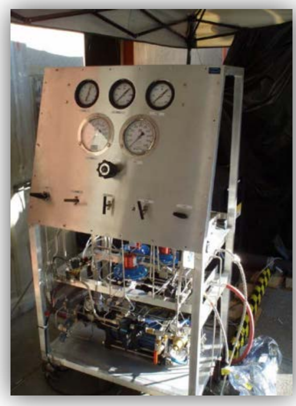
Permeability Measurements



Adsorbent System: BoP-Composite Tank

Milestone	Metric Outcome
Report on ability to **develop testing capability** to burst test Type 4 composite and Type 1 (metal) tanks at 40K and demonstrate tanks meeting minimally 2.5x nominal operating burst pressure.	The cryogenic test facility was completed, but funding was exhausted prior to tank testing. Cimeron composites has been identified as having the capability to perform these tests within budget. **Metric Met.**
Report on ability to **develop Type 4 (composite) and Type 1 (metal) tanks** capable of use between 40 and 160K meeting ASME pressure vessel code for use at 60 bar having a mass less than 10 kg and a volume less than 120 liters.	Based on these results single piece 120 liter Type 1 and Type 4 tanks will be designed and masses calculated. It is anticipated that the Type 1 tank will not meet the mass target while the **Type 4 tank will meet the mass metric.**
Report on ability to **identify Type IV tank liner materials** suitable for 40K operation having a mass less than 8 kg and a volume less than 3 liters (2.55 mm thickness).	**Metric not achievable**

Cryo-burst test facility competed



Segmented Al tank design

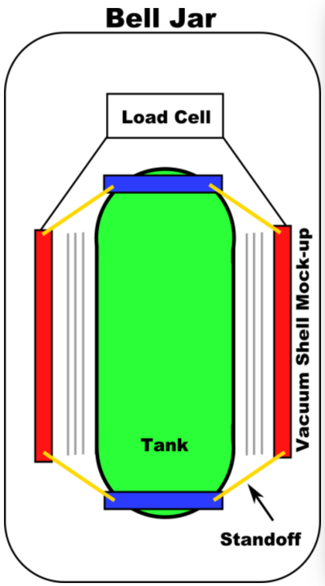
Composite tank design

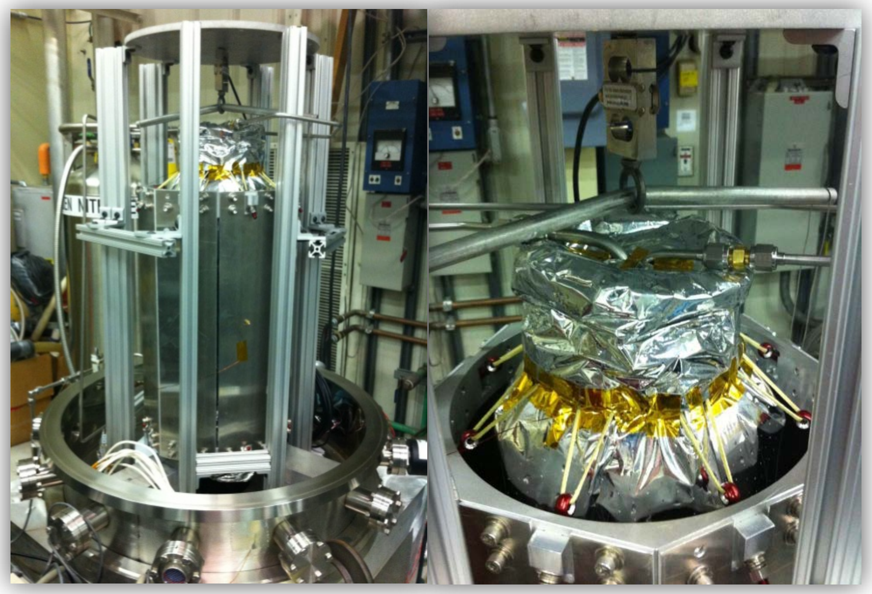
Cryogenic Tank Testing

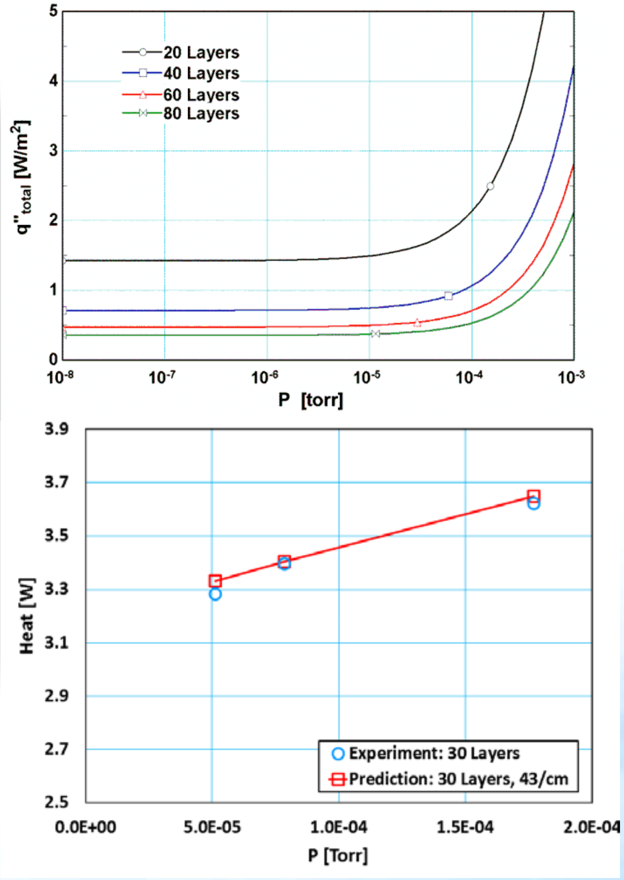



Adsorbent System: BoP-Insulation Development

Milestone	Metric Outcome
Report on ability to develop a thermal insulation design having less than a 5 W heat leak at 40K having a mass less than 11 kg and volume less than 35 liters.	25% scale experimental verification has been started, and preliminary results are being analyzed which should prove **exceeding of metric**.





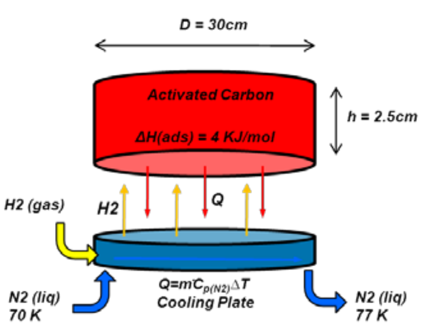


Adsorbent System: BoP-Internal Heat Exchange

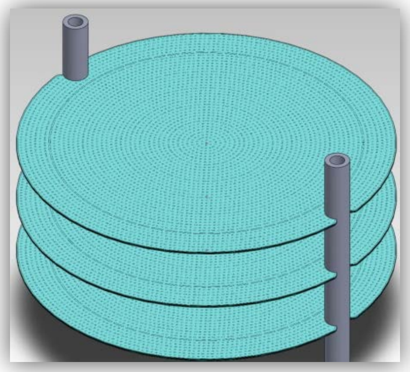
Milestone	Metric Outcome
Report on ability to **develop and demonstrate a Modular Adsorption Tank Insert** capable of allowing less than 3 min. refueling time and H2 release rate of 0.02 g H2/(sec. kW) with a mass less than 9.4 kg and a volume less than 4.2 liters.	**Exceeded metric** Laboratory testing is being used to confirm simulations and manufacturing studies have confirmed that aluminum can be used for this component.

Modular Adsorption Tank Insert (MATI)

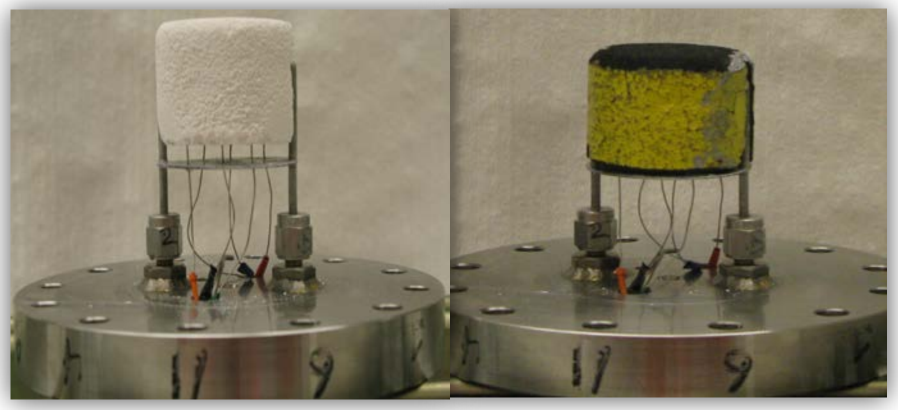
System Concept

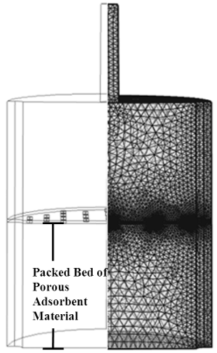


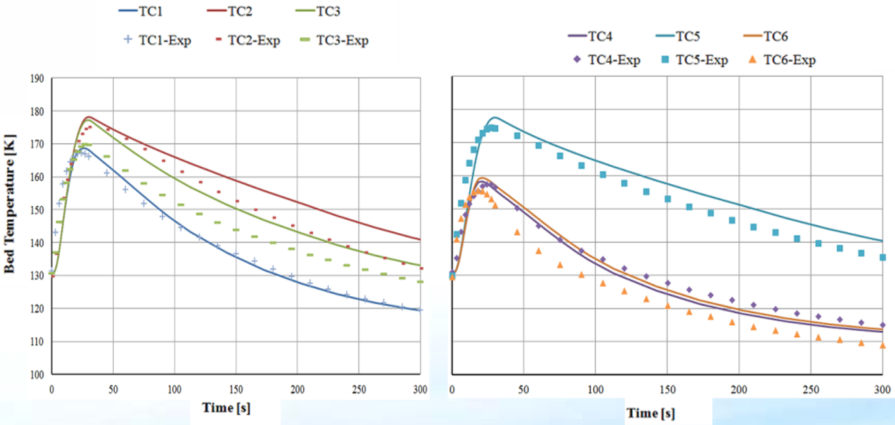
- Cross-flow HX
- Heat of adsorption removed by LN2
- Radial H2 access to adsorption bed



MATI v1 – Combined LN2 cooling and H2 distribution



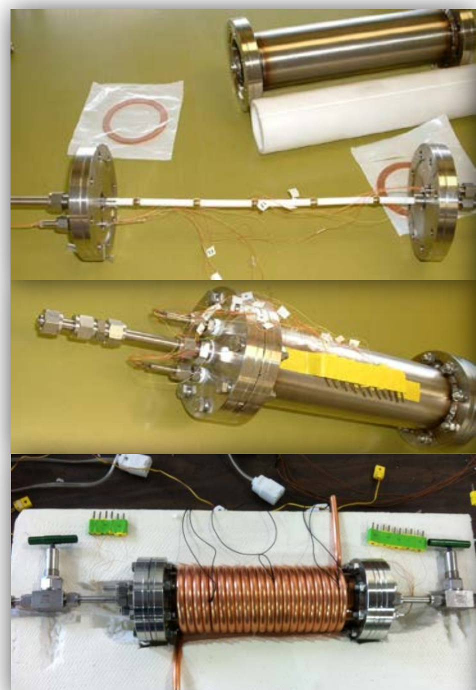


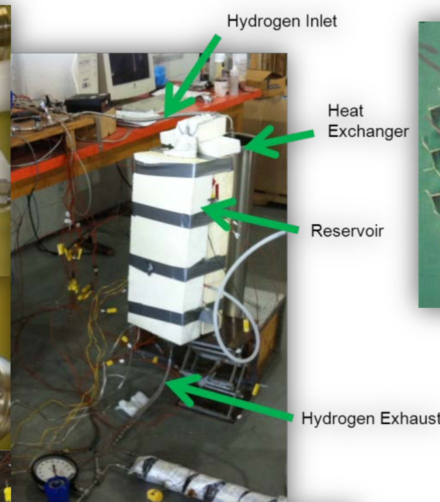


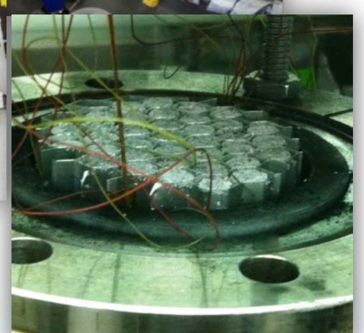
Adsorbent System: BoP-Internal Heat Exchange

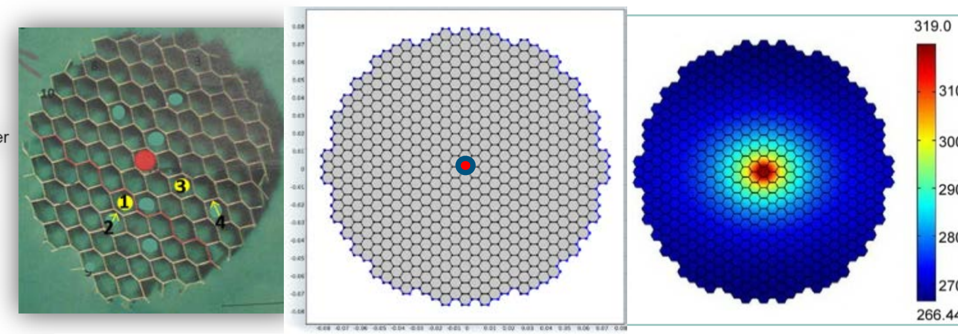
Milestone	Metric Outcome
Report on ability to **develop and demonstrate an internal flow through HX** system based on compacted media capable of allowing less than 3 min. scaled refueling time and H2 release rate of 0.02 g H2/(sec. kW) with a mass less than 6.5 kg and a volume less than 6 liters.	**Met metric**

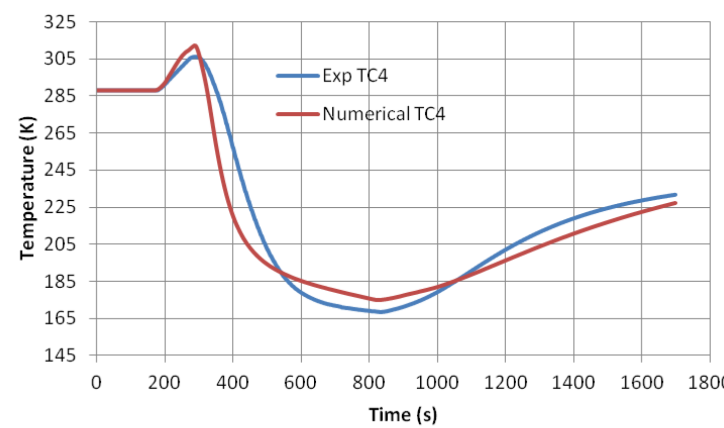
Powder & Pellet HexCell HX







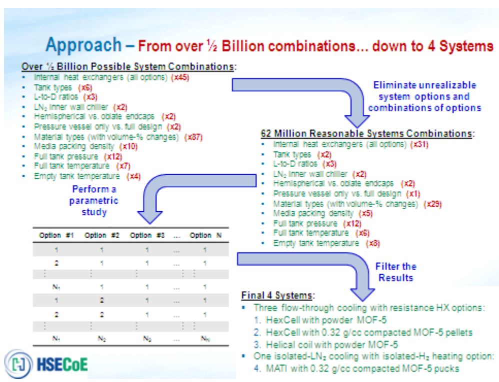




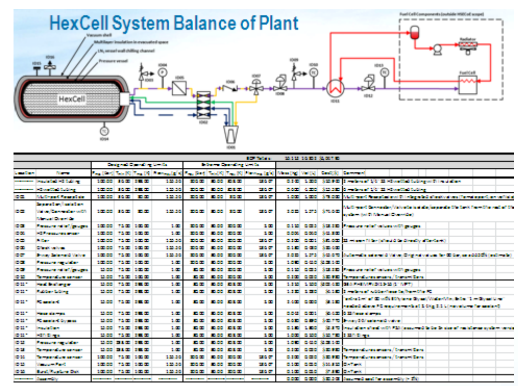
Accomplishment

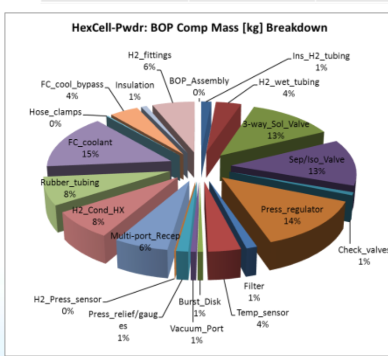
Adsorbent System: System Design

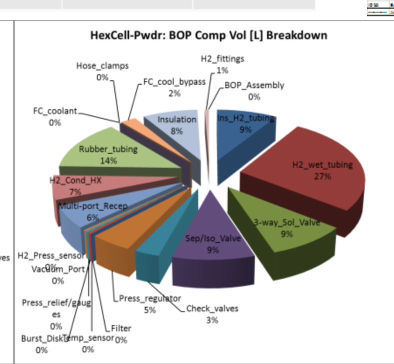
Milestone	Metric Outcome
Report on ability to **identify BoP materials** (excluding internal HX, external HX, and combustor) suitable for 60 bar cryogenic adsorbent system having mass less than 17 kg and a volume less than 18.5 liters.	**Metric exceeded**
Report on ability to **identify a system design** having a mass less than 137 kg and a volume less than 279 liters meeting the all of the HSECoE drive cycles	**Metric exceeded**

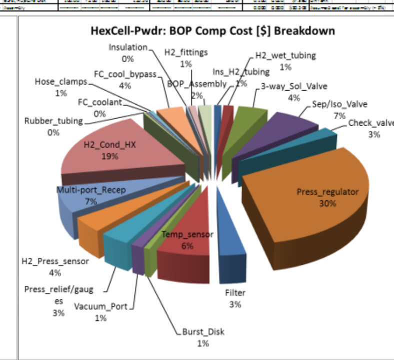


Internal HX and Media	Helical Coil + powder MOF-5	HexCell + powder MOF-5	HexCell + 0.32 g/cc MOF-5 pellets	MATI + 0.32 g/cc MOF-5 pucks
System Mass [kg]	178.4	159.2	175.0	164.3
System Volume [L]	328.7	320.2	288.8	270.4
Estimate System Cost [$]	$2,486	$2,376	$2,671	$2,883
System Rank {Ford}	5.742	6.020	5.899	5.964
Gravimetric Capacity [g/g]	0.0314	0.0352	0.0320	0.0341
Volumetric Capacity [g/L]	17.04	17.49	19.40	20.72







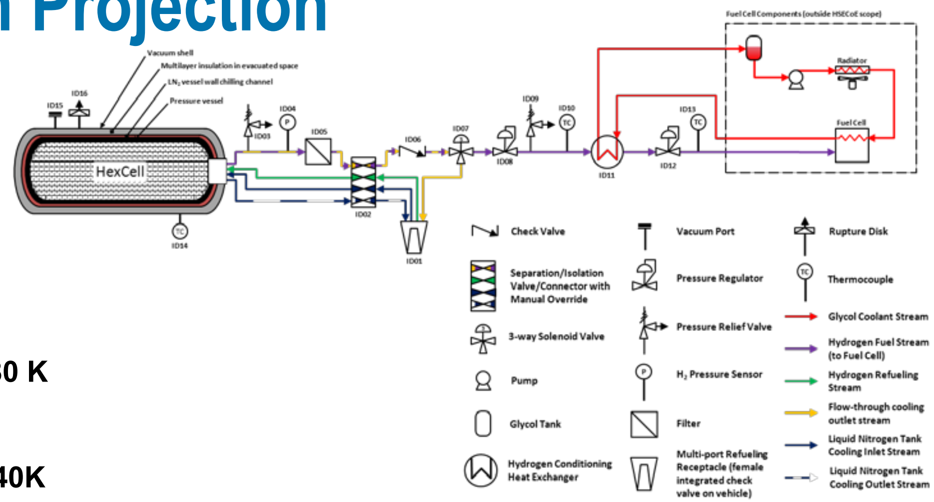


HSECoE

Accomplishment

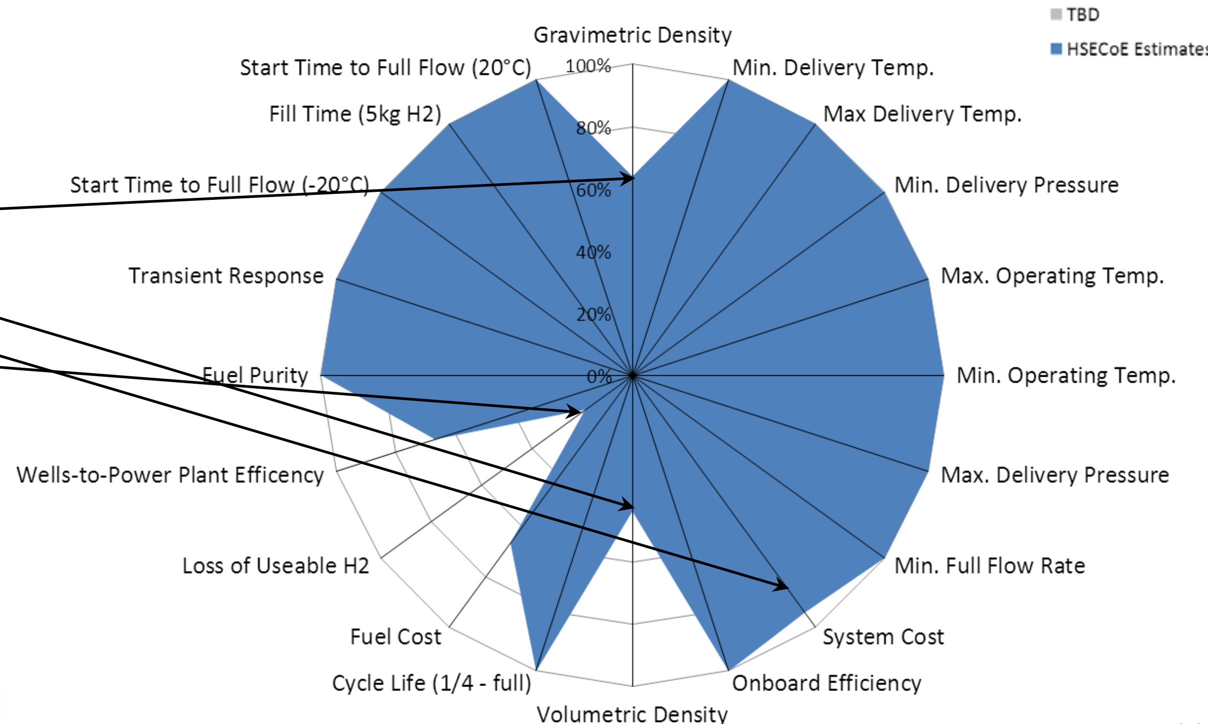
HexCell Adsorbent System Projection
End of Phase 2

2017 Targets



- **MOF-5, no thermal enhancement, 80 K initial fill**
- **Type 1 Al pressure vessel, 100 bar**
- **Double-wall 60-layer MLVI jacket design, 5W heat leak @ 80 K**
- **Adsorption: Porous-bed "flow-through" cooling/fueling**
- **Desorption: Electrical resistance heater/honeycomb HX 140K**

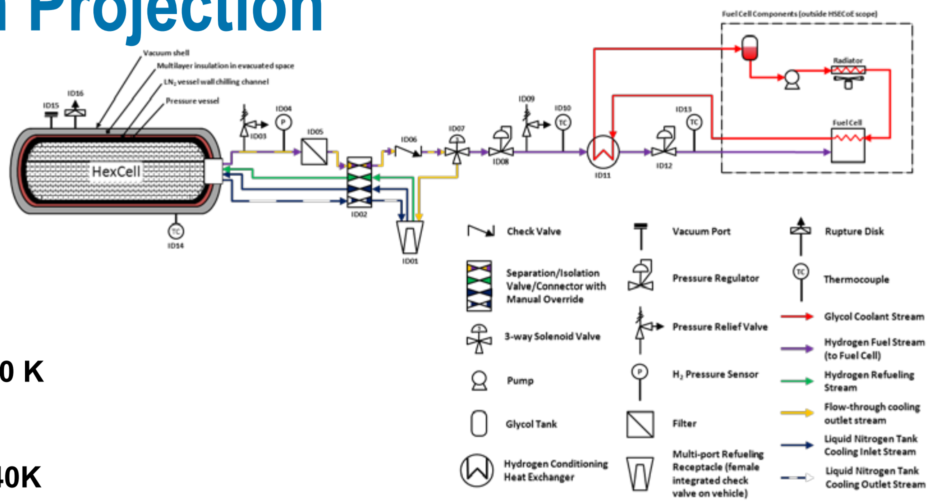
1. Gravimetric Density
2. Volumetric Density
3. System Cost
4. Loss of Usable H_2



HSECoE

HexCell Adsorbent System Projection End of Phase 2

2017 Targets



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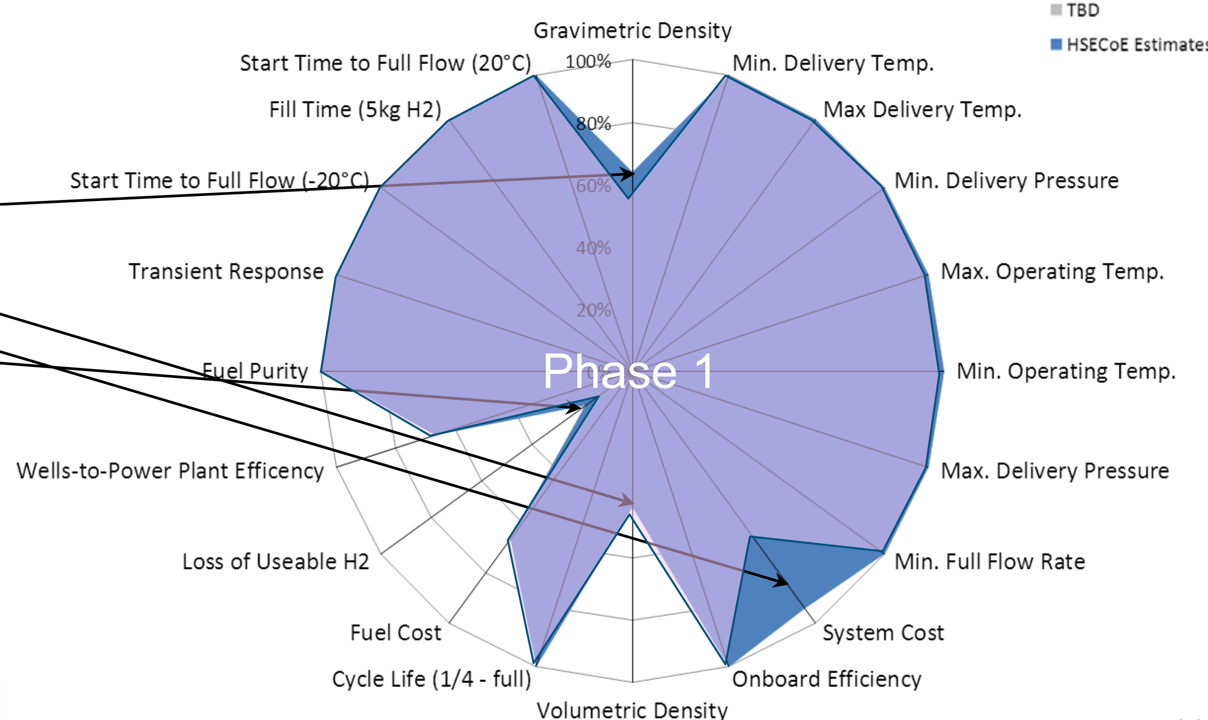
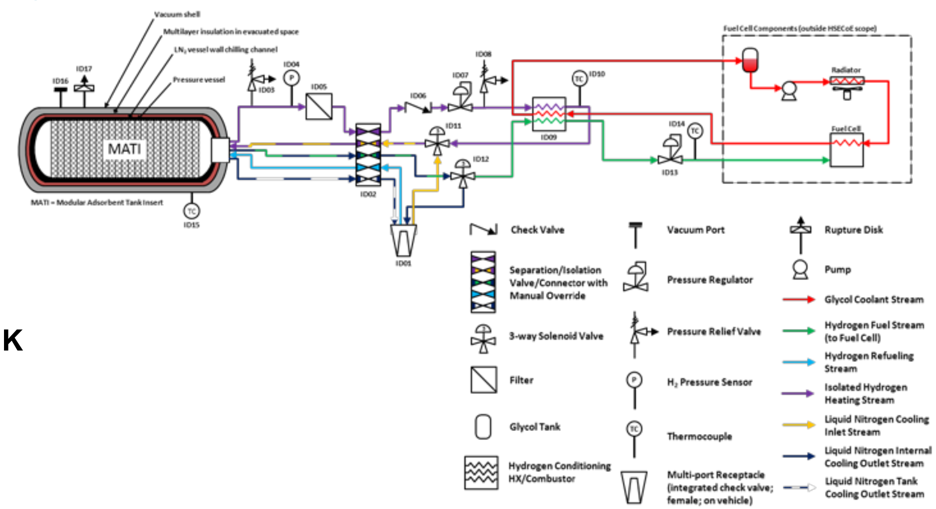


HSECoE

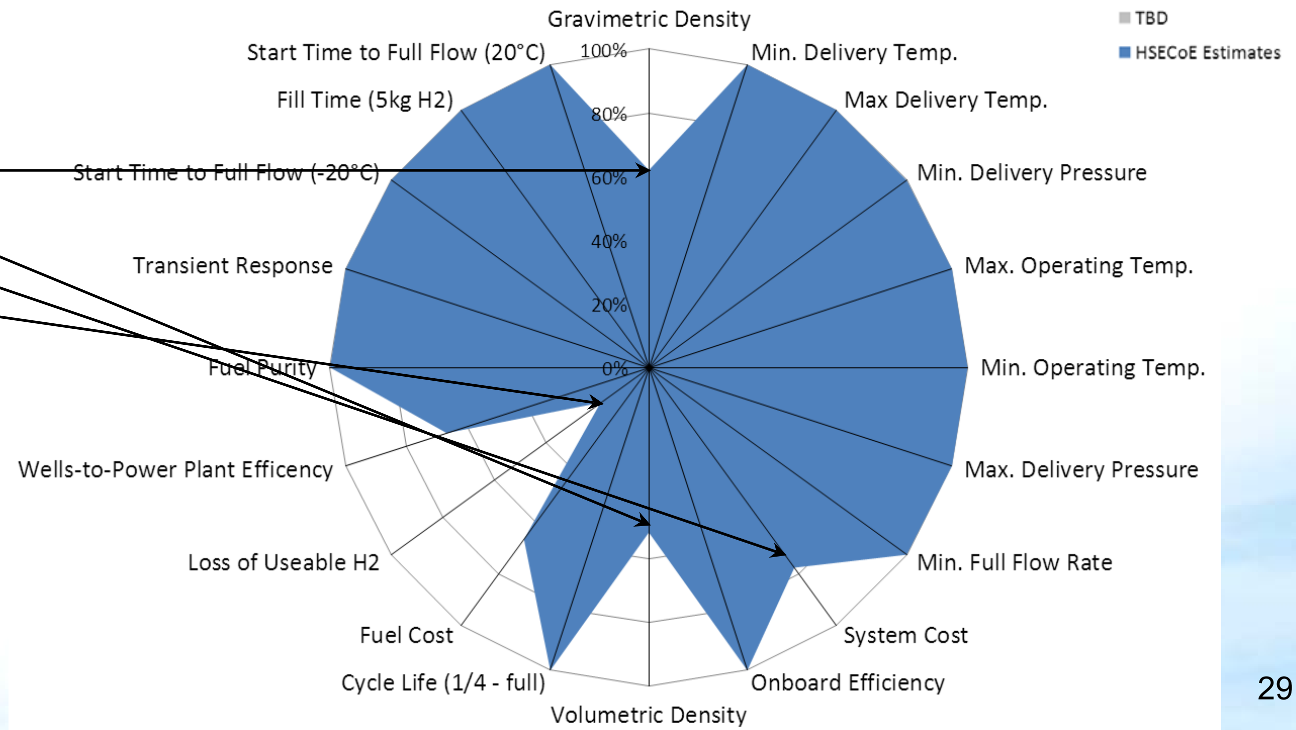
MATI Adsorbent System Projection End of Phase 2

2017 Targets



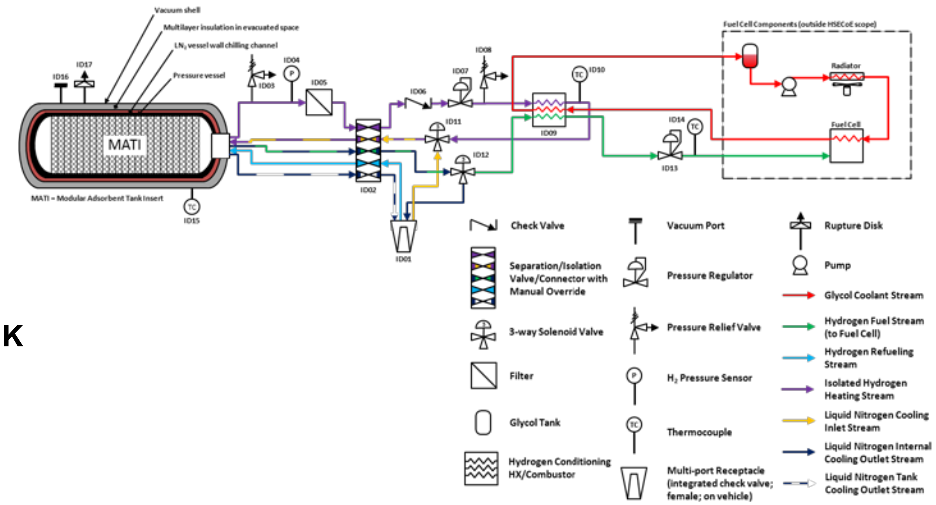
- **Compacted MOF-5, no thermal enhancement, 80 K initial fill**
- **Type 1 Al pressure vessel, 100 bar**
- **Double-wall 60-layer MLVI jacket design, 5W heat leak @ 80 K**
- **Adsorption: LN2 chilled plates**
- **Desorption: BoP heated H2/140K**

1. Gravimetric Density
2. Volumetric Density
3. System Cost
4. Loss of Usable H_2



MATI Adsorbent System Projection End of Phase 2

2017 Targets



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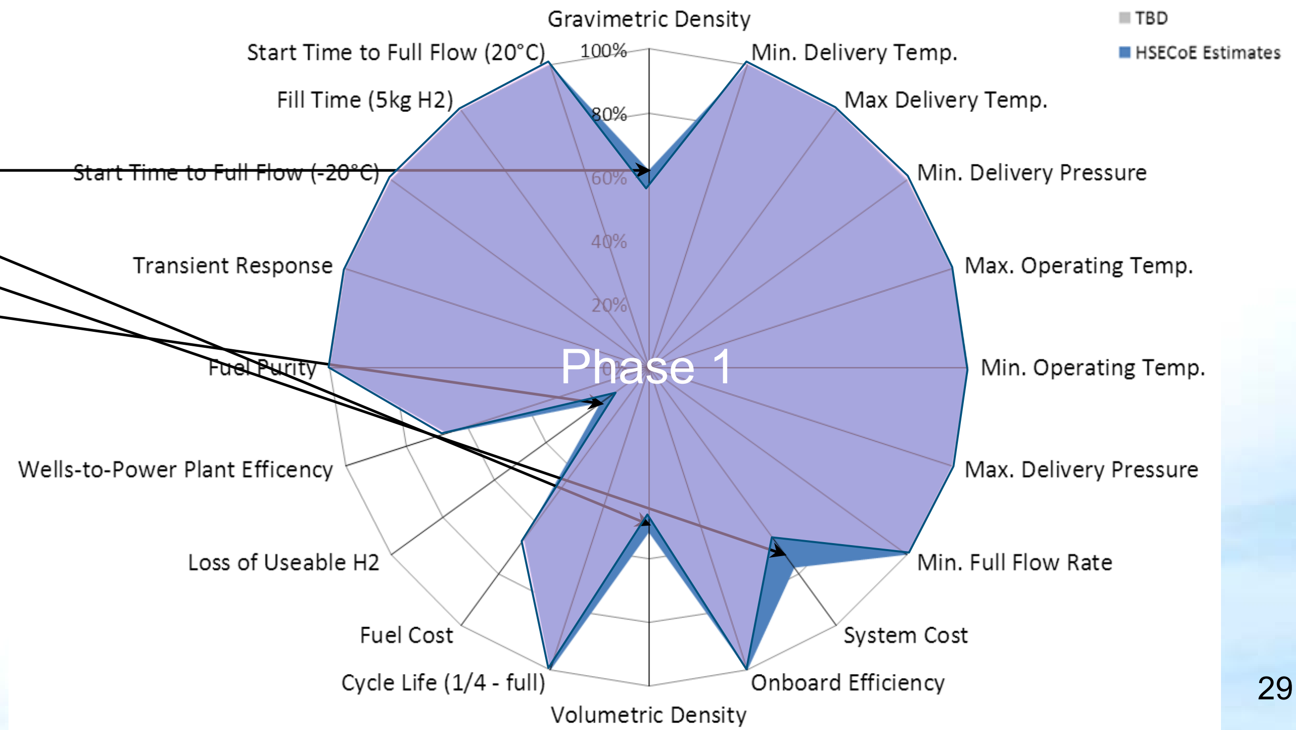
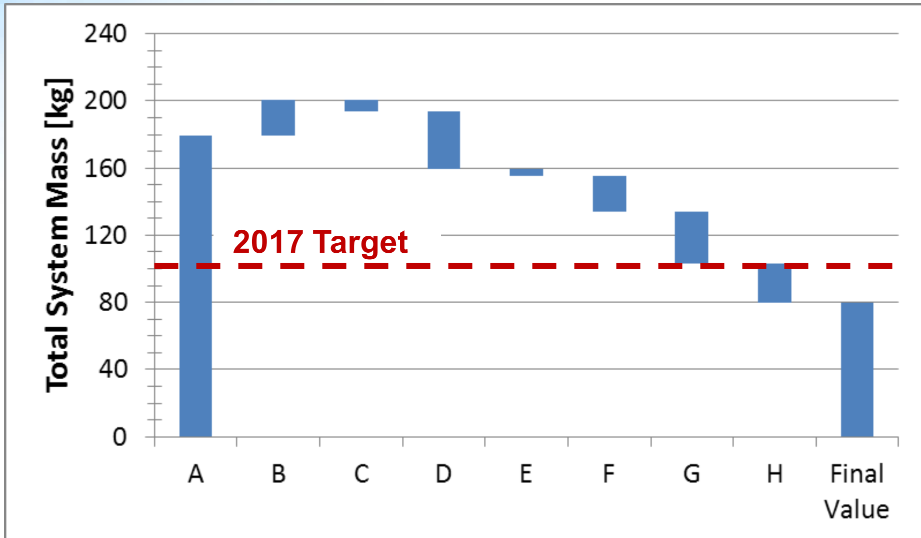
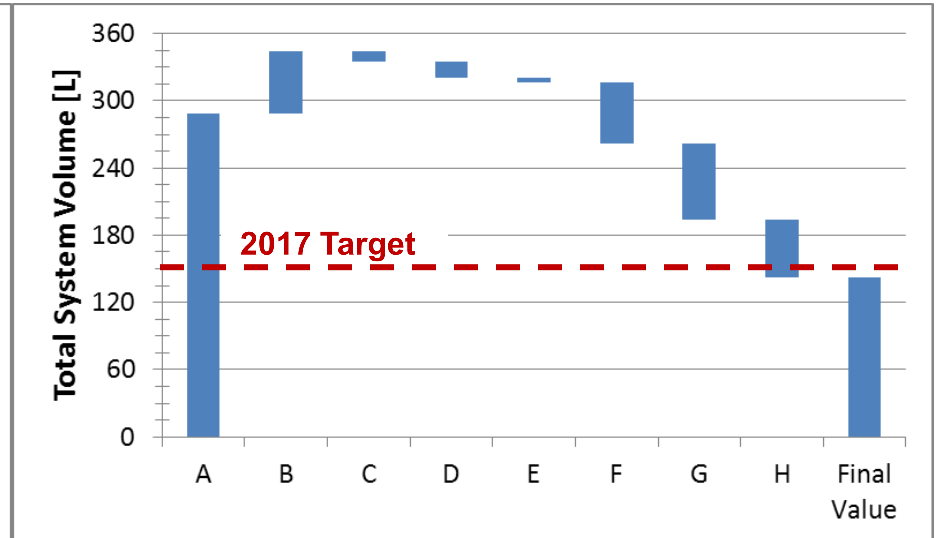
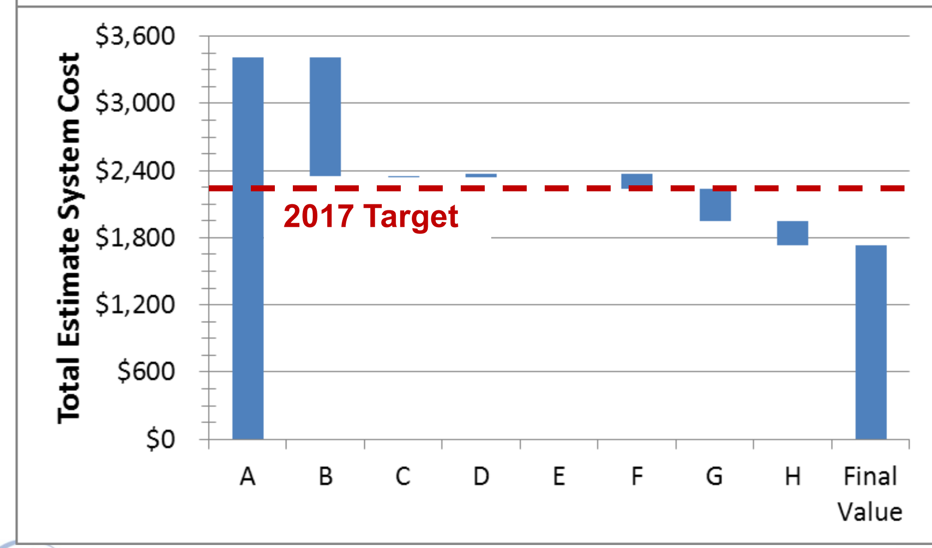


Waterfall Charts for 80 K, 100 bar HexCell System







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

Adsorbent System FMEA Updated

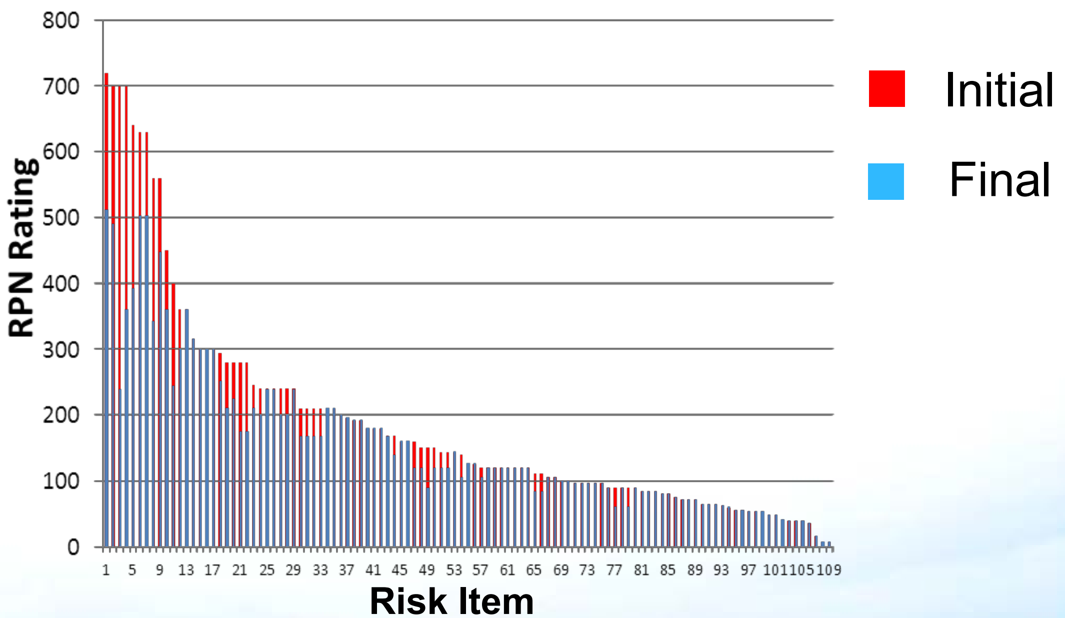
Failure Modes and Effects Analysis

Highest risk items identified from initial FMEA
Corrective actions taken
Example actions during phase 2 for reducing the Risk Priority Number (RPN)

- Completed initial homogenous material analysis and heat exchanger testing
- Revised tank construction from composite to aluminum and completed cryogenic testing
- Developed designs with deep-dive technical reviews, controls, and test plans for Phase 3

Initial Phase 2 RPN values
- High: 720
- Mean: 188

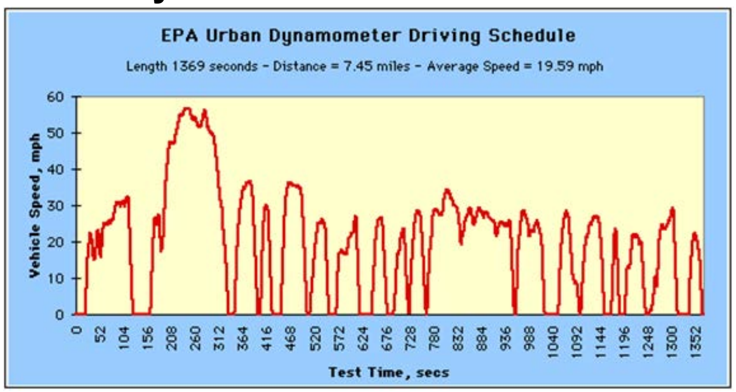
Final Phase 2 RPN values
- High: 512
- Mean: 113



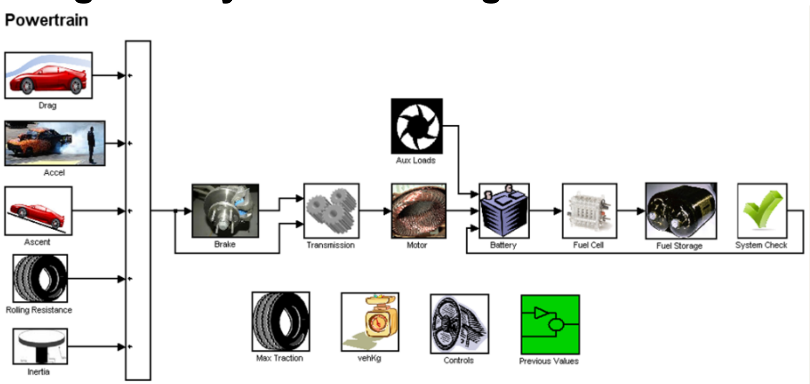
Wells-to-Power Plant Analyses

Milestone	Metric Outcome
Calculate and **model the well-to-power plant (WTPP) efficiency** for two adsorbent and one chemical storage system designs and compare results relative to the 60% technical target.	**Met metric for one adsorbent system in process of completion.**

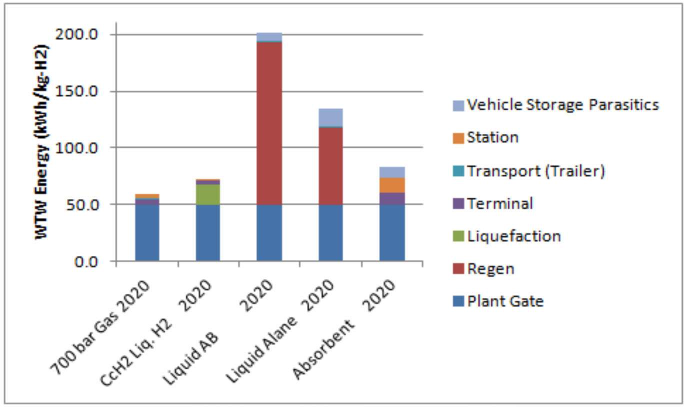
Drive Cycles



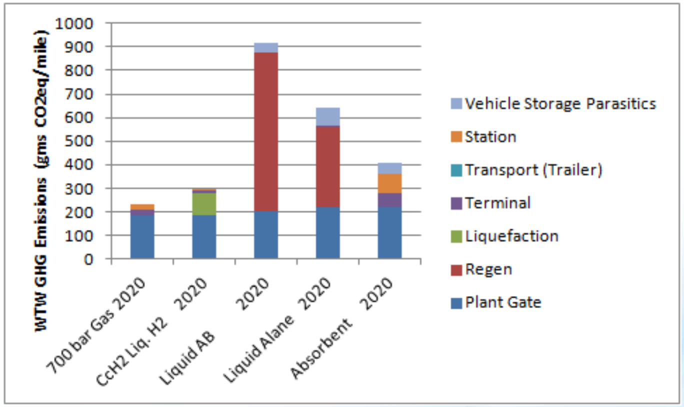
Integrated System Modeling



Energy Efficiency



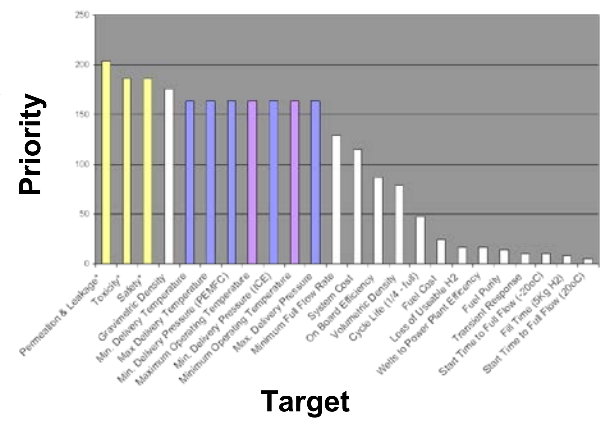
GHG Emissions



Technical Target Prioritization

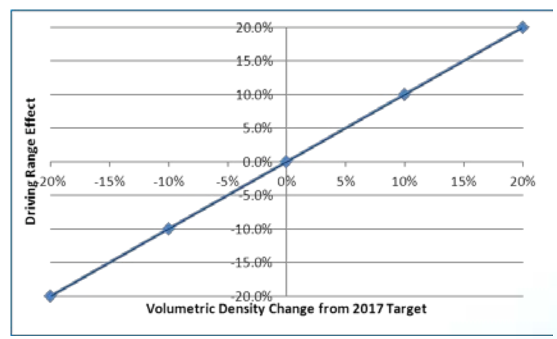
- **All targets must still be met simultaneously**
- Prioritization identifies **performance must-have** vs. **design choice** targets
- Guides design trade-offs to optimize overall system/vehicle performance to meet customer expectations
- QFD approach originally taken

Original Target Ranking



- **Method for the refined analysis**
  - Quantify the storage system linkage to vehicle attributes
  - Subjective scale of cause-effect relationships are revised based on correlation analysis
  - Limited to the key system targets: **gravimetric density, volumetric density, and cost**

Correlation of Driving Range vs. Volumetric Density



- **Refined Analysis**
  - **System Score = Grav. Score + Cost Score + Vol. Score**
    - **Target Score** = (% of Target Obtained)*∑(Importance * Correlation Constant)
    - Gravimetric Score = $S_{GD\%}$ (I_{FE} x C_{GFE} + I_{DR} x C_{GDR} + I_{VA} x C_{GVA} + I_{VC} x C_{GVC})
    - Cost Score = $S_{C\%}$ x I_{VC} x C_{CVC}
    - Volumetric Score = $S_{VD\%}$ x I_{VDR} x C_{VDR}

HSECoE

Accomplishment

WEB Site Models Added

www.HSECoE.org

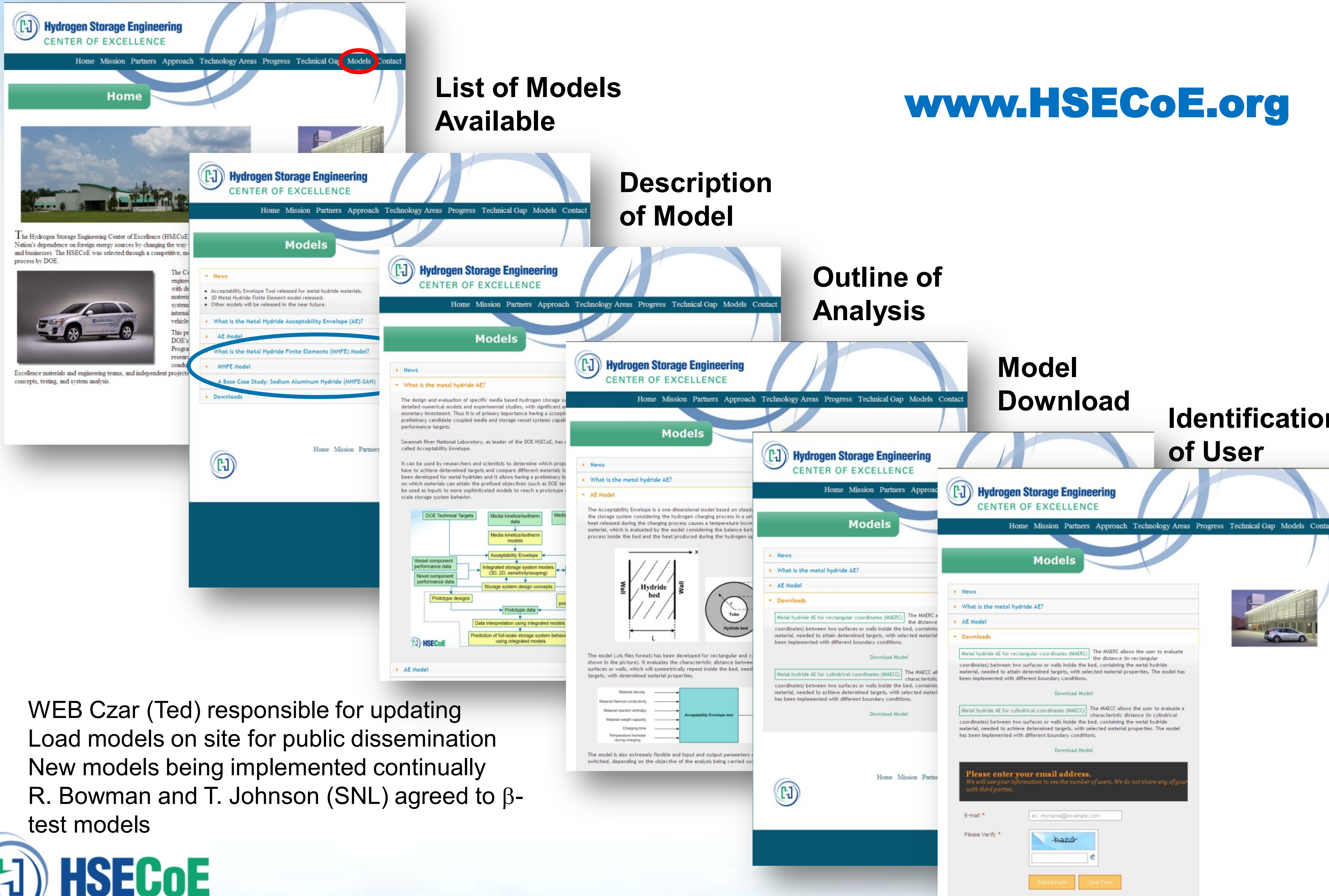
List of Models Available

Description of Model

Outline of Analysis

Model Download

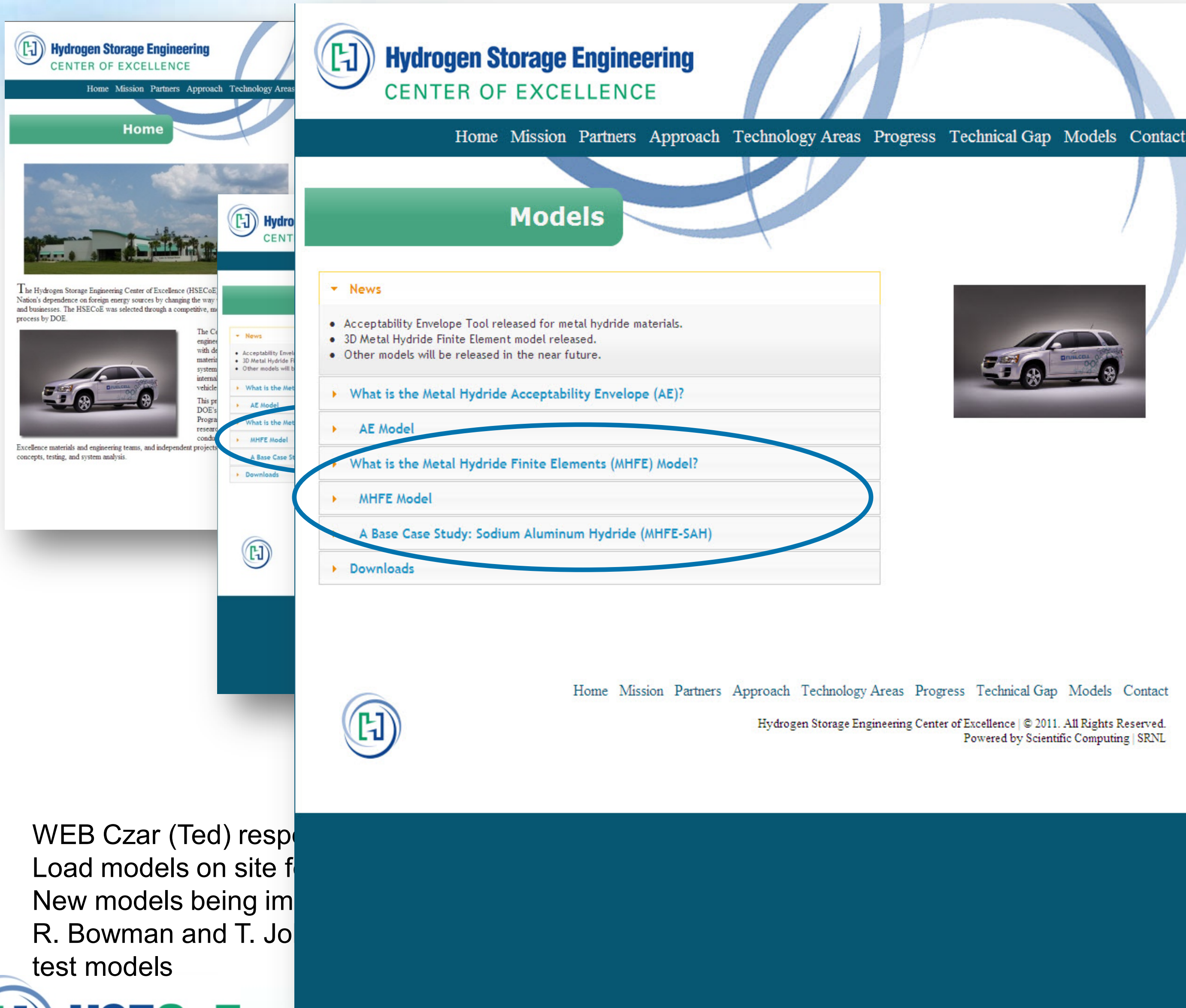
Identification of User



- WEB Czar (Ted) responsible for updating
- Load models on site for public dissemination
- New models being implemented continually
- R. Bowman and T. Johnson (SNL) agreed to β-test models

HSECoE

WEB Site Models Added



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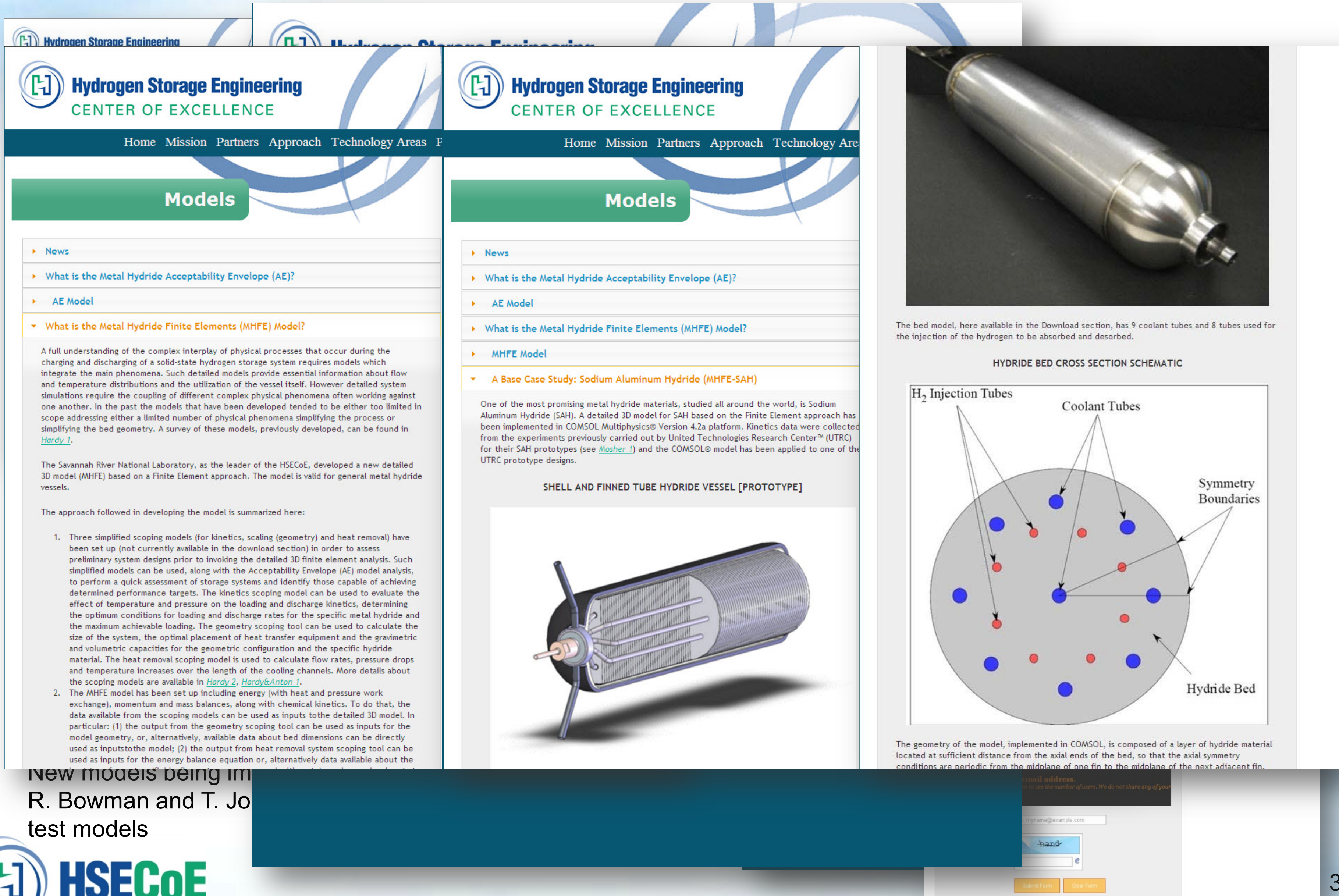
Identification of User

- WEB Czar (Ted) resp
- Load models on site f
- New models being im
- R. Bowman and T. Jo
  test models

HSECoE

Accomplishment

WEB Site Models Added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What is the Metal Hydride Acceptability Envelope (AE)?
AE Model
What is the Metal Hydride Finite Elements (MHFE) Model?

A full understanding of the complex interplay of physical processes that occur during the charging and discharging of a solid-state hydrogen storage system requires models which integrate the main phenomena. Such detailed models provide essential information about flow and temperature distributions and the utilization of the vessel itself. However detailed system simulations require the coupling of different complex physical phenomena often working against one another. In the past the models that have been developed tended to be either too limited in scope addressing either a limited number of physical phenomena simplifying the process or simplifying the bed geometry. A survey of these models, previously developed, can be found in Hardy 1.

The Savannah River National Laboratory, as the leader of the HSECoE, developed a new detailed 3D model (MHFE) based on a Finite Element approach. The model is valid for general metal hydride vessels.

The approach followed in developing the model is summarized here:

1. Three simplified scoping models (for kinetics, scaling (geometry) and heat removal) have been set up (not currently available in the download section) in order to assess preliminary system designs prior to invoking the detailed 3D finite element analysis. Such simplified models can be used, along with the Acceptability Envelope (AE) model analysis, to perform a quick assessment of storage systems and identify those capable of achieving determined performance targets. The kinetics scoping model can be used to evaluate the effect of temperature and pressure on the loading and discharge kinetics, determining the optimum conditions for loading and discharge rates for the specific metal hydride and the maximum achievable loading. The geometry scoping tool can be used to calculate the size of the system, the optimal placement of heat transfer equipment and the gravimetric and volumetric capacities for the geometric configuration and the specific hydride material. The heat removal scoping model is used to calculate flow rates, pressure drops and temperature increases over the length of the cooling channels. More details about the scoping models are available in Hardy 2, Hardy&Anton 1.
2. The MHFE model has been set up including energy (with heat and pressure work exchange), momentum and mass balances, along with chemical kinetics. To do that, the data available from the scoping models can be used as inputs tothe detailed 3D model. In particular: (1) the output from the geometry scoping tool can be used as inputs for the model geometry, or, alternatively, available data about bed dimensions can be directly used as inputstothe model; (2) the output from heat removal system scoping tool can be used as inputs for the energy balance equation or, alternatively data available about the

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What is the Metal Hydride Acceptability Envelope (AE)?
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What is the Metal Hydride Finite Elements (MHFE) Model?
MHFE Model
A Base Case Study: Sodium Aluminum Hydride (MHFE-SAH)

One of the most promising metal hydride materials, studied all around the world, is Sodium Aluminum Hydride (SAH). A detailed 3D model for SAH based on the Finite Element approach has been implemented in COMSOL Multiphysics® Version 4.2a platform. Kinetics data were collected from the experiments previously carried out by United Technologies Research Center™ (UTRC) for their SAH prototypes (see Mosher 1) and the COMSOL® model has been applied to one of the UTRC prototype designs.

SHELL AND FINNED TUBE HYDRIDE VESSEL [PROTOTYPE]

The bed model, here available in the Download section, has 9 coolant tubes and 8 tubes used for the injection of the hydrogen to be absorbed and desorbed.

HYDRIDE BED CROSS SECTION SCHEMATIC

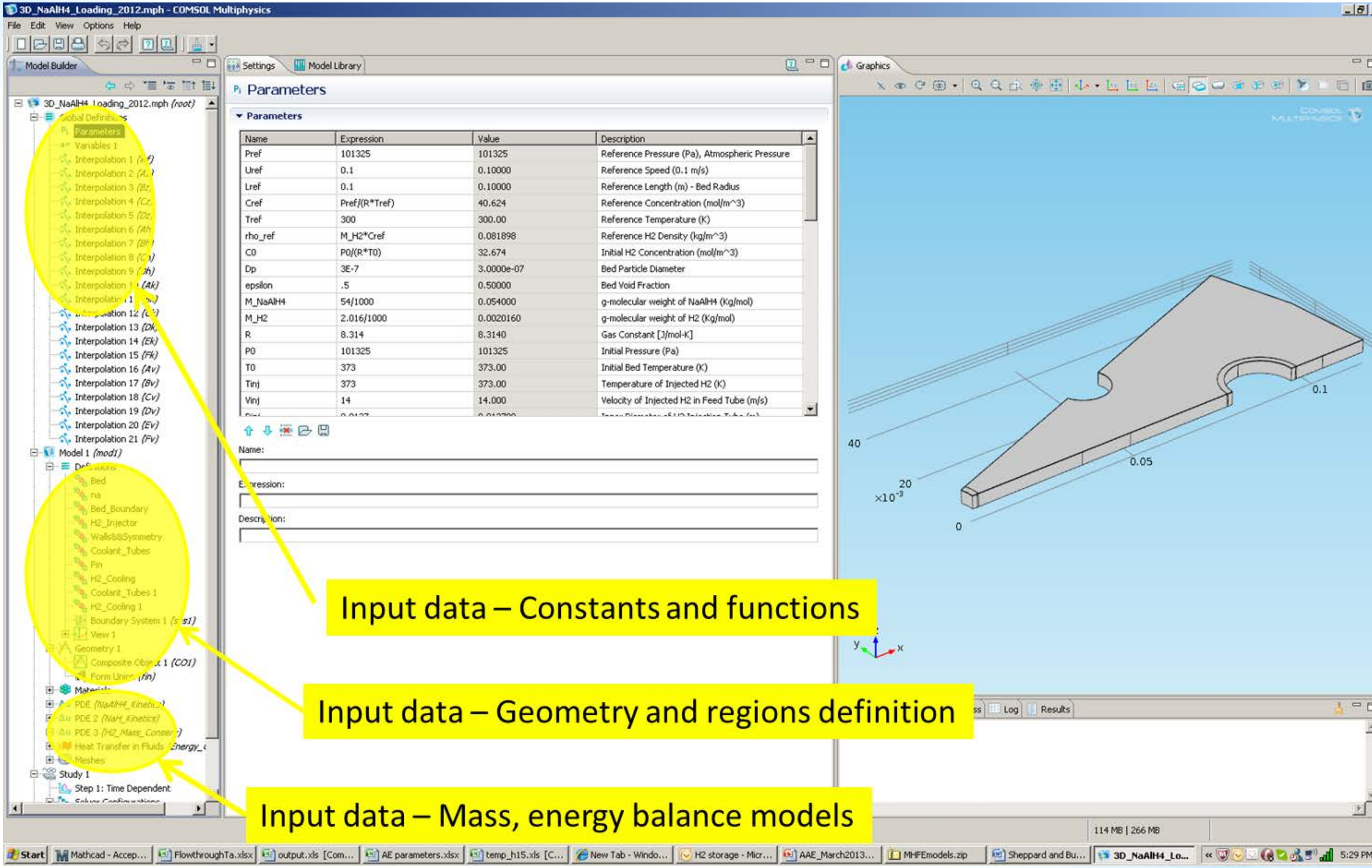
The geometry of the model, implemented in COMSOL, is composed of a layer of hydride material located at sufficient distance from the axial ends of the bed, so that the axial symmetry conditions are periodic from the midplane of one fin to the midplane of the next adjacent fin.

- New models being im
- R. Bowman and T. Jo
  test models

HSECoE

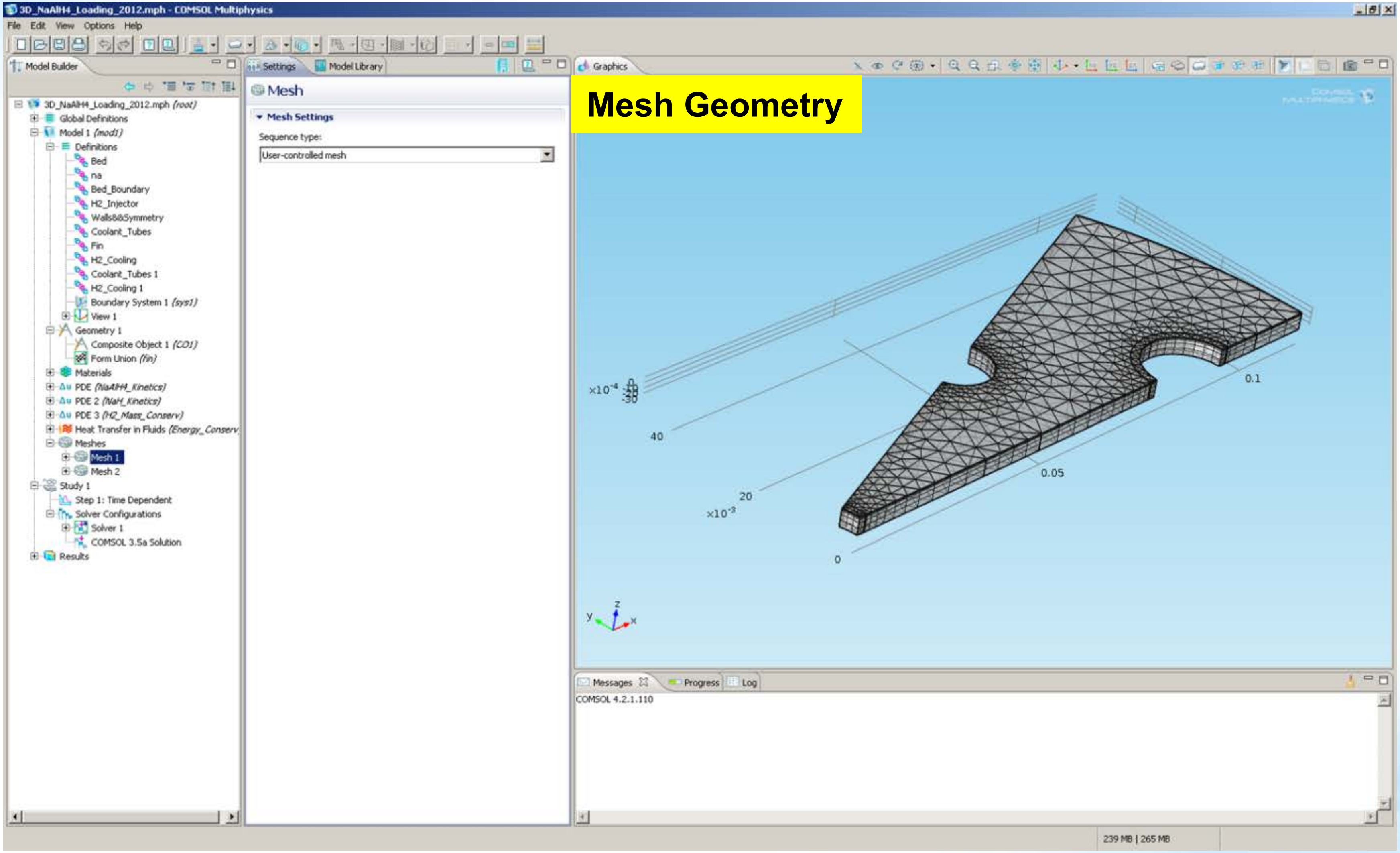
Metal Hydride FEM Model

COMSOL MULTIPHYSICS



Metal Hydride FEM Model

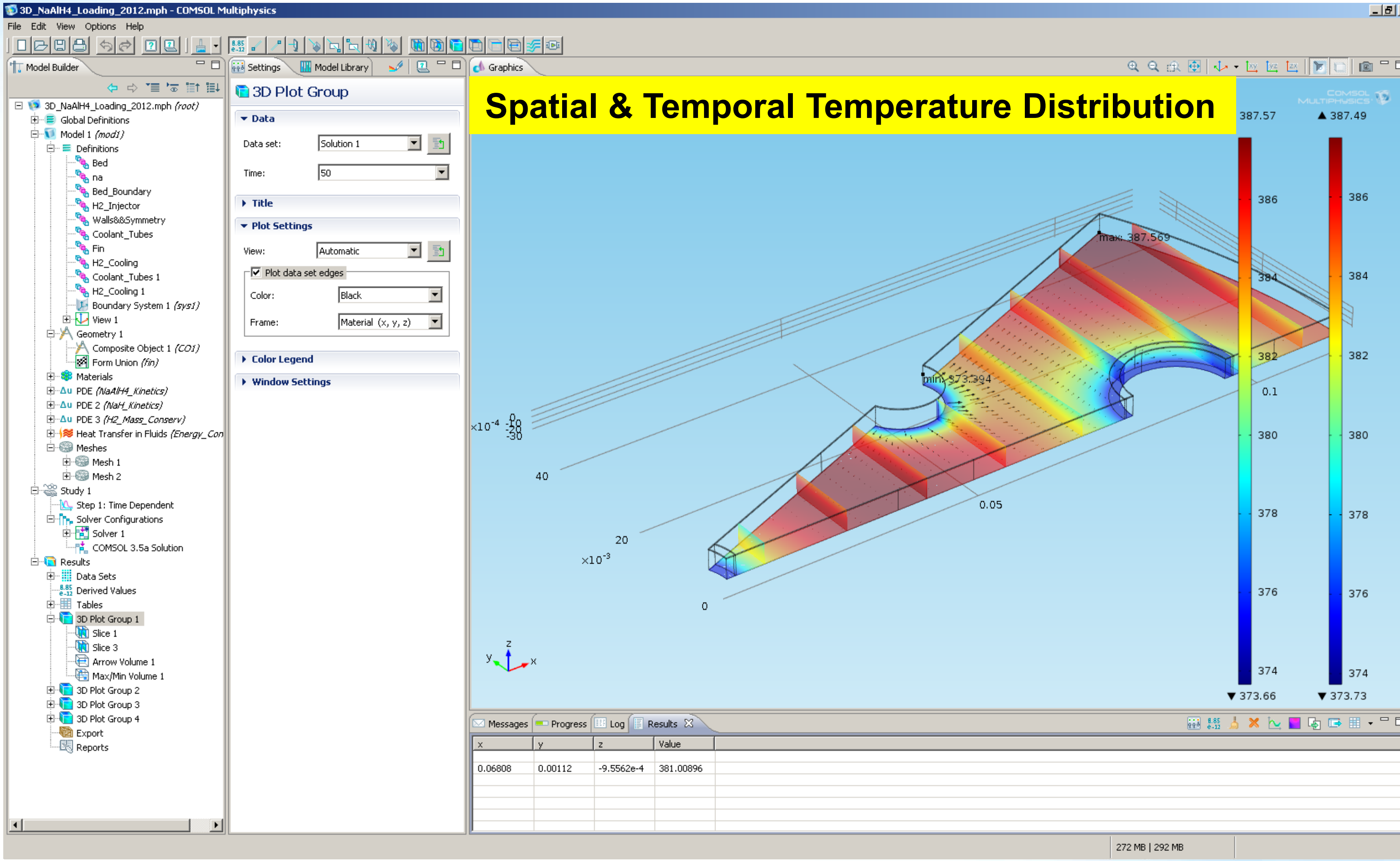
COMSOL MULTIPHYSICS®



HSECoE

Metal Hydride FEM Model

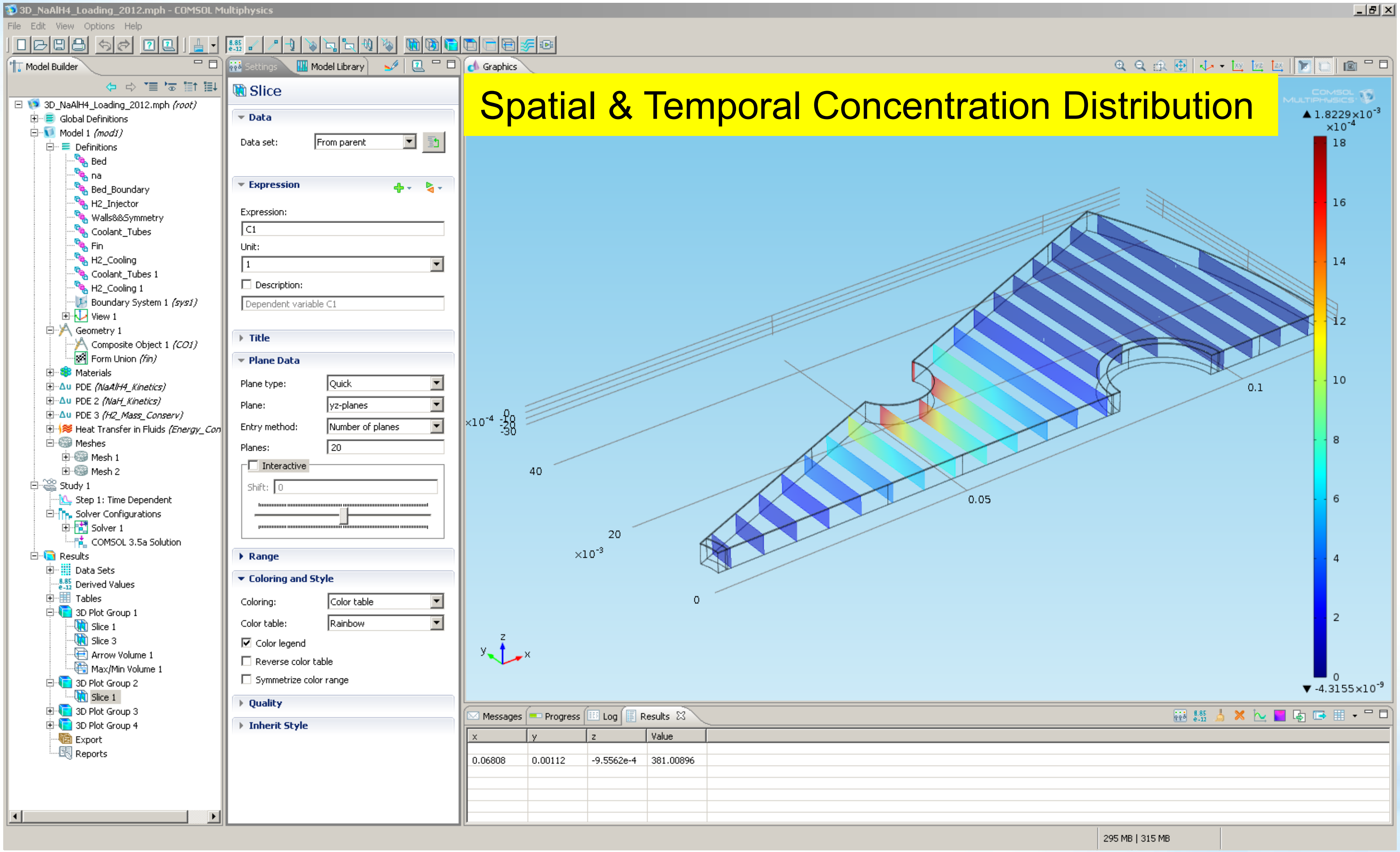
COMSOL MULTIPHYSICS®



Accomplishment

Metal Hydride FEM Model

COMSOL MULTIPHYSICS®



HSECoE

HSECoE Website Status/Plan

	Model Name	Lead	Status
1	MH Acceptability Envelope	SRNL	Complete
2	MH Finite Element Model	SRNL	Complete
3	MH Framework Model	UTRC	Model complete *(TBR)*
4	Tank Volume/Cost Model	PNNL	Model Complete *(TBR)*
5	Electric/Hybrid Vehicle Performance*	NREL	6/13
6	AD Finite Element Model	SRNL	9/13
7	AD Framework Model	SRNL	3/14
8	Chemical Hydride Model(s)	PNNL	6/14

** NREL model to be linked to HSECoE website*

Phase 3 Go/NoGo Review Held

- **Where we are now?**
  - Phase 2 Spider Charts
  - Phase 2 SMART Milestone Status
  - Phase 2 Waterfall Charts
- **Why this demonstration will be valuable?**
  - Validate models
  - Materials Properties Requirements
  - Demonstrate Engineering Concepts
- **What will be demonstrated in Phase 3?**
  - Scale of test and justification
  - Specific designs/components (mass/volume/cost)
  - Design status/plan
- **How will it be demonstrated in Phase 3?**
  - Specific test plan for each target
  - What will be learned from each test
  - Test facility status/plan
  - Decommissioning plan
- **Who will participate and how?**
  - Partner's roles
  - Phase 3 Draft SMART Milestones
- **When will this come about?** *Planned Phase 3 Gantt chart*

Green text indicates deliverable to DOE

System Test Matrixes

Phase 3 ideas for testing specific targets: MOF-5 cryoadsorbent system
Phase 3 goal for this system:
System/material form: powder/compacted? Flow-through/MATI?

Target	Gravimetric capacity	Volumetric capacity	System cost	Fuel cost	Ambient temperature	Min/max delivery temperature	Operational cycle life (1/4 tank to full)
Unit	wt%	g-H_2/L	$/kWh net	$/gge at pump	°C	°C	cycles
2017	5.5	40		2-6	-40 - 60 (sun)	-40/85	1500
Ultimate	7.5	70		2-3	-40 - 60 (sun)	-40/85	1500
Will this target be tested?	Yes-Partial	Yes-Partial	Maybe	No	Indirect via modeling	Indirect via modeling	Yes-Partial
What is the test or model approach?	Actual weights instrumented BOP list; Instrumentation and hardware adds to system;What we could build today;	Separate lists of volumes (as for weights)	Cost of lab system will be known. Production system costs at 500K units/year will be estimated by HSECoE and DTI	Cost to refuel will be estimated by Paster and Thornton	Test will be at room temperature	Will measure H2 delivery temperature Separate component test	Stress models ASME. Limited material cycling test (possibly 500 cycles?) + extrapolation
What exactly should be measured in this test to verify the target or model?	Usable capacity. Include 5 bar & 3 bar operating pressure as test matrix and see effect on gravimetric	Usable capacity	Estaimated costs of lab scale system to actual cost of lab scale system	Amount of LN2 and H2 consumed during refill	External temperature	H2 outlet temperature	Fatigue behavior. Structure of tank internals before/after cycling (tomography?). H2 purity before/after
What is the reference test or model nar E' refers to experiments; 'M' refers to models	4.3 - System Fill Test 4.4 - System Delivery Test E: Chahine M: Tamburello	4.3 - System Fill Test 4.4 - System Delivery Test E: Chahine M: Tamburello	Sytem Cost Projections M: Weimar & Veenstra	WTW Efficiency Projections M: Thornton	<Insert model name> M: Tamburello	<Insert model name> M: Tamburello	Cycle Tests; E: Chahine and Simmons
Does the test involve possible scaling? (Will the system size be varied in Phase 3 to examine finite-size effects?)	No. Only one size will be tested	No. Only one size will be tested	Yes. Scaling for higher volume volume manufacturing will be included in the analysis	Yes. Models should scale to account for economies of scale (large number of vehicles and fueling stations)	No. Only one size will be tested	No. Only one size will be tested	No. Only one size will be tested
Is modeling required to justify scaling? (Should modeling be used to determine the size of the system or magnitude of effect to be tested?)	Yes. Need to quantify tradeoff between finite-size effects and the size of system which can realistically be tested.	Yes. Need to quantify tradeoff between finite-size effects and the size of system which can realistically be tested.	Yes	Yes	No	No	No
Is there any contraints to the test set-up (i.e. test facility limits, materials availability, etc.) ?	See UQTR limits below	See UQTR limits below	N/A	N/A	Unlikely that heating or cooling system to these temperatures will be possible.	Chahine	Cycle test is limited by time to complete a cycle and consumables (H2, N2)

Target	Min delivery pressure to FC	Max delivery pressure to FC	On-board efficiency	Well to power plant efficiency	System fill rate	Min full flow rate	Start time to full flow (20°C)
Unit	bar (abs)	bar (abs)	%	%	kg-H_2/min	(g/s)/kW	s
2017	5	12			1.5	0.02	5
Ultimate	3	12	90	60	2	0.02	5
Will this target be tested?	Yes	Yes	Yes	Indirect via modeling	Yes	Indirect via modeling	Yes
What is the test or model approach?	Test both 3 and 5 bar.	Verify pressure regulation to 12 bar functions over specified operating conditions	Determine work/heat input to release H2 and warm system to specified final temperature. Modeing:	Modeling: Thornton, Hardy	Detailed model can estimate what flow rates / sorbent/ minimum temperature and what pressure?	Modeling: Tamburello & Hardy, Pasini	Experiments: Chahine
What exactly should be measured in this test to verify the target or model?	H2 outlet pressure at a function of charge state and discharge rate	H2 outlet pressure at a function of charge state and discharge rate	Energy input to tank to induce H2 release	Cost and energy inputs during refill	Time to complete fill as a function of tank starting temperature and state of charge	H2 outlet flow as a function of state of charge and "drive cycle"	Time to achieve full flow
What is the reference test or model nar E' refers to experiments; 'M' refers to models	4.4 System Delivery Test; E: Chahine	4.4 System Delivery Test; E: Chahine	4.4 System Delivery Test; E: Chahine	4.3 System Fill test; M: Thornton, Hardy	4.3 System Fill Test; E: Chahine, M: Hardy & Tamburrello	4.4 System Delivery Test and 4.6 System Dynamic Test; M: Pasini, Tamburello, Hardy; E: Chahine	4.5 - System start-up test; E: Chahine
Does the test involve possible scaling? (Will the system size be varied in Phase 3 to examine finite-size effects?)	No. Only one size will be tested	No. Only one size will be tested	No. Only one size will be tested	No. Only one size will be tested	Possibly. Should detemine how fill time varies with state of charge and initital temperature	No. Only one size will be tested	No. Only one size will be tested
Is modeling required to justify scaling? (Should modeling be used to determine the size of the system or magnitude of effect to be tested?)	No	No	Yes	No	Yes. Need to quantify tradeoff between finite-size effects and the size of system which can realistically be tested.	Yes	No
Is there any contraints to the test set-up (i.e. test facility limits, materials availability, etc.) ?	No	No	No	N/A	Note limitations on UQTR cooling rate of compressed H2	N/A	No? Chahine

Target	Start time to full flow (-20°C)	Transient response (10%-90% & 90%-0%)	Fuel purity (SAE J2719 & ISO/PDTS 14687-2)	Permeation & leakage	Toxicity	Safety	Loss of usable H_2
Unit	s	s	%H_2	Scch/h	-	-	(g/h)/kg-H2 stored
2017	15	0.75	99.97	See note	See note	See note	0.05
Ultimate	15	0.75	99.97	See note	See note	See note	0.05
Will this target be tested?	Indirect via modeling	Yes	Yes	No	Yes-Partial	Yes	Yes
What is the test or model approach?	Modeling: Tamburello & Hardy	Modeling: Hardy; Experiments: Chahine	Direct measurement of H2 purity from storage tank via mass spec or RGA. Done at beginning of tests and	Consider for Phase 2 at JPL with composite tank. Reiter and Simmons	Dust cloud ignition	Design should be robust and testing procedures should be vetted in advance for possible risks	Clarify whether Phase 3 will require a MLVI and jacket
What exactly should be measured in this test to verify the target or model?	Time to achieve full flow. Consider extrapolating 20 C data to -20 C.	Time to achieve desired response in flow rate	Composition of desorbed gas using Mass spectrometer or RGA.	Transport of H2 through liner. Other?	N/A. BASF and/or UTRC will conduct dust cloud tests?	Meets appicable safety standards	Temperature of tank vs time. Vacuum level in insulated jacket.
What is the reference test or model nar E' refers to experiments; 'M' refers to models	4.5 - System start-up test; M: Tamburello and Hardy	4.6 System Dynamic Test; E: Chahine	H2 Purity Test: E: Veenstra, Siegel, and Chahine	Permeation Test: E: Reither and Simmons	Dust cloud test; E: Khalil and/or BASF	Safety Protocols; E: Chahine	Insulation Test; E: Reiter
Does the test involve possible scaling? (Will the system size be varied in Phase 3 to examine finite-size effects?)	No. Only one size will be tested	No. Only one size will be tested	N/A	Consider for Phase 2 at JPL	N/A	N/A	Yes, examine different amounts of insulation
Is modeling required to justify scaling? (Should modeling be used to determine the size of the system or magnitude of effect to be tested?)	No	Yes	No	No	No	No	Yes
Is there any contraints to the test set-up (i.e. test facility limits, materials availability, etc.) ?	N/A	Chahine	Test rig should be designed to enable sampling of H2 purity	Reiter	N/A	Chahine	Availability of MLVI is a concern. JPL to address

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System Test Matrixes

Target	Gravimetric capacity	Volumetric capacity	System cost	Fuel cost	Ambient temperature
Unit	wt%	g-H_2/L	\$/kWh net	\$/gge at pump	°C
2017	5.5	40		2-6	-40 - 60 (sun)
Ultimate	7.5	70		2-3	-40 - 60 (sun)

Phase 3 ideas for testing specific ta
Phase 3 goal for this system:
System/material form: powder/compacted?

Target	capacity	capacity	System cost	Fuel cost	temperature	temperature	life (1/4 tank to full)	pressure to FC	pressure to FC	efficiency	plant efficiency	System fill rate	Min full flow rate	flow (20°C)	flow (-20°C)	(10%-90% & 90%-0%)	J2719 & ISO/PDTS 14687-2)	leakage	Toxicity	Safety	Loss of usable H_2
Unit	wt%	g-H_2/L	\$/kWh net	\$/gge at pump	°C	°C	cycles	bar (abs)	bar (abs)	%	%	kg-H_2/min	(g/s)/kW	s	s	s	%H_2	Scch/h	-	-	(g/h)/kg-H2 stored
2017	5.5	40		2-6	-40 - 60 (sun)	-40/85	1500	5	12			1.5	0.02	5	15	0.75	99.97	See note	See note	See note	0.05
Ultimate	7.5	70		2-3	-40 - 60 (sun)	-40/85	1500	3	12	90	60	2	0.02	5	15	0.75	99.97	See note	See note	See note	0.05
Will this target be tested?	Yes-Partial	Yes-Partial	Maybe	No	Indirect via modeling	Indirect via modeling	Yes-Partial	Yes	Yes	Yes	Indirect via modeling	Yes	Indirect via modeling	Yes	Indirect via modeling	Yes	Yes	No	Yes-Partial	Yes	Yes
What is the test or model approach?	Actual weights instrumented BOP list; Instrumentation and hardware adds to system;What we could build today;	Separate lists of volumes (as for weights)	Cost of lab system will be known. Production system costs at 500K units/year will be estimated by HSECoE and DTI	Cost to refuel will be estimated by Paster and Thornton	Test will be at room temperature	Will measure H2 delivery temperature Separate component test	Stress models ASME. Limited material cycling test (possibly 500 cycles?) + extrapolation	Test both 3 and 5 bar.	Verify pressure regulation to 12 bar functions over specified operating conditions	Determine work/heat input to release H2 and warm system to specified final temperature. Modeing:	Modeling: Thornton, Hardy	Detailed model can estimate what flow rates / sorbent/ minimum temperature and what pressure?	Modeling: Tamburello & Hardy, Pasini	Experiments: Chahine	Modeling: Tamburello & Hardy	Modeling: Hardy; Experiments: Chahine	Direct measurement of H2 purity from storage tank via mass spec or RGA. Done at beginning of tests and	Consider for Phase 2 at JPL with composite tank. Reiter and Simmons	Dust cloud ignition	Design should be robust and testing procedures should be vetted in advance for possible risks	Clarify whether Phase 3 will require a MLVI and jacket
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What is the reference test or model nai E' refers to experiments; 'M' refers to models	4.3 - System Fill Test 4.4 - System Delivery Test E: Chahine M: Tamburello	4.3 - System Fill Test 4.4 - System Delivery Test E: Chahine M: Tamburello	Sytem Cost Projections M: Weimar & Veenstra	WTW Efficiency Projections M: Thornton	<Insert model name> M: Tamburello	<Insert model name> M: Tamburello	Cycle Tests; E: Chahine and Simmons	4.4 System Delivery Test; E: Chahine	4.4 System Delivery Test; E: Chahine	4.4 System Delivery Test; E: Chahine	4.3 System Fill test; M: Thornton, Hardy	4.3 System Fill Test; E: Chahine, M: Hardy & Tamburrello	4.4 System Delivery Test and 4.6 System Dynamic Test; M: Pasini, Tamburello, Hardy; E: Chahine	4.5 - System start-up test; E: Chahine	4.5 - System start-up test; M: Tamburello and Hardy	4.6 System Dynamic Test; E: Chahine	H2 Purity Test: E: Veenstra, Siegel, and Chahine	Permeation Test: E: Reither and Simmons	Dust cloud test; E: Khalil and/or BASF	Safety Protocols; E: Chahine	Insulation Test; E: Reiter
Does the test involve possible scaling? (Will the system size be varied in Phase 3 to examine finite-size effects?)	No. Only one size will be tested	No. Only one size will be tested	Yes. Scaling for higher volume volume manufacturing will be included in the analysis	Yes. Models should scale to account for economies of scale (large number of vehicles and fueling stations)	No. Only one size will be tested	No. Only one size will be tested	No. Only one size will be tested	No. Only one size will be tested	No. Only one size will be tested	No. Only one size will be tested	No. Only one size will be tested	Possibly. Should detemine how fill time varies with state of charge and initital temperature	No. Only one size will be tested	No. Only one size will be tested	No. Only one size will be tested	No. Only one size will be tested	N/A	Consider for Phase 2 at JPL	N/A	N/A	Yes, examine different amounts of insulation
Is modeling required to justify scaling? (Should modeling be used to determine the size of the system or magnitude of effect to be tested?)	Yes. Need to quantify tradeoff between finite-size effects and the size of system which can realistically be tested.	Yes. Need to quantify tradeoff between finite-size effects and the size of system which can realistically be tested.	Yes	Yes	No	No	No	No	No	Yes	No	Yes. Need to quantify tradeoff between finite-size effects and the size of system which can realistically be tested.	Yes	No	No	Yes	No	No	No	No	Yes
Is there any contraints to the test set-up (i.e. test facility limits, materials availability, etc.) ?	See UQTR limits below	See UQTR limits below	N/A	N/A	Unlikely that heating or cooling system to these temperatures will be possible.	Chahine	Cycle test is limited by time to complete a cycle and consumables (H2, N2)	No	No	No	N/A	Note limitations on UQTR cooling rate of compressed H2	N/A	No? Chahine	N/A	Chahine	Test rig should be designed to enable sampling of H2 purity	Reiter	N/A	Chahine	Availability of MLVI is a concern. JPL to address

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System Test Matrixes

Target	Gravimetric capacity	Volumetric capacity	System cost	Fuel cost	Ambient temperature
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Ultimate	7.5	70		2-3	-40 - 60 (sun)

Phase 3 ideas for testing specific ta
Phase 3 goal for this system:
System/material form: powder/compacted?

Will this target be tested?

What is the test or model approach?

What exactly should be measured in this test to verify the target or model?

uel cost	temperature	temperature	ife (1/4 tank to full)	pressure to FC	pressure to FC	efficiency	plant efficiency	System fill rate	Min full flow rate	flow (20°C)	flow (-20°C)	(10%-90% & 90%-0%)	J2719 & ISO/PDTS 14687-2)	leakage	Toxicity	Safety	Loss of usable H_2
ge at pump	°C	°C	cycles	bar (abs)	bar (abs)	%	%	kg-H_2/min	(g/s)/kW	s	s	s	%H_2	Scch/h	-	-	(g/h)/kg-H2 stored
2-6	-40 - 60 (sun)	-40/85	1500	5	12			1.5	0.02	5	15	0.75	99.97	See note	See note	See note	0.05
2-3	-40 - 60 (sun)	-40/85	1500	3	12	90	60	2	0.02	5	15	0.75	99.97	See note	See note	See note	0.05
No	Indirect via modeling	Indirect via modeling	Yes-Partial	Yes	Yes	Yes	Indirect via modeling	Yes	Indirect via modeling	Yes	Indirect via modeling	Yes	Yes	No	Yes-Partial	Yes	Yes
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nt of LN2 and nsumed refill	External temperature	H2 outlet temperature	Fatigue behavior. Structure of tank internals before/after cycling (tomography?). H2 purity before/after	H2 outlet pressure at a function of charge state and discharge rate	H2 outlet pressure at a function of charge state and discharge rate	Energy input to tank to induce H2 release	Cost and energy inputs during refill	Time to complete fill as a function of tank starting temperature and state of charge	H2 outlet flow as a function of state of charge and "drive cycle"	Time to achieve full flow	Time to achieve full flow. Consider extrapolating 20 C data to -20 C.	Time to achieve desired response in flow rate	Composition of desorbed gas using Mass spectrometer or RGA.	Transport of H2 through liner. Other?	N/A. BASF and/or UTRC will conduct dust cloud tests?	Meets appicable safety standards	Temperature of tank vs time. Vacuum level in insulated jacket.
Efficiency tions M: ton	<Insert model name> M: Tamburello	<Insert model name> M: Tamburello	Cycle Tests; E: Chahine and Simmons	4.4 System Delivery Test; E: Chahine	4.4 System Delivery Test; E: Chahine	4.4 System Delivery Test; E: Chahine	4.3 System Fill test; M: Thornton, Hardy	4.3 System Fill Test; E: Chahine, M: Hardy & Tamburrello	4.4 System Delivery Test and 4.6 System Dynamic Test; M: Pasini, Tamburello, Hardy; E: Chahine	4.5 - System start-up test; E: Chahine	4.5 - System start-up test; M: Tamburello and Hardy	4.6 System Dynamic Test; E: Chahine	H2 Purity Test: E: Veenstra, Siegel, and Chahine	Permeation Test: E: Reither and Simmons	Dust cloud test; E: Khalil and/or BASF	Safety Protocols; E: Chahine	Insulation Test; E: Reiter
lodels should o account for mies of scale number of es and g stations)	No. Only one size will be tested	No. Only one size will be tested	No. Only one size will be tested	No. Only one size will be tested	No. Only one size will be tested	No. Only one size will be tested	No. Only one size will be tested	Possibly. Should detemine how fill time varies with state of charge and initital temperature	No. Only one size will be tested	No. Only one size will be tested	No. Only one size will be tested	No. Only one size will be tested	N/A	Consider for Phase 2 at JPL	N/A	N/A	Yes, examine different amounts of insulation
	No	No	No	No	No	Yes	No	Yes. Need to quantify tradeoff between finite-size effects and the size of system which can realistically be tested.	Yes	No	No	Yes	No	No	No	No	Yes
	Unlikely that heating or cooling system to these temperatures will be possible.	Chahine	Cycle test is limited by time to complete a cycle and consumables (H2, N2)	No	No	No	N/A	Note limitations on UQTR cooling rate of compressed H2	N/A	No? Chahine	N/A	Chahine	Test rig should be designed to enable sampling of H2 purity	Reiter	N/A	Chahine	Availability of MLVI is a concern. JPL to address

System Test Matrixes

Phase 3 ideas for testing specific ta
Phase 3 goal for this system:
System/material form: powder/compacted

Target	Gravimetric capacity	Volumetric capacity	System cost	Fuel cost	Ambient temperature
Unit	wt%	$g\text{-}H_2/L$	$/kWh net	$/gge at pump	°C
2017	5.5	40		2-6	-40 - 60 (sun)
Ultimate	7.5	70		2-3	-40 - 60 (sun)
Will this target be tested?	Yes-Partial	Yes-Partial	Maybe	No	Indirect via modeling
What is the test or model approach?	Actual weights instrumented BOP list; Instrumentation and hardware adds to system;What we could build today; Alternate list of what it could be.; actual capacity of system	Separate lists of volumes (as for weights)	Cost of lab system will be known. Production system costs at 500K units/year will be estimated by HSECoE and DTI	Cost to refuel will be estimated by Paster and Thornton	Test will be at room temperature
What exactly should be measured in this test to verify the target or model?	Usable capacity. Include 5 bar & 3 bar operating pressure as test matrix and see effect on gravimetric capacity.	Usable capacity	Estaimated costs of lab scale system to actual cost of lab scale system	Amount of LN2 and H2 consumed during refill	External temperature

System Component Specification

Component	Assumed Validation in Phase II	Responsible Design Organization	What can be validated with modeling rather than experimental work?	Rationale for including/excluding from Phase III	Areas of Concern Requiring Testing	Limitations on Scaling	Include in Phase
Internal Heat Exchanger: **HexCell Resistance Heater with Flow-Through Cooling**	Modeling and partial experimental validation of individual components/capabilities	SRNL / UQTR	1st-order thermal behavior (already completed).	Simple, low-cost design; Verify capability for rapid cooling: dynamic behavior (such as channeling) can only be evaluated experimentally	Cool-down time; non-uniform temperature distribution; robustness of HX with respect to temperature/pressure cycling; efficiency (energy consumed during fill)	N/A	Yes
Cryo-Adsorbent Material: **Powder MOF-5**	Modeling and experimental validation	SRNL / UQTR / Ford (BASF)	Theoretical H2 uptake; heat transfer (partial)	Integral part of system; validate capacity projections; Quantify effects due to bed inhomogeneities (non-uniform packing)	Packing density, heat transfer, and adsorption capacity	N/A	Yes
Inter-Wall LN_2 Pre-chiller: **"Thermos Bottle"**	Modeling only; Constant wall temperature models to show the need/benefit	PNNL / Lincoln Composites	1st-order thermal behavior can be modeled	Validate system thermal models; Phase-change within the channel must be evaluated experimentally	Choked flow due to LN2 phase change	Channel cross-section must remain intact	Yes – partially
Internal Heat Exchanger: **MATI with Isolated-H2 Heating and Isolated-LN2 Cooling**	Modeling and partial experimental validation of individual components/capabilities	OSU	1st-order thermal behavior has already been verified.	Quantify advantages in cooling rate and system volume; Verify rapid cooling capability and desorption performance	Welds, cycling, and verification of adsorption/desorption behavior, design complexity/robustness	N/A	Yes – partially
Cryo-Adsorbent Material: **Compacted MOF-5 "pucks" (0.32 g/cc)**	Modeling and partial experimental validation	OSU / Ford (BASF)	Theoretical H2 uptake; heat transfer (partial)	Integral part of system; validate capacity and kinetic projections; Assess robustness and heat transfer limitations	Cracking/crumbling, heat transfer, and adsorbent behavior	N/A	Yes – partially
Type 1 Aluminum pressure vessel	Design and partial experimental validation	LC	Mass, volume, and cost	Integral part of system; validate capacity projections	Cryo-burst testing	N/A	Yes
Multi-layer vacuum insulation	Modeling of heating rate/dormancy performance	JPL	Partial dormancy performance	Validate dormancy model; vacuum level stability; robustness of design	No supplier (JPL work scope reduction)	N/A	No

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System Component Specification

Component	Assumed Validation in Phase II	Responsible Design Organization	What can be validated with modeling rather than experimental work?

Exchanger: **HexCell Resistance Heater with Flow-Through Cooling**	experimental validation of individual components/capabilities	SRNL / UQTR	1^{st}-order thermal behavior (already completed).	cooling: dynamic behavior (such as channeling) can only be evaluated experimentally	of HX with respect to temperature/pressure cycling; efficiency (energy consumed during fill)	N/A	Yes
Cryo-Adsorbent Material: **Powder MOF-5**	Modeling and experimental validation	SRNL / UQTR / Ford (BASF)	Theoretical H2 uptake; heat transfer (partial)	Integral part of system; validate capacity projections; Quantify effects due to bed inhomogeneities (non-uniform packing)	Packing density, heat transfer, and adsorption capacity	N/A	Yes
Inter-Wall LN$_2$ Pre-chiller: **"Thermos Bottle"**	Modeling only; Constant wall temperature models to show the need/benefit	PNNL / Lincoln Composites	1^{st}-order thermal behavior can be modeled	Validate system thermal models; Phase-change within the channel must be evaluated experimentally	Choked flow due to LN2 phase change	Channel cross-section must remain intact	Yes – partially
Internal Heat Exchanger: **MATI with Isolated-H2 Heating and Isolated-LN2 Cooling**	Modeling and partial experimental validation of individual components/capabilities	OSU	1^{st}-order thermal behavior has already been verified.	Quantify advantages in cooling rate and system volume; Verify rapid cooling capability and desorption performance	Welds, cycling, and verification of adsorption/desorption behavior, design complexity/robustness	N/A	Yes – partially
Cryo-Adsorbent Material: **Compacted MOF-5 "pucks" (0.32 g/cc)**	Modeling and partial experimental validation	OSU / Ford (BASF)	Theoretical H2 uptake; heat transfer (partial)	Integral part of system; validate capacity and kinetic projections; Assess robustness and heat transfer limitations	Cracking/crumbling, heat transfer, and adsorbent behavior	N/A	Yes – partially
Type 1 Aluminum pressure vessel	Design and partial experimental validation	LC	Mass, volume, and cost	Integral part of system; validate capacity projections	Cryo-burst testing	N/A	Yes
Multi-layer vacuum insulation	Modeling of heating rate/dormancy performance	JPL	Partial dormancy performance	Validate dormancy model; vacuum level stability; robustness of design	No supplier (JPL work scope reduction)	N/A	No

System Component Specification

Component	Assumed Validation in Phase II		Responsible Design Organization	What can be validated with modeling rather than experimental work?
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"Thermos Bottle"	models to show the need/benefit	Composites	can be modeled	within the channel must be evaluated experimentally	phase change	remain intact	
Internal Heat Exchanger: **MATI with Isolated-H2 Heating and Isolated-LN2 Cooling**	Modeling and partial experimental validation of individual components/capabilities	OSU	1st-order thermal behavior has already been verified.	Quantify advantages in cooling rate and system volume; Verify rapid cooling capability and desorption performance	Welds, cycling, and verification of adsorption/desorption behavior, design complexity/robustness	N/A	Yes – partially
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Multi-layer vacuum insulation	Modeling of heating rate/dormancy performance	JPL	Partial dormancy performance	Validate dormancy model; vacuum level stability; robustness of design	No supplier (JPL work scope reduction)	N/A	No

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System Component Specification

Component	Assumed Validation in Phase II	Responsible Design Organization	What can be validated with modeling rather than experimental work?	
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Cryo-Adsorbent Material: **Powder MOF-5**	Modeling and experimental validation	SRNL / UQTR / Ford (BASF)	Theoretical H2 uptake; heat transfer (partial)	Integral part of system; validate capacity projections; Quantify effects due to bed inhomogeneities (non-uniform packing)

Type 1 Aluminum pressure vessel	Design and partial experimental validation	LC	Mass, volume, and cost	Integral part of system; validate capacity projections	Cryo-burst testing	N/A	Yes
Multi-layer vacuum insulation	Modeling of heating rate/dormancy performance	JPL	Partial dormancy performance	Validate dormancy model; vacuum level stability; robustness of design	No supplier (JPL work scope reduction)	N/A	No

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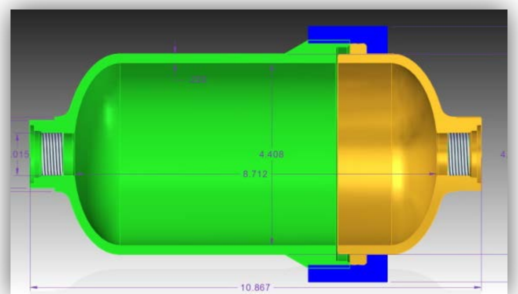
Adsorbent System Phase 3 Proposal

Heat Exchange Systems

HexCell/MOF-5 Powder
Flow-Through Cooling
Resistance Heating

Containment

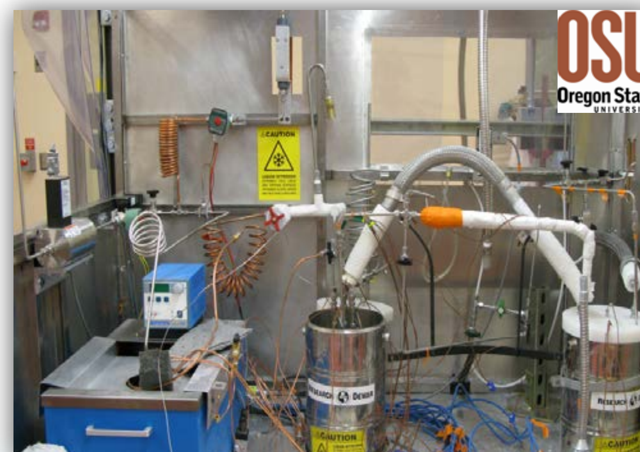


2 Liter Type 1
Segmented Al Tank

Test Facilities

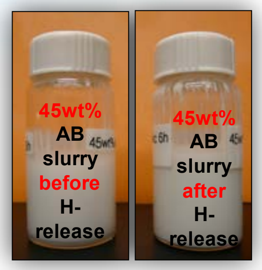
0.3g/cc MOF-5 Puck
MATI Heating/Cooling

Type 1 SS
Pressure Vessel



Chemical System Phase 3 Proposal

Materials

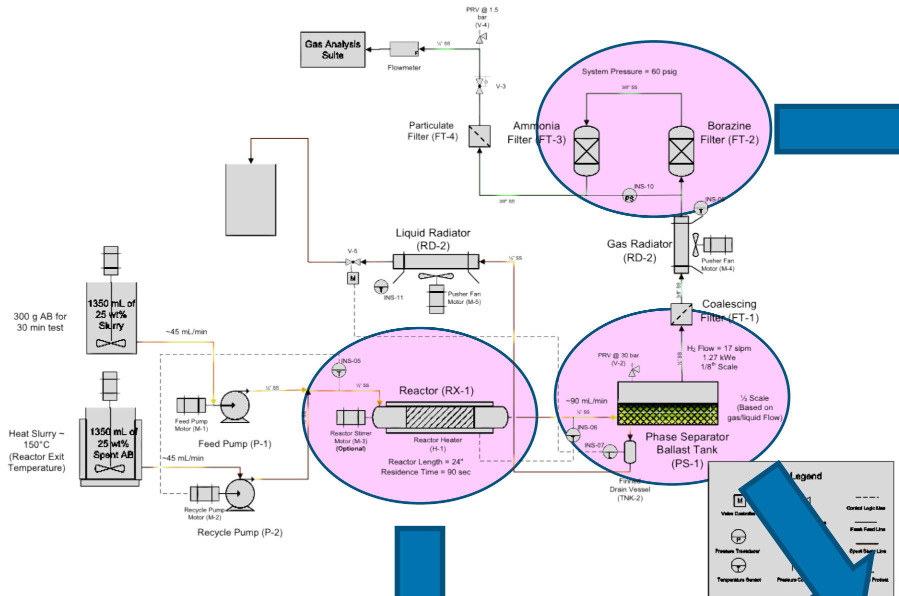


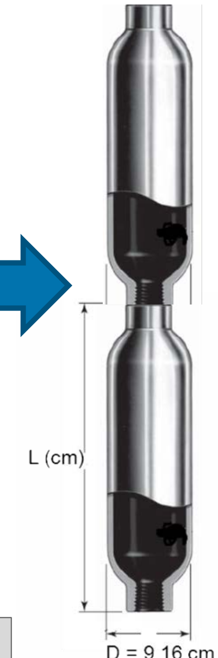
20-40$^{w}/_{o}$ AB/Si-oil

20-40$^{w}/_{o}$ AlH_3/Si-oil

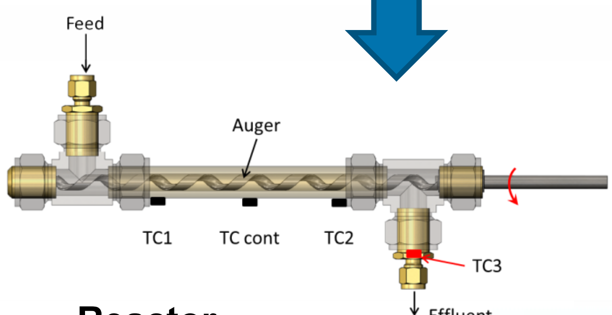
MPAB

System

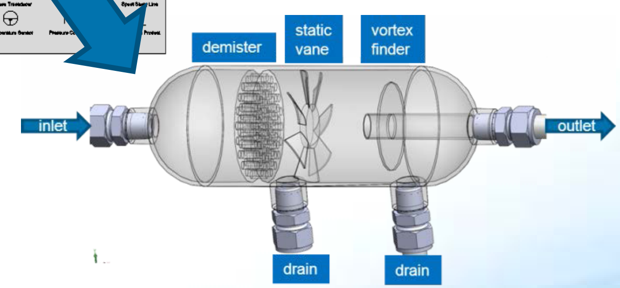




Ammonia & Borazine Scrubbers



Reactor



Gas/Liquid Separator

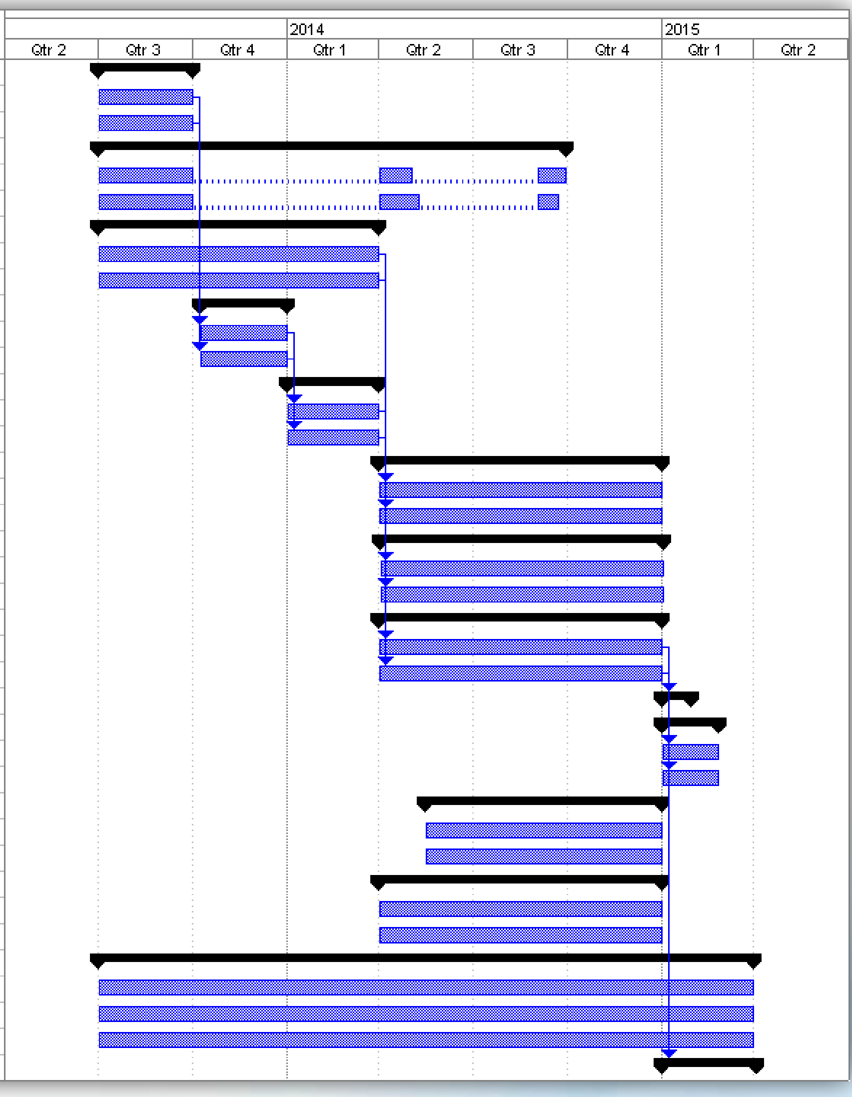
Phase 3 Approach

- Design subscale prototype systems
- Synthesize materials
- Complete test facilities
- Acquire BoP components
- Fabricate/assemble prototype system
- Evaluate prototype under static conditions assessing performance against targets
- Compare to and refine models
- Modify test apparatus/prototype
- Post updated models on WEB
- Decommission prototypes as necessary
- Write Final Report

Future Work

Phase 3 Gantt Chart

WBS	Task Name	Resource Names	Duration	Start	Finish
3.1	**Design subscale prototype systems**		**66 days**	**Mon 7/1/13**	**Mon 9/30/13**
3.1.1	Adsorbent	SRNL/OSU	66 days	Mon 7/1/13	Mon 9/30/13
3.1.2	Chemical	LANL/PNNL	66 days	Mon 7/1/13	Mon 9/30/13
3.2	**Synthesize/Modify Materials**		**326 days**	**Mon 7/1/13**	**Mon 9/29/14**
3.2.1	Adsorbent	FMC	111 days	Mon 7/1/13	Mon 9/29/14
3.2.2	Chemical	PNNL	111 days	Mon 7/1/13	Mon 9/22/14
3.3	**Complete test facilities**		**196 days**	**Mon 7/1/13**	**Mon 3/31/14**
3.3.1	Adsorbent	UQTR/OSU	196 days	Mon 7/1/13	Mon 3/31/14
3.3.2	Chemical	lanl	196 days	Mon 7/1/13	Mon 3/31/14
3.4	**Acquire BoP/System Components**		**60 days**	**Wed 10/9/13**	**Tue 12/31/13**
3.4.1	Adsorbent	UQTR/OSU/LC	60 days	Wed 10/9/13	Tue 12/31/13
3.4.2	Chemical	LANL/UTRC	60 days	Wed 10/9/13	Tue 12/31/13
3.5	**Fabricate/assemble prototype system**		**64 days**	**Wed 1/1/14**	**Mon 3/31/14**
3.5.1	Adsorbent	UQTR/OSU	64 days	Wed 1/1/14	Mon 3/31/14
3.5.2	Chemical	LANL/UTRC	64 days	Wed 1/1/14	Mon 3/31/14
3.6	**Evaluate prototype & assess performance**		**197 days**	**Tue 4/1/14**	**Wed 12/31/14**
3.6.1	Adsorbent	UQTR/OSU	197 days	Tue 4/1/14	Wed 12/31/14
3.6.2	Chemical	lanl	197 days	Tue 4/1/14	Wed 12/31/14
3.7	**Compare to and refine models**		**197 days**	**Wed 4/2/14**	**Thu 1/1/15**
3.7.1	Adsorbent	SRNL/OSU	197 days	Wed 4/2/14	Thu 1/1/15
3.7.2	Chemical	PNNL	197 days	Wed 4/2/14	Thu 1/1/15
3.8	**Modify test apparatus/prototype**		**197 days**	**Tue 4/1/14**	**Wed 12/31/14**
3.8.1	Adsorbent	SRNL/UQTR/OSU	197 days	Tue 4/1/14	Wed 12/31/14
3.8.2	Chemical	lanl	197 days	Tue 4/1/14	Wed 12/31/14
3.9	**Post updated models on WEB**	SRNL/UTRC/PNNL/NREL	20 days	Thu 1/1/15	Wed 1/28/15
3.10	**Decommission prototypes as necessary**		**40 days**	**Thu 1/1/15**	**Wed 2/25/15**
3.10.1	Adsorbent	UQTR/OSU	40 days	Thu 1/1/15	Wed 2/25/15
3.10.2	Chemical	lanl	40 days	Thu 1/1/15	Wed 2/25/15
3.11	**Performance/Cost Model Updates**		**164 days?**	**Fri 5/16/14**	**Wed 12/31/14**
3.11.1	Adsorbent	NREL,PNNL,UTRC,FMC	164 days?	Fri 5/16/14	Wed 12/31/14
3.11.2	Chemical	NREL,PNNL,FMC,UTRC	164 days?	Fri 5/16/14	Wed 12/31/14
3.12	**Maaterials' Requirements Refinement**		**198 days?**	**Mon 3/31/14**	**Wed 12/31/14**
3.12.1	Adsorbent	FMC/SRNL	198 days?	Mon 3/31/14	Wed 12/31/14
3.12.2	Chemical	LANL/PNNL	198 days?	Mon 3/31/14	Wed 12/31/14
3.13	**Project Management**		**457 days**	**Mon 7/1/13**	**Tue 3/31/15**
3.13.1	Center	SRNL	457 days	Mon 7/1/13	Tue 3/31/15
3.13.2	Adsorbent	UM	457 days	Mon 7/1/13	Tue 3/31/15
3.13.3	Chemical	lanl	457 days	Mon 7/1/13	Tue 3/31/15
3.14	**Write Final Report**	All	66 days	Thu 1/1/15	Thu 4/2/15



Phase 3 Gantt Chart

SMART Milestones Being Developed for Each Contribution in Resources

WBS	Task Name	Resource Names	Duration	Start	Finish
3.1	**Design subscale prototype systems**		**66 days**	**Mon 7/1/13**	**Mon 9/30/13**
3.1.1	Adsorbent	SR			
3.1.2	Chemical	LA			
3.2	**Synthesize/Modify Materials**				
3.2.1	Adsorbent				
3.2.2	Chemical				
3.3	**Complete test facilities**		**196 d**	**Mon 7/1/13**	**Mon 3/31/14**
3.3.1	Adsorbent	UQTR/OSU	196 d	Mon 7/1/13	Mon 3/31/14
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3.4.1	Adsorbent	UQTR/OSU/LC	60 days	Wed 10/9/13	Tue 12/31/13
3.4.2	Chemical	LANL/UTRC	60 days	Wed 10/9/13	Tue 12/31/13
3.5	**Fabricate/assemble prototype system**		**64 days**	**Wed 1/1/14**	**Mon 3/31/14**
3.5.1	Adsorbent	UQTR/OSU	64 days	Wed 1/1/14	Mon 3/31/14
3.5.2	Chemical	LANL/UTRC	64 days	Wed 1/1/14	Mon 3/31/14
3.6	**Evaluate prototype & assess performance**		**197 days**	**Tue 4/1/14**	**Wed 12/31/14**
3.6.1	Adsorbent	UQTR/OSU	197 days	Tue 4/1/14	Wed 12/31/14
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3.7.2	Chemical	PNNL	197 days	Wed 4/2/14	Thu 1/1/15
3.8	**Modify test apparatus/prototype**		**197 days**	**Tue 4/1/14**	**Wed 12/31/14**
3.8.1	Adsorbent	SRNL/UQTR/OSU	197 days	Tue 4/1/14	Wed 12/31/14
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3.9	**Post updated models on WEB**	SRNL/UTRC/PNNL/NREL	20 days	Thu 1/1/15	Wed 1/28/15
3.10	**Decommission prototypes as necessary**		**40 days**	**Thu 1/1/15**	**Wed 2/25/15**
3.10.1	Adsorbent	UQTR/OSU	40 days	Thu 1/1/15	Wed 2/25/15
3.10.2	Chemical	lanl	40 days	Thu 1/1/15	Wed 2/25/15
3.11	**Performance/Cost Model Updates**		**164 days?**	**Fri 5/16/14**	**Wed 12/31/14**
3.11.1	Adsorbent	NREL,PNNL,UTRC,FMC	164 days?	Fri 5/16/14	Wed 12/31/14
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3.12.2	Chemical	LANL/PNNL	198 days?	Mon 3/31/14	Wed 12/31/14
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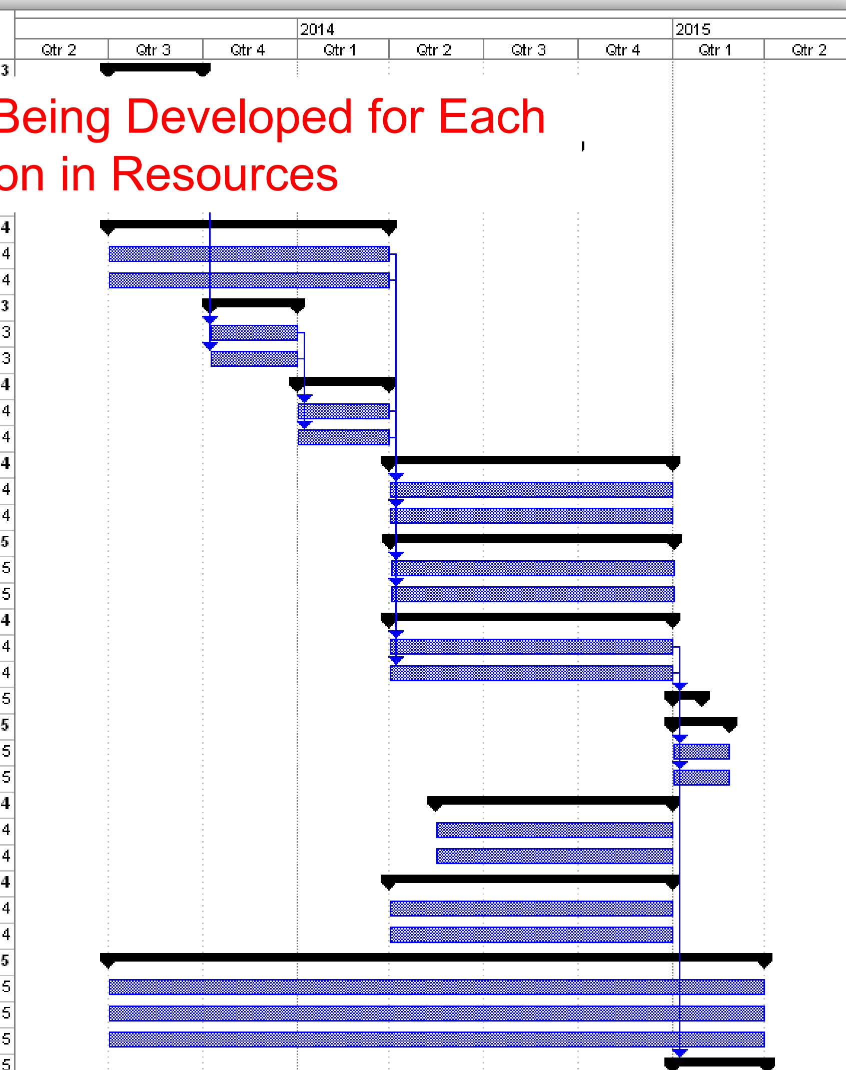
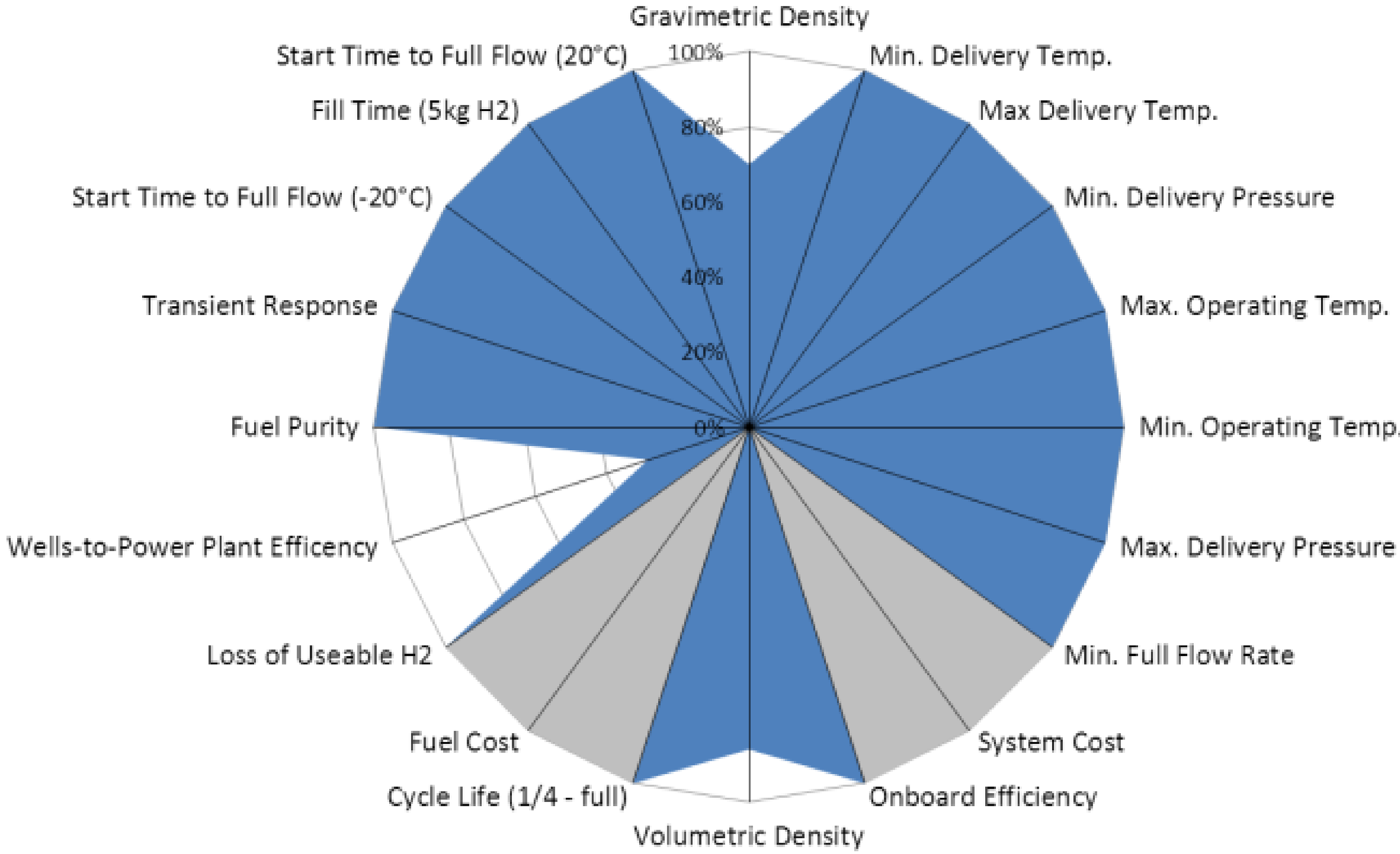
3.13.3	Chemical	lanl	457 days	Mon 7/1/13	Tue 3/31/15
3.14	**Write Final Report**	All	66 days	Thu 1/1/15	Thu 4/2/15



Preliminary vs. Demonstrated Spider Chart

Why Phase 3 demonstration is critical in model validation

Chemical Hydrogen Storage System (2012)



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Preliminary vs. Demonstrated Spider Chart

Why Phase 3 demonstration is critical in model validation

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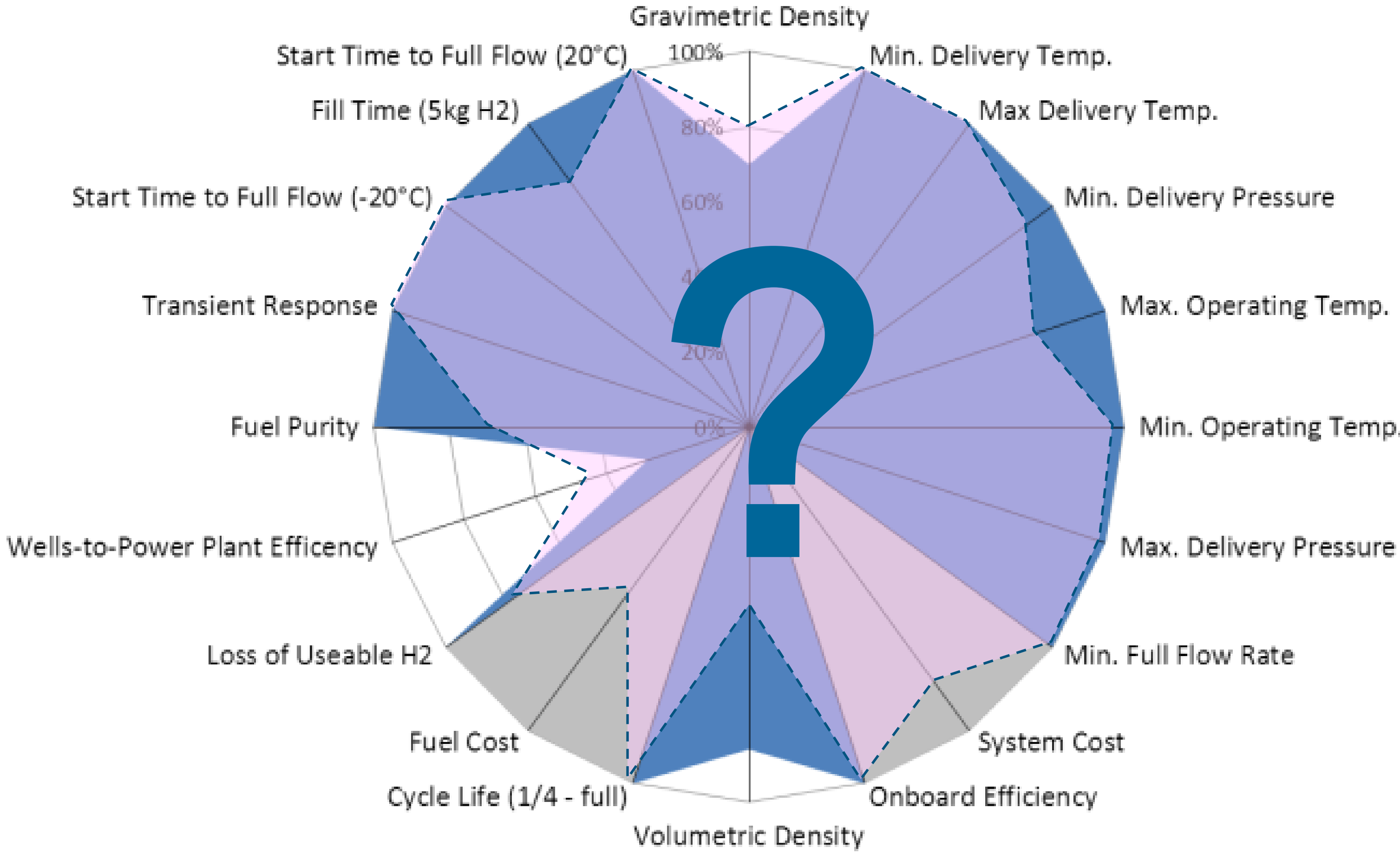
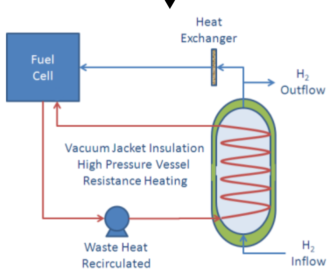


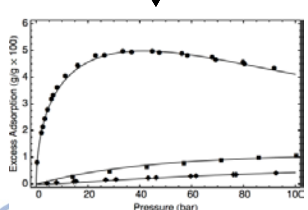
Technology Readiness Levels

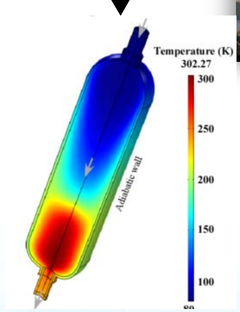
Materials Based Hydrogen Storage Systems for Automotive Applications

Materials CoEs — **HSECoE**

TRL 1	TRL 2	TRL 3	TRL 4	TRL 5	TRL 6	TRL 7	TRL 8	TRL 9
Basic Technology Research		Research to Prove Feasibility	Technology Development		Technology Demonstration	System Commissioning		System Operation
Basic Principals	Concept Formulation	Characteristic Proof of Concept	System Validation in Laboratory Environment	System Validation in Relevant Environment	Pilot Scale System Validation	Full Scale System Validation	Actual System Qualification	Actual System Operation







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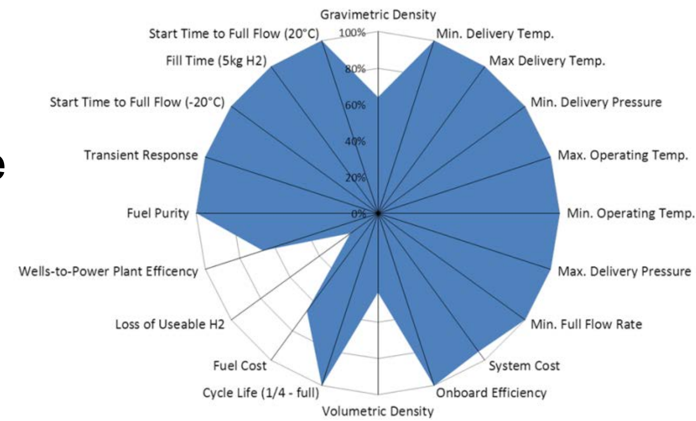
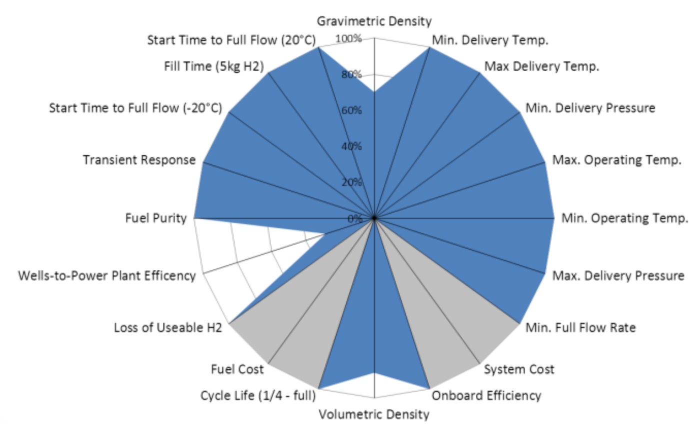
Summary

- **Adsorption Systems**
  - Limited in volumetric density and dormancy at ~77K due to materials
  - Temperature assisted PSA using a Type I tank at 60 bar is proposed for subscale prototype demonstration.
- **Chemical Systems**
  - Limited in gravimetric density and efficiency due to materials.
  - Liquid/Slurry flow through reactors with GLS and purification is proposed for subscale prototype demonstration.
- **Phase 3 Go/NoGo meetings held with DoE with results forthcoming.**

Adsorbent System



Chemical System



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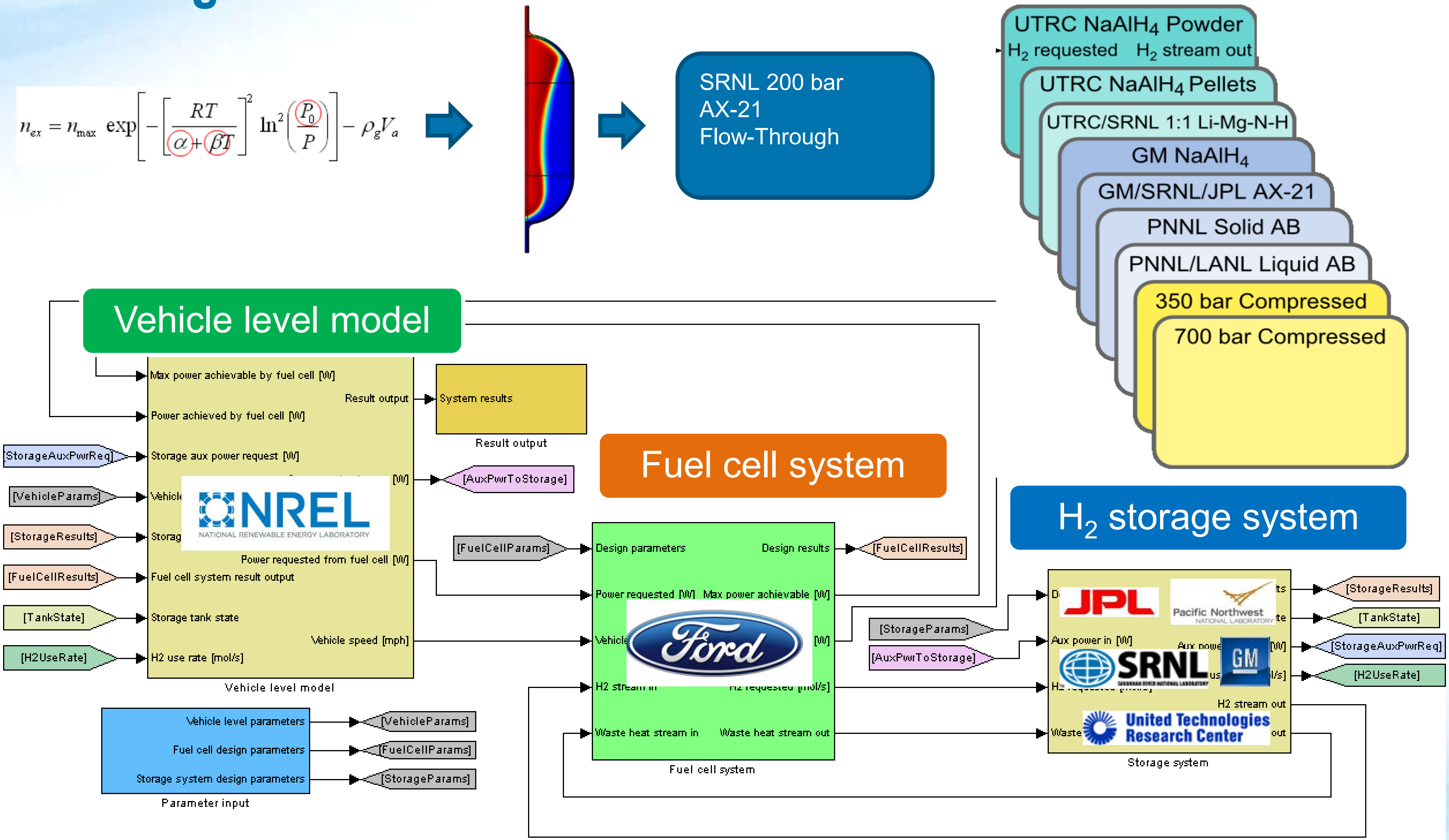
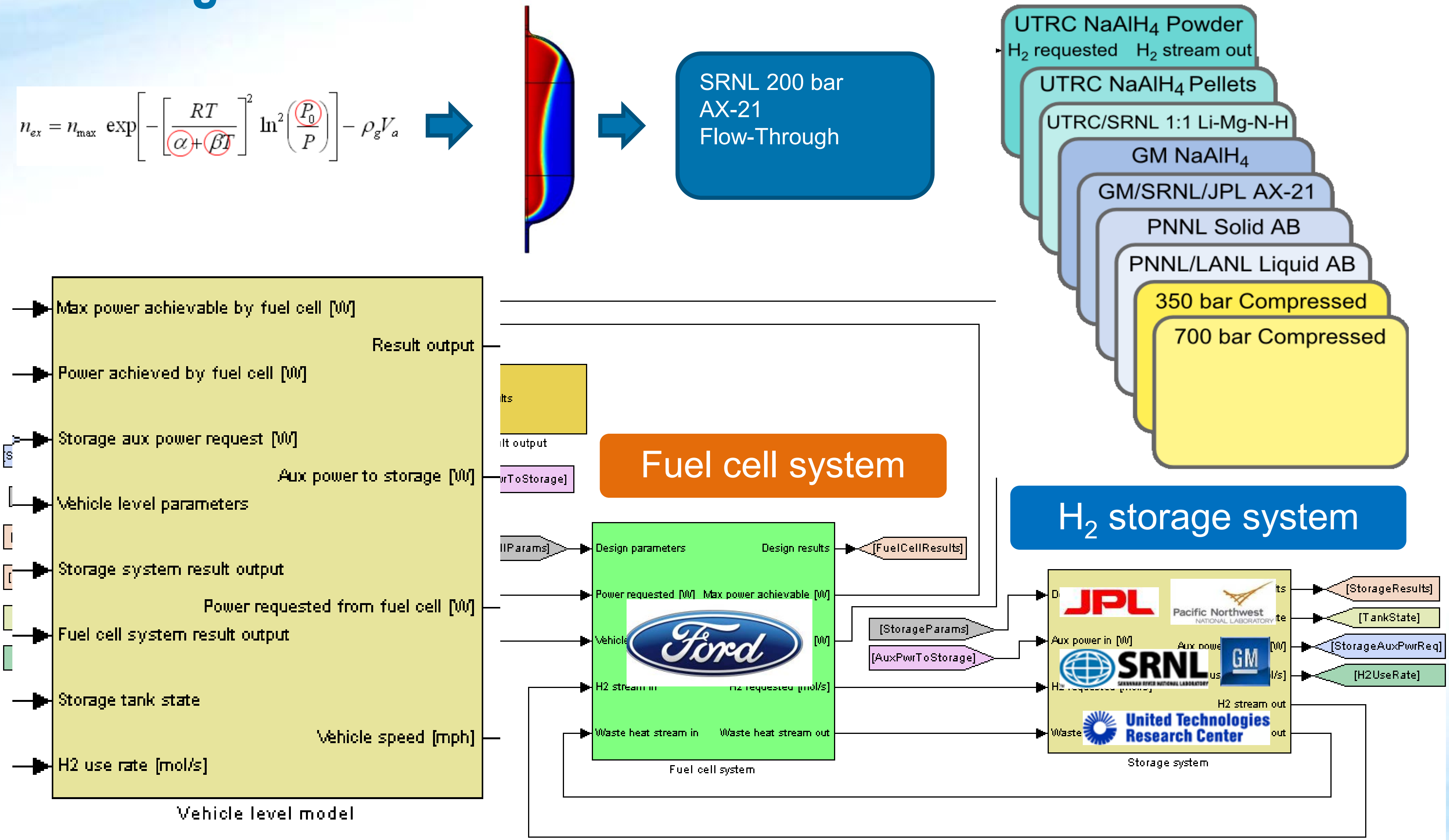
Technical Back-Up Slides

Integrated Model Framework

$$n_{ex} = n_{max} \exp\left[-\left[\frac{RT}{\alpha+\beta T}\right]^2 \ln^2\left(\frac{P_0}{P}\right)\right] - \rho_g V_a$$



Integrated Model Framework



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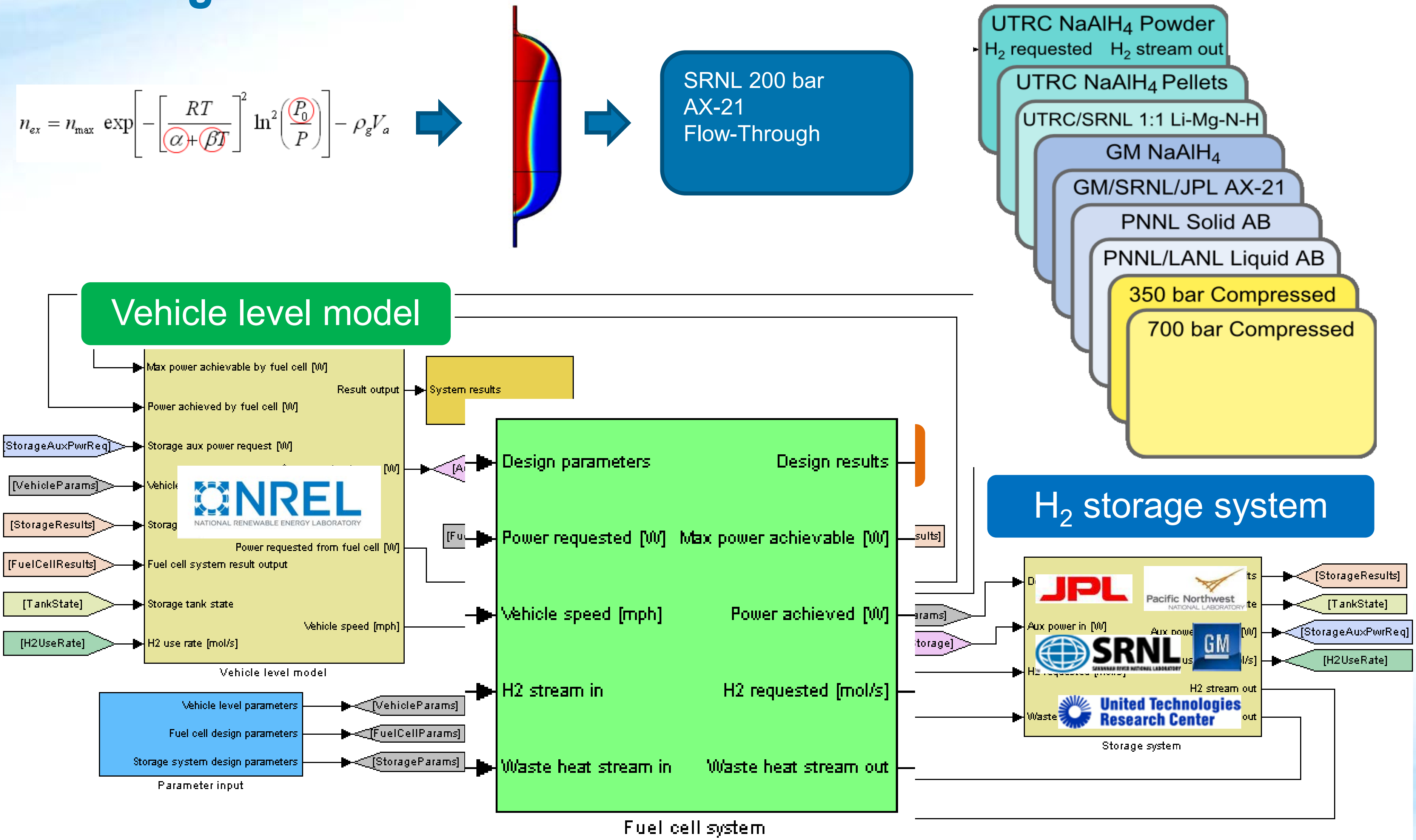
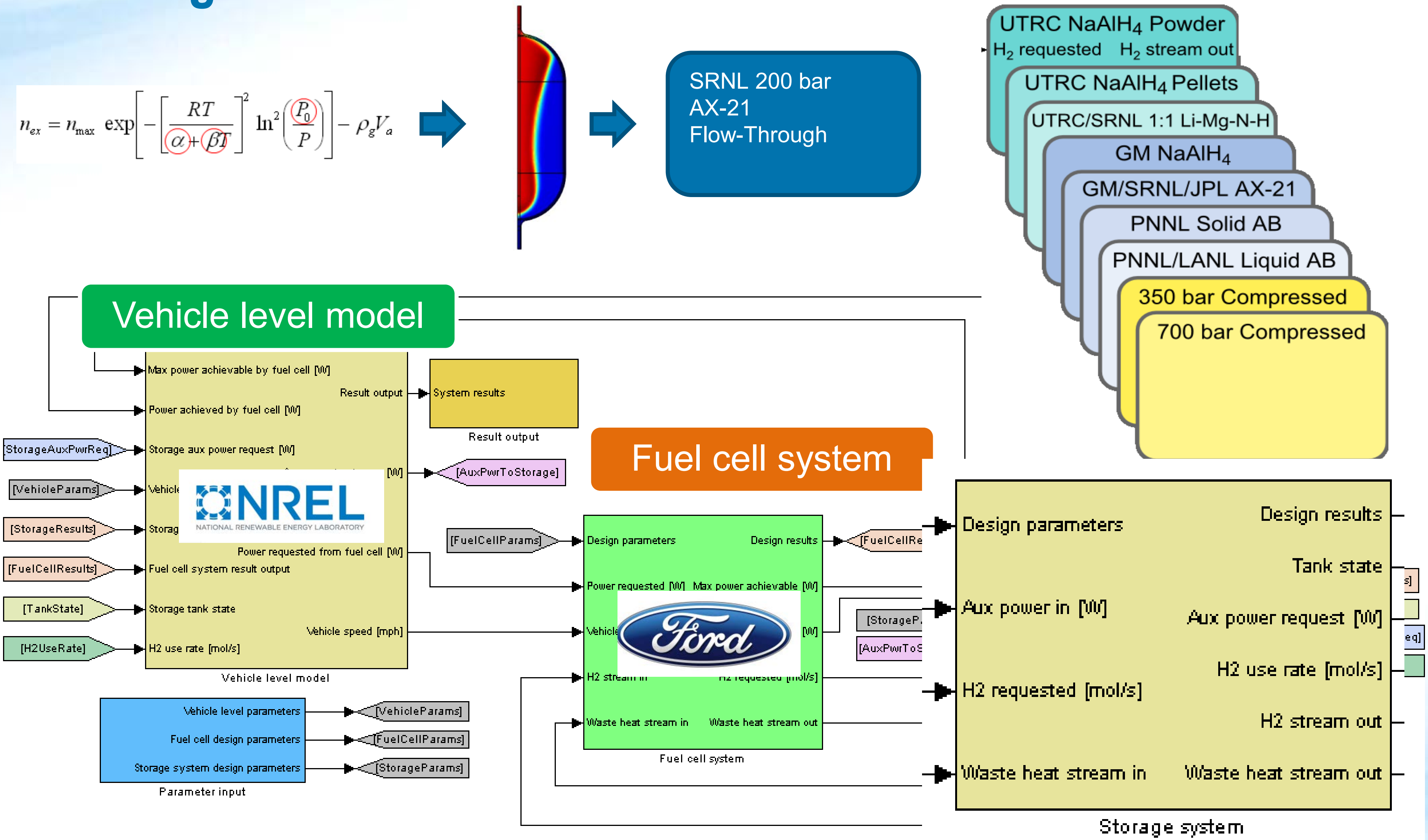
Integrated Model Framework



Integrated Model Framework

$$n_{ex} = n_{max} \exp\left[-\left[\frac{RT}{\alpha+\beta T}\right]^2 \ln^2\left(\frac{P_0}{P}\right)\right] - \rho_g V_a$$



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Integrated Model Framework