



# Hydrogen Storage Engineering

## CENTER OF EXCELLENCE

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Director

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**Savannah River National Laboratory**

June 18, 2014



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

*Project ID#  
ST004*

SRNL-STI-2014-00176

# Overview

## Timeline

- **Start: February 1, 2009**
- **End: June 30, 2015**
- **90% Complete (as of 3/1/14)**

## Budget

- **Total Center Funding:**
  - DOE Share: \$ 35,275,000
  - Cost Share: \$ 3,322,000
  - FY '13 Funding: \$ 6,059,000
  - FY '14 Funding: \$3,138,000
- **Prog. Mgmt. Funding**
  - FY '13: \$ 300,000
  - FY '14: \$ 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



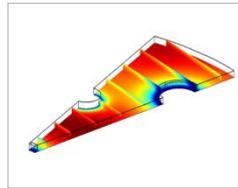
## HSECoE Technical Objectives

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  
through the integrated model  
identifying materials requirements



Materials → Thermal Management → H<sub>2</sub> Storage BoP → Fuel Cell → Vehicle → Wheels



Engineered  
Materials  
Properties

Heat Transfer  
Designs

BoP  
Component  
Requirements

What is Needed  
of the Hydrogen Storage  
Media & System

# HSECoE Organization

DoE Program Management  
N. Stetson  
J. Adams  
R. Bowman

## Center Coordinating Council

D. Anton, Center Director  
T. Motyka, Assistant Director

### OEMs

M. Cai, GM  
M. Veenstra, Ford

### Technology Area Leads

*Performance Cost & Energy Analysis*  
M. Thornton

*Materials Operating Requirements*  
E. Rönnebro

*Transport Phenomena*  
B. Hardy

*Integrated Storage System/Power Plant Modeling*  
B. van Hassel

*Enabling Technologies*  
K. Simmons

*Subscale Prototype Construction, Testing, & Evaluation*  
T. Semelsberger

### System Architects

*MH System*  
T. Motyka

*CH System*  
T. Semelsberger

*A System*  
D. Siegel

### DOE Program Liaisons

*Independent Projects*  
T. Motyka

*Hydrogen Safety*  
J. Khalil

*External Communications*  
T. Motyka

Intellectual Property Management Committee

Safety Review Committee

# Technical Matrix

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



# Internal Communications



**Annual F2F meetings (Sept.-Oct.)**

**AMR Pre-Meeting (May-June)**

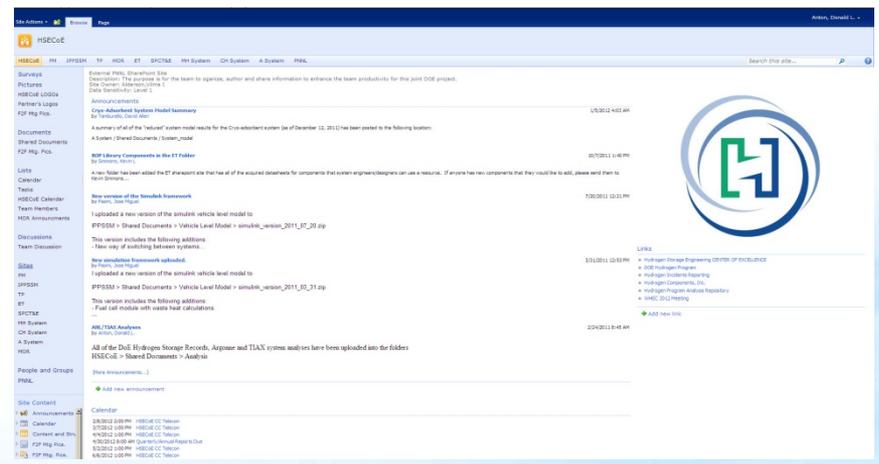
**Tech Team Review F2F Meeting (Feb.-March)**

**Monthly System Architect Telecoms**

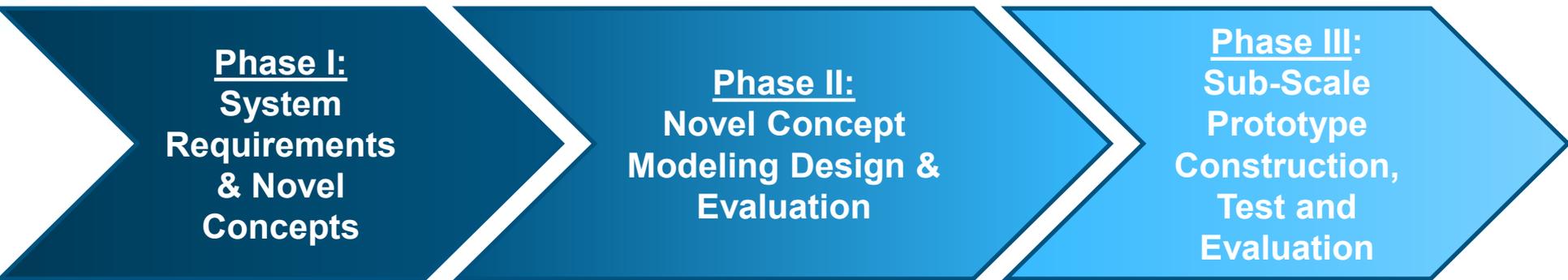
**Monthly Coordinating Council Telecoms**

**Semi-monthly technical team telecoms**

**SharePoint Site used extensively to share documents and data**



# Phased Approach



• **Where were 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?**

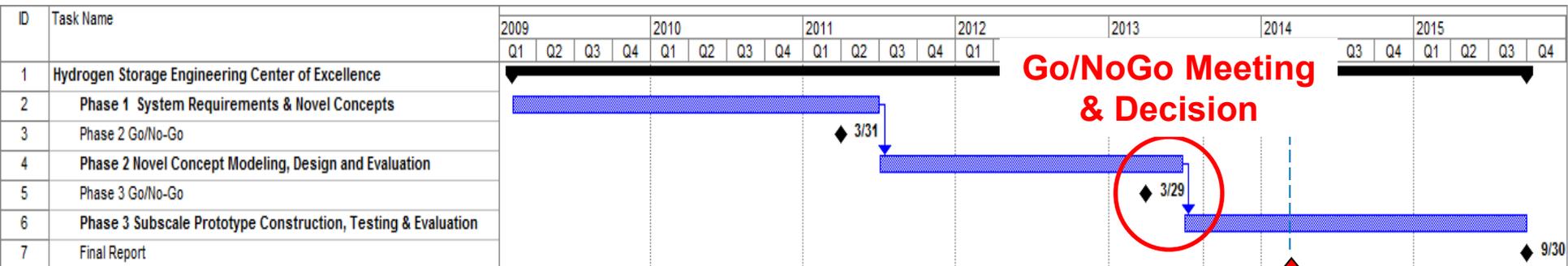
- Novel Concepts
- Concept Validation
- Integration Testing
- System Design

• **Put it all together and confirm claims.**

- System Integration
- System Assessments
- Model Validation
- Gap Analysis
- Performance Projections

# Important Dates

- Duration: 6.7 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, 2015**



**Go/NoGo Meeting & Decision**

**Here we are today.**

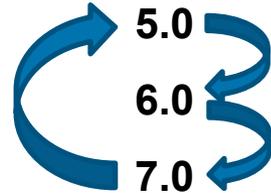
## Phase 3 Go/NoGo Review Held

- **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*

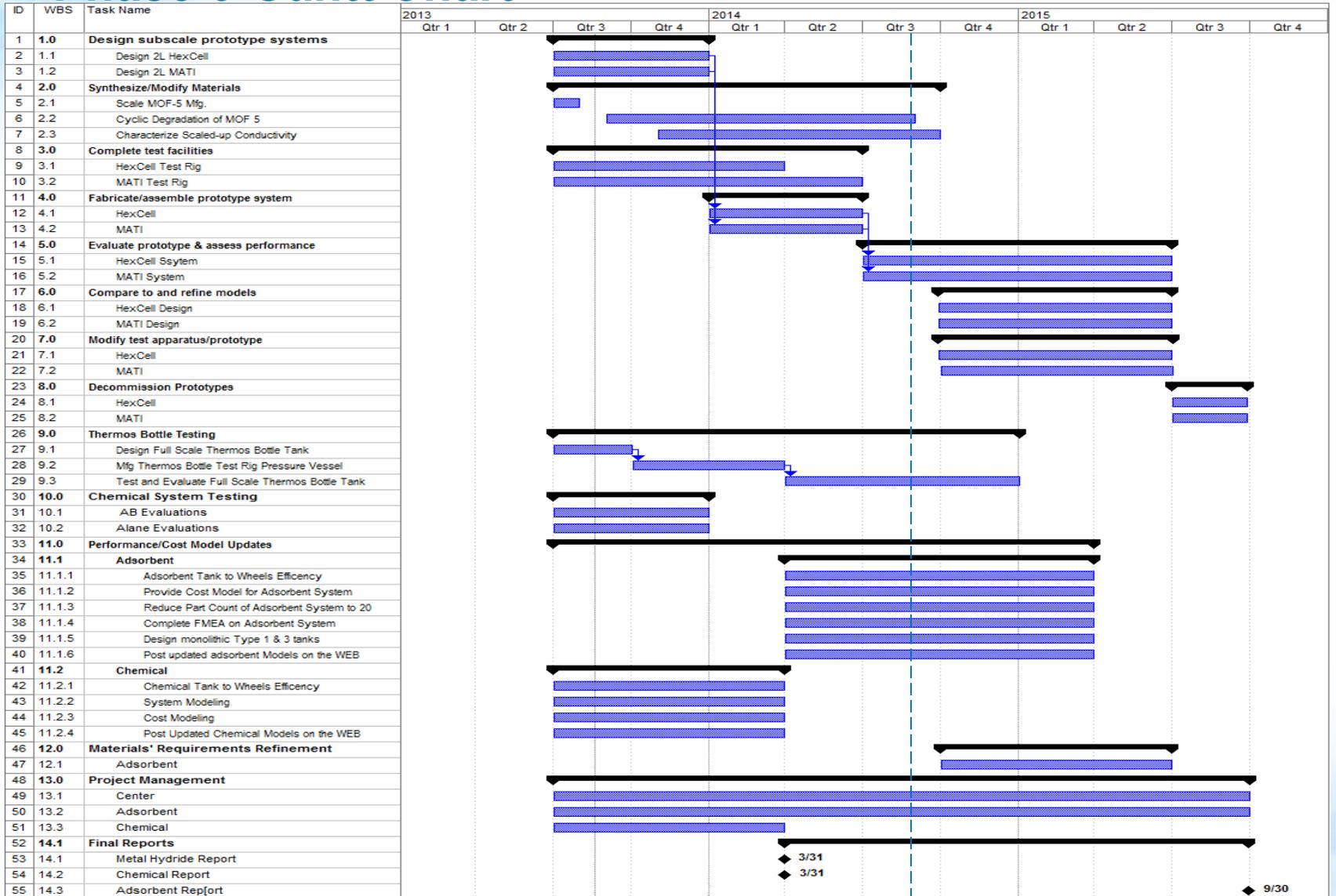
## Phase 3 Go/NoGo Decisions

- ✓ **Complete a Unified Comprehensive Report of Metal Hydride System Efforts.**
- ✓ **Draw Down Chemical System Work to Systematic Conclusion**
  - **Complete a Unified Comprehensive Report on Chemical System Efforts.**
  - **Continue Phase 3 Demonstration Efforts of HexCell Adsorbent System to Validate Models**
  - **Continue Phase 3 Demonstration Efforts of MATI Adsorbent System to Validate Models**
  - **Complete a Unified Comprehensive Report of Adsorbent System Efforts.**
  - **Make Models Generally Available to the Public**

## Phase 3 Task Structure

- 1.0 Design subscale prototype systems
  - 2.0 Synthesize/modify materials
  - 3.0 Complete test facilities
  - 4.0 Fabricate/assemble prototype system
  - 5.0 Evaluate prototype & assess performance
  - 6.0 Compare to and refine models
  - 7.0 Modify test apparatus/prototype
  - 8.0 Decommission prototypes
  - 9.0 Thermos bottle testing
  - 10.0 Chemical system completion
  - 11.0 Performance/cost model updates
  - 12.0 Materials' requirements refinement
  - 13.0 Project management
  - 14.0 Final Reports
- 

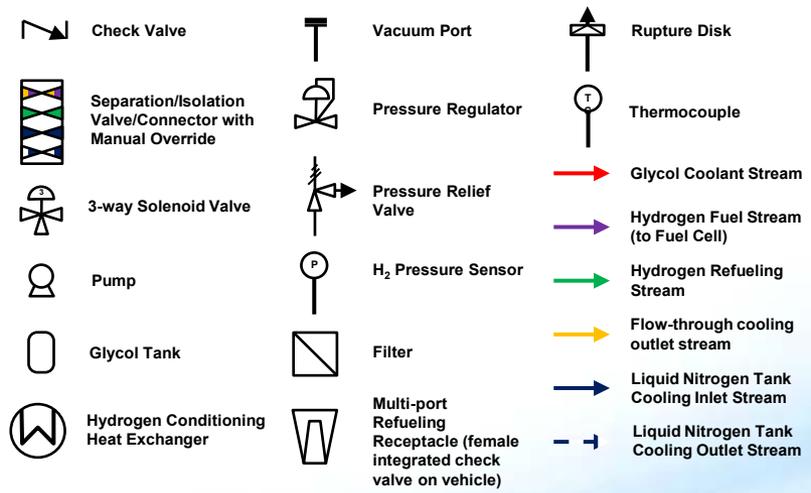
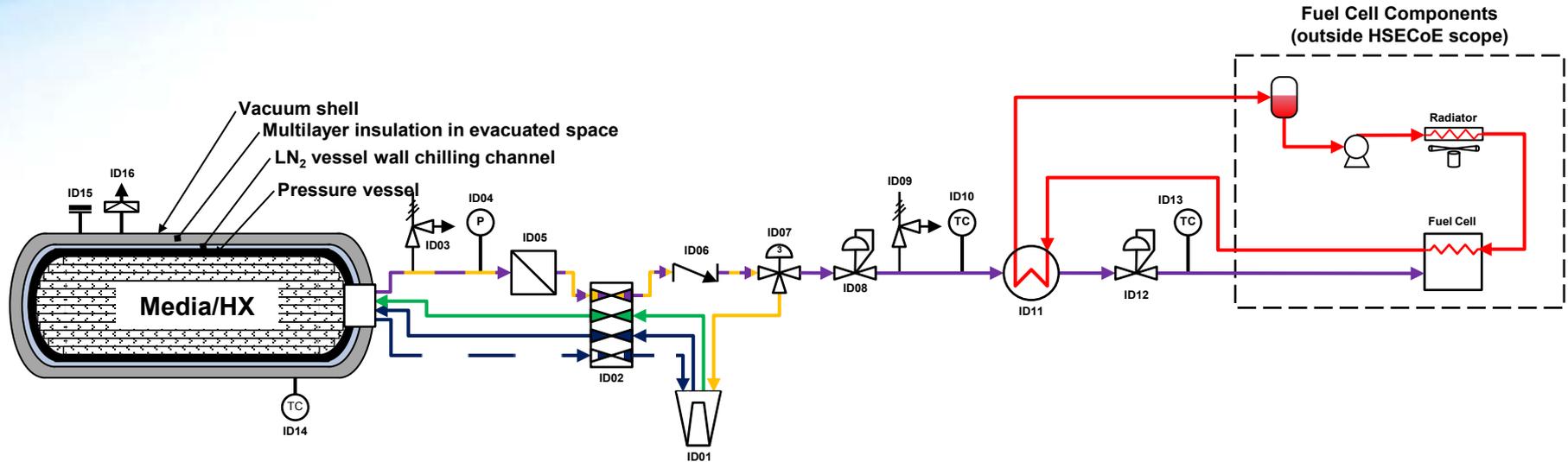
# Phase 3 Gantt Chart



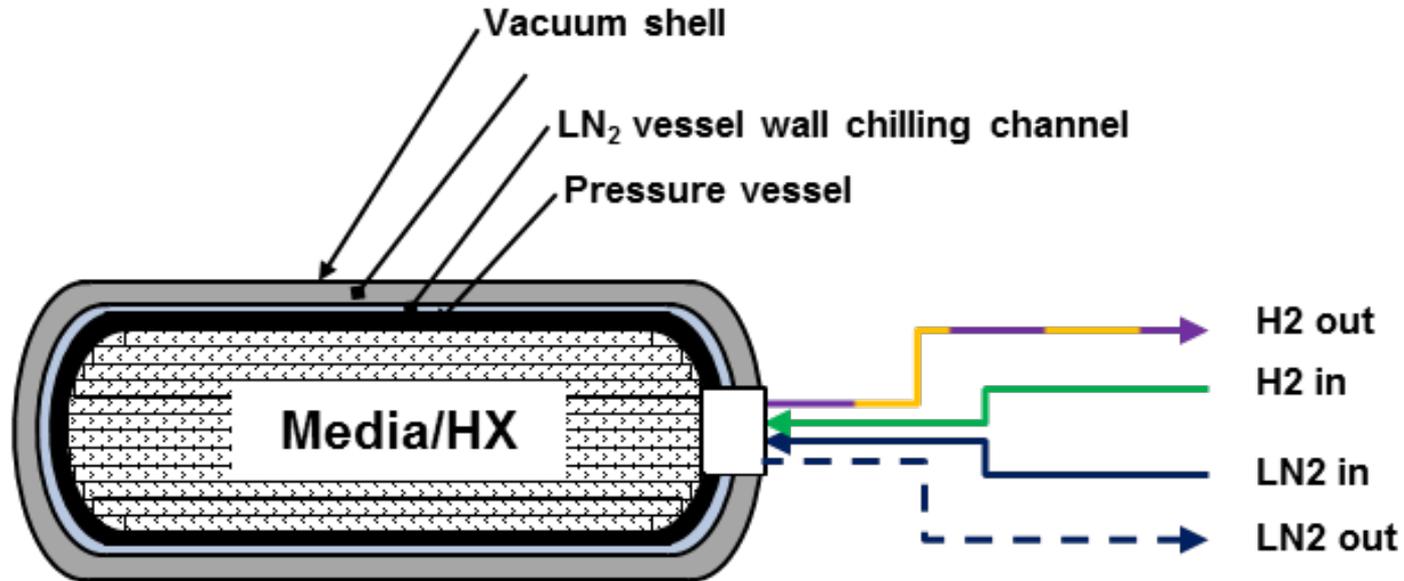
◆ 3/31  
◆ 3/31

◆ 9/30

# Adsorbent System Overview



# Adsorbent System Overview



# Adsorbent System

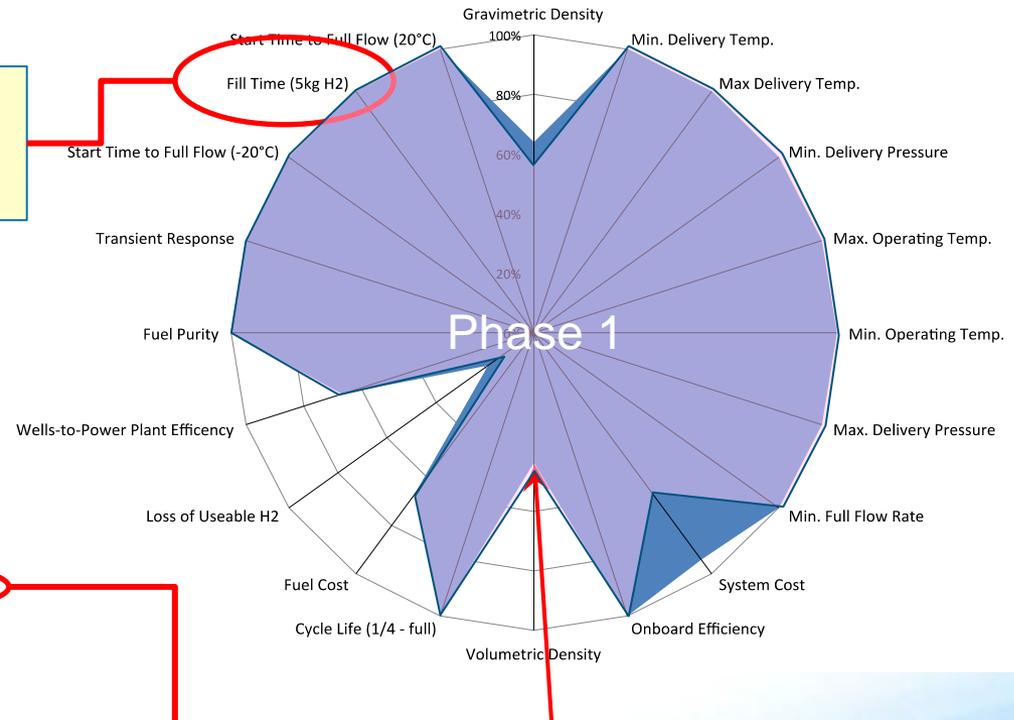
Media: MOF-5

P: 5-60 bar – Type I AI Pressure Vessel

T: 80-160K - MLVI

## HexCell Heat Exchanger

Fill time targets achieved due to advanced heat exchanger designs



Further work needed to approach volumetric target

### Technical Hurdles

Gravimetric Capacity – BoP Mass

System Cost – BoP cost

Volumetric Capacity – Media Density

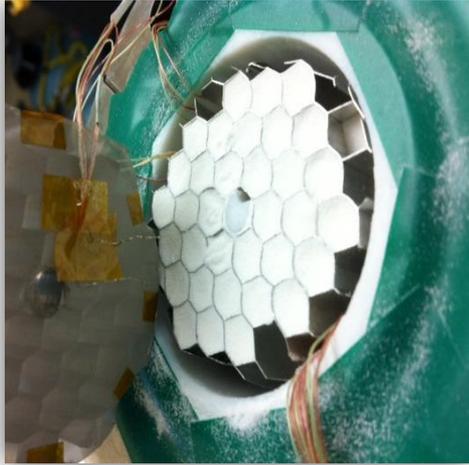
Fuel Cost – LN2 Chilled H<sub>2</sub>

Loss of Useable H<sub>2</sub> - Insulation

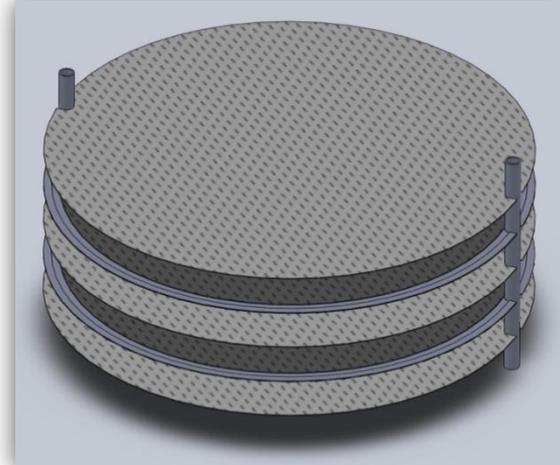
Well to Power Plant Efficiency – LN2 chilled H<sub>2</sub>

# Adsorbent Heat Exchanger Types

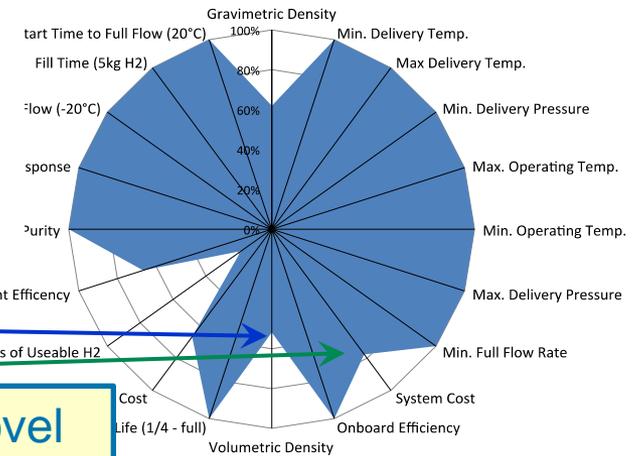
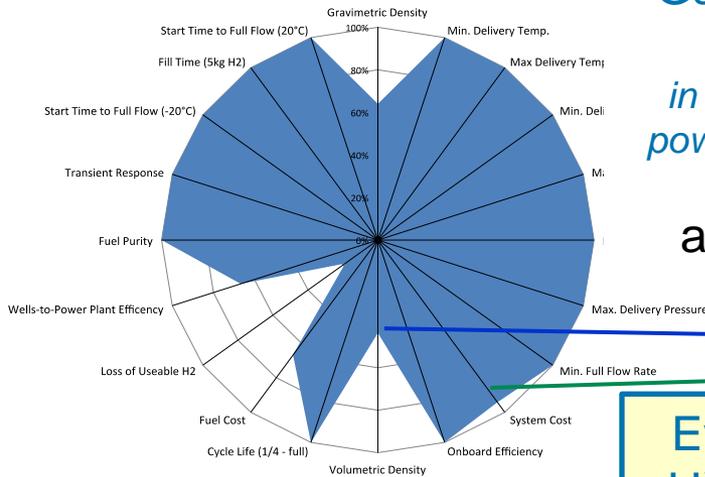
## HexCell



## MATI



Gain Volumetric Density  
in going from loose powder to compacted pucks  
at expense of Cost



Evaluation of Novel HX Design to Prove Efficacy & Utility

# HSECoE Adsorbent System

## S\*M\*A\*R\*T Milestones

Adsorbent System						
Component	Partner	Proposed SMART Milestones	Due Date	Modified Date	Status	Reason
Adsorbent Media	Ford/UM/BASF	Conduct a scale-up of the MOF-5 manufacturing process to deliver >9 kg of material while maintaining performance, as measured by surface area and particle size, to within 10% of lab-scale procedure.	12/31/2015			Adsorbent Media
Adsorbent Media	Ford/UM/BASF	Evaluate MOF-5 degradation beyond 300 cycles based on maximum allowable impurity levels as stated in SAE J2719 and report on the ability to mitigate to less than 10%.	9/30/2015			
Adsorbent Media	LANL	Perform a minimum of 10 heat capacity or thermal conductivity measurements at temperatures ranging from 70-200K on compacted MOF-5 samples prepared by Ford and to support validating system models and system level designs.	9/30/2015			
MATI HX	OSU	Design a 2L adsorbent subscale prototype utilizing a MATI thermal management system having 54 g available hydrogen, internal densities of 0.10g/g gravimetric, and 27g/L volumetric.	12/31/2015			MATI System
MATI Prototype	SRNL	Design and construct a hydrogen cryo-adsorbent test station capable of evaluating the performance of a two liter cryo-adsorbent prototype between 80-160K and which would meet all of the performance metrics for the DoE Technical Targets for On-Board Hydrogen Storage Systems.	9/30/2015			
MATI HX	OSU	Demonstrate performance of subscale system evaluations and model validation of a 2L adsorbent system utilizing a MATI thermal management system having 54 g available hydrogen, internal densities of 0.10g/g gravimetric, and 27 g/L volumetric.	6/30/2015			
MATI Prototype	SRNL	Demonstrate a two liter hydrogen adsorption system containing a MATI internal heat exchanger provided by Oregon State University characterizing its performance against each of the sixteen performance DoE Technical Targets for On-Board Hydrogen Storage Systems.	9/30/2015			HexCell System
HexCell HX	SRNL/UQTR	Design a 2L adsorbent subscale prototype utilizing a HexCell heat exchanger having 46g available hydrogen, internal densities of 0.13g/g gravimetric, and 23.4g/L volumetric.	12/31/2015			
HexCell Prototype	SRNL/UQTR	Demonstrate performance of subscale system evaluations and model validation of a 2L adsorbent system utilizing a HexCell heat exchanger having 46g available hydrogen, internal densities of 0.13g/g gravimetric, and 23.4g/L volumetric.	6/30/2015			
Pressure Vessel	Hexagon-Lincoln	<b>Design and manufacture a baseline, separable Type 1 tank</b> in accordance with size (2L - 6L), pressure (100 bar service pressure), operating temperatures (80K - 160K) and interfaces specified by HSECoE team members, and with a 10% reduction in weight per unit volume compared with the Type 1 tank tested in Phase 2.	12/31/13			Pressure Vessel
Pressure Vessel Cooling	PNNL / Hexagon-Lincoln	Evaluate the thermal-mechanical stresses in the thermos bottle concept during refueling considering a fatigue life of 1500 cycles. Identify any necessary design criteria to avoid failure of the pressure vessel under combined thermal-mechanical loading. Design a scale thermos bottle tank using LN2 cooling having a cooling rate capable of meeting the DoE technical targets for refueling from 160K to 77K in 4.2 mins and meet any necessary fatigue design criteria.	9/30/2014			
Pressure Vessel	Hexagon-Lincoln	Design alternate tank configurations, such as monolithic Type 1, Type 3 with suitable cryogenic liner, and Type 4 with suitable cryogenic liner, that can operate at 100 bar service pressure, at temperatures of 80K - 160K, and offer a further 10% reduction in weight compared with the Phase 3 baseline Type 1 tank, and are consistent with safety requirements established by industry for hydrogen fuel containers.	3/31/2015			
Pressure Vessel Cooling	PNNL/Hexagon-Lincoln	Hexagon-Lincoln will fabricate and PNNL will demonstrate a minimum one liter scale thermos bottle tank. With this device they will measure the transient heat loss for dormancy and demonstrate the LN2 thermos bottle tank cooling concept. This experiment will be scaled to the full size 5.6 kgH2 size and shown experimentally to meet the DoE technical targets for dormancy and refueling time.	6/30/2015			Particulate Filter
Particulate Filter	UTRC	<b>Demonstrate a particulate filter for a cryo-adsorbent bed passing less than 1mg/L and 10mm diameter (SAE J2719 guideline).</b>	3/31/2014			
System Modeling	NREL	Prepare a report on the impact of system design changes on the tank to wheels efficiency and document progress relative to a 300 mile range for adsorbent systems.	9/30/2014			System Modeling
System Modeling	NREL/SRNL/PNNL/Ford/UTRC	Update the cryo-adsorbent system model with Phase 3 performance data, integrate into the framework; document and release models to the public.	9/30/2014			
System Modeling	Ford/UM/BASF	Complete the failure mode and effects analysis (FMEA) associated with real-world operating conditions for a MOF-5-based system, for both HexCell and MATI concepts based on the Phase 3 test results. Report on the ability to reduce the risk priority numbers (RPN) from the phase 2 peak/mean and identify key failure modes.	6/30/2015			
System Modeling	GM	Attend Center F2F meetings and submit a letter memo indicating technical or programic areas the Center should be pursuing with more emphasis. Actively participate in Center Coordinating Council Telecons. Actively participate in testing and evaluation of models to be published on the WEB.	6/30/2015			

Complete
On Schedule
Behind Schedule

# Adsorbent Media Preparation



**Conduct a scale-up of the MOF-5 manufacturing process to deliver > 9 kg of material while maintaining performance, as measured by surface area and particle size, to within 10% of lab-scale procedure.**

**Evaluate MOF-5 degradation beyond 300 cycles based on maximum allowable impurity levels as stated in SAE J2719 and report on the ability to mitigate to less than 10%.**

**Perform a minimum of 10 heat capacity or thermal conductivity measurements at temperatures ranging from 70-200K on compacted MOF-5 samples prepared by Ford and to support validating system models and system level designs.**

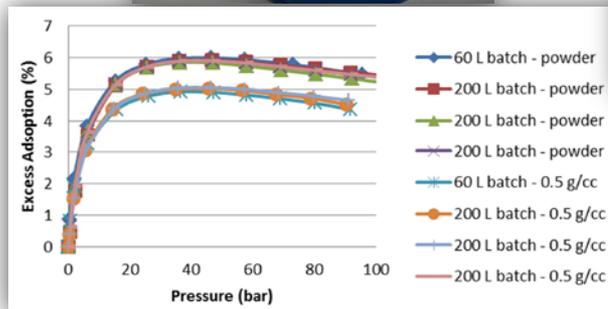
## 10 kg of MOF-5 Received and Characterized



## Hydrogen Impurity Concentrations Selected

	J2719 SPEC PPM	Airgas Research Grade Hydrogen	OPTION A Airgas Proposal PPM
Water <sup>a</sup>	5	.06 to .2	5 to 10 (H2)
Total Hydrocarbons <sup>b</sup> (C1 basis)	2	< .02 (MDL)	2 (H2)
Oxygen	5	.1 to .2	5 (H2)
Helium	300	< 50 (MDL)	500 (H2)
Nitrogen, Argon	100	.1 to 1	100 (H2)
Carbon dioxide	2	< .03 (MDL)	5 (H2)
Carbon monoxide	0.2	< .01 (MDL)	2 (H2)
Total sulfur <sup>c</sup>	0.004	< .02 (MDL)	0.25 (N)
Formaldehyde	0.01	< .1 (MDL)	not included
Formic acid	0.2	< .1 (MDL)	not included
Ammonia	0.1	< .05 (MDL)	2.5 (N)
Total halogenates <sup>d</sup>	0.05	< .05 (MDL)	1 (N)

## Cryogenic thermal conductivity apparatus upgraded for Powder Testing



## MATI Half-Pucks Fabricated



# MATI Heat Exchanger & Test Systems



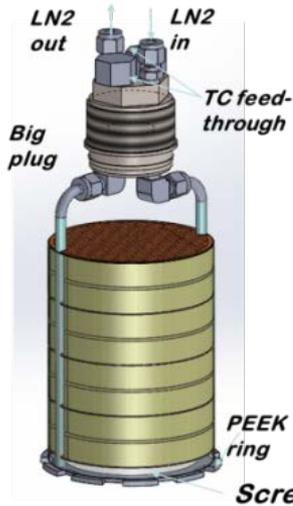
**Design a 2L adsorbent subscale prototype utilizing a MATI thermal management system** having 54 g available hydrogen, internal densities of 0.10g/g gravimetric, and 27g/L volumetric.

**Design and construct a hydrogen cryo-adsorbent test station** capable of evaluating the performance of a two liter cryo-adsorbent prototype between 80-160K and which would meet all of the performance metrics for the DoE Technical Targets for On-Board Hydrogen Storage Systems.

**Demonstrate performance of subscale system evaluations and model validation of a 2L adsorbent system utilizing a MATI thermal management system** having 54 g available hydrogen, internal densities of 0.10g/g gravimetric, and 27 g/L volumetric.

**Demonstrate a two liter hydrogen adsorption system containing a MATI internal heat exchanger** provided by Oregon State University characterizing its performance against each of the sixteen performance DoE Technical Targets for On-Board Hydrogen Storage Systems.

## MATI System Design Completed



*MATI connected to the Plug*

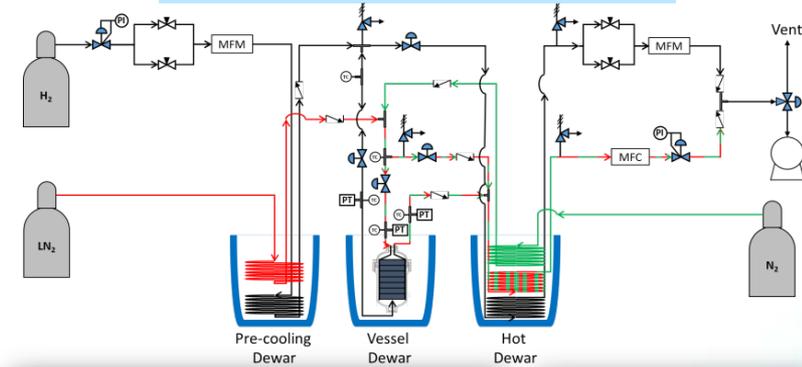


*Dome threaded onto the Plug*



*Housing attached to the dome*

## MATI Test Station Design

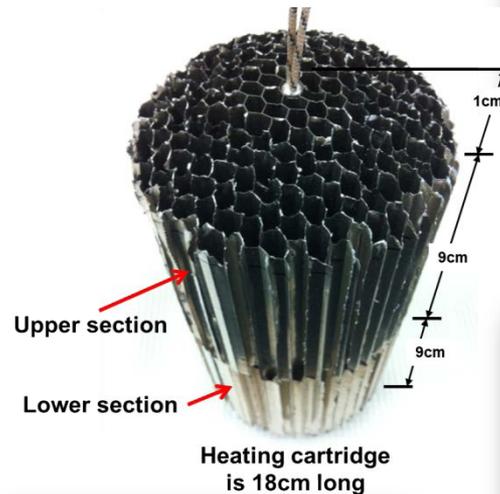
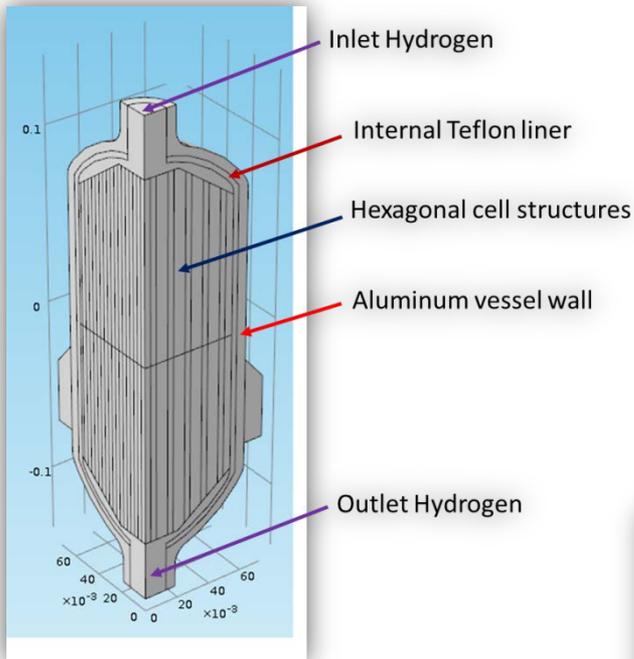


# HexCell Heat Exchanger & Test System

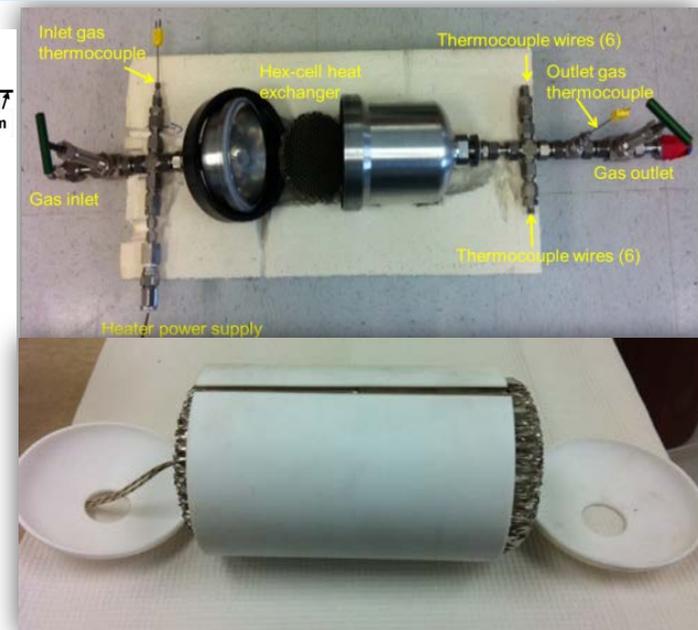
**Design a 2L adsorbent subscale prototype utilizing a HexCell heat exchanger having 46g available hydrogen, internal densities of 0.13g/g gravimetric, and 23.4g/L volumetric.**

**Demonstrate performance of subscale system evaluations and model validation of a 2L adsorbent system utilizing a HexCell heat exchanger having 46g available hydrogen, internal densities of 0.13g/g gravimetric, and 23.4g/L volumetric.**

## HexCell 2L System Design



## HexCell 2L System Assembly



## HexCell 2L Test System

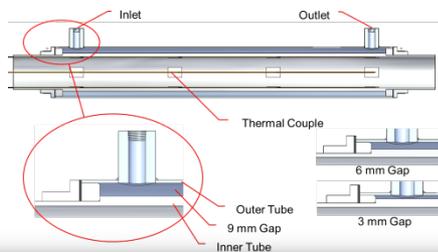
## Pressure Vessel Demonstration

**Evaluate the thermal-mechanical stresses in the thermos bottle concept** during refueling considering a fatigue life of 1500 cycles. Identify any necessary design criteria to avoid failure of the pressure vessel under combined thermal-mechanical loading. Design a scale thermos bottle tank using LN<sub>2</sub> cooling having a cooling rate capable of meeting the DoE technical targets for refueling from 160K to 77K in 4.2 mins and meet any necessary fatigue design criteria.

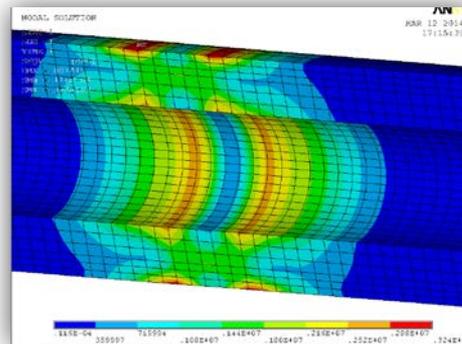
**Design alternate tank configurations, such as monolithic Type 1, Type 3 with suitable cryogenic liner, and Type 4 with suitable cryogenic liner,** that can operate at 100 bar service pressure, at temperatures of 80K – 160K, and offer a further 10% reduction in weight compared with the Phase 3 baseline Type 1 tank, and are consistent with safety requirements established by industry for hydrogen fuel containers.

**Hexagon-Lincoln will fabricate and PNNL will demonstrate a minimum one liter scale thermos bottle tank.** With this device they will measure the transient heat loss for dormancy and demonstrate the LN<sub>2</sub> thermos bottle tank cooling concept. This experiment will be scaled to the full size 5.6 kgH<sub>2</sub> size and shown experimentally to meet the DoE technical targets for dormancy and refueling time.

### Tank Cooling Design and Test Apparatus

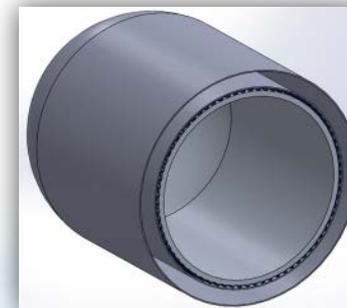
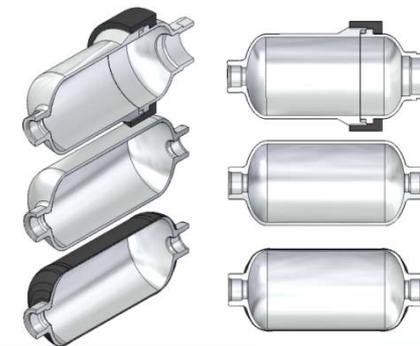


### Thermal and Fatigue Stress Calculated



Peak thermal stress is 3.2 MPa (von Mises). Fatigue strength of 100 MPa is required for 5000 cycle life.

### Alternate Tank Configurations

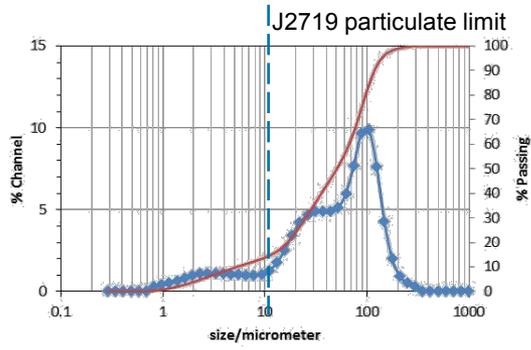


Thermos®  
Bottle Tank  
Design

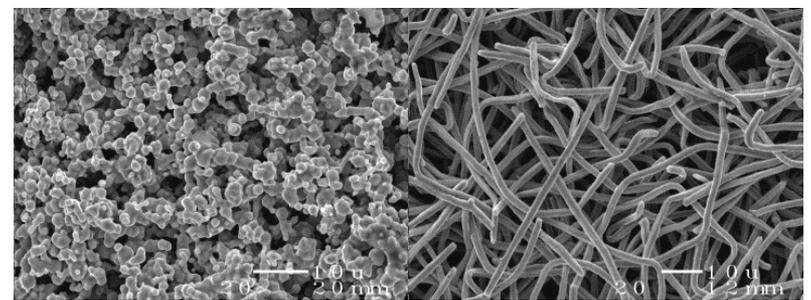
# Particle Filter Demonstration

Demonstrate a particulate filter for a cryo-adsorbent bed passing less than 1mg/L and 10mm diameter (SAE J2719 guideline).

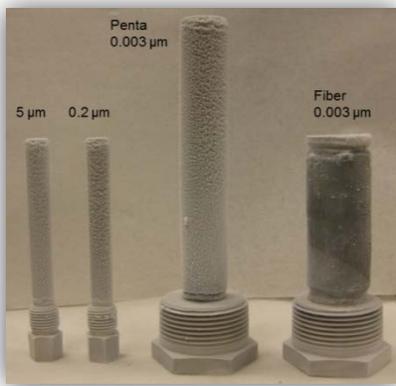
MOF-5 particle size distribution



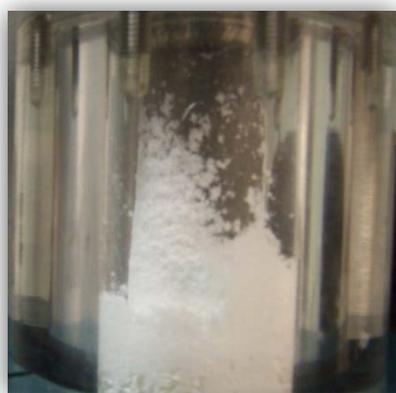
Both particle and fiber filters evaluated



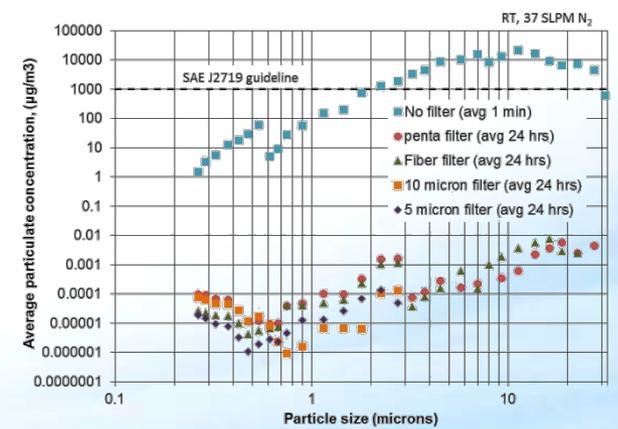
All filters survive LN2 thermal shock testing



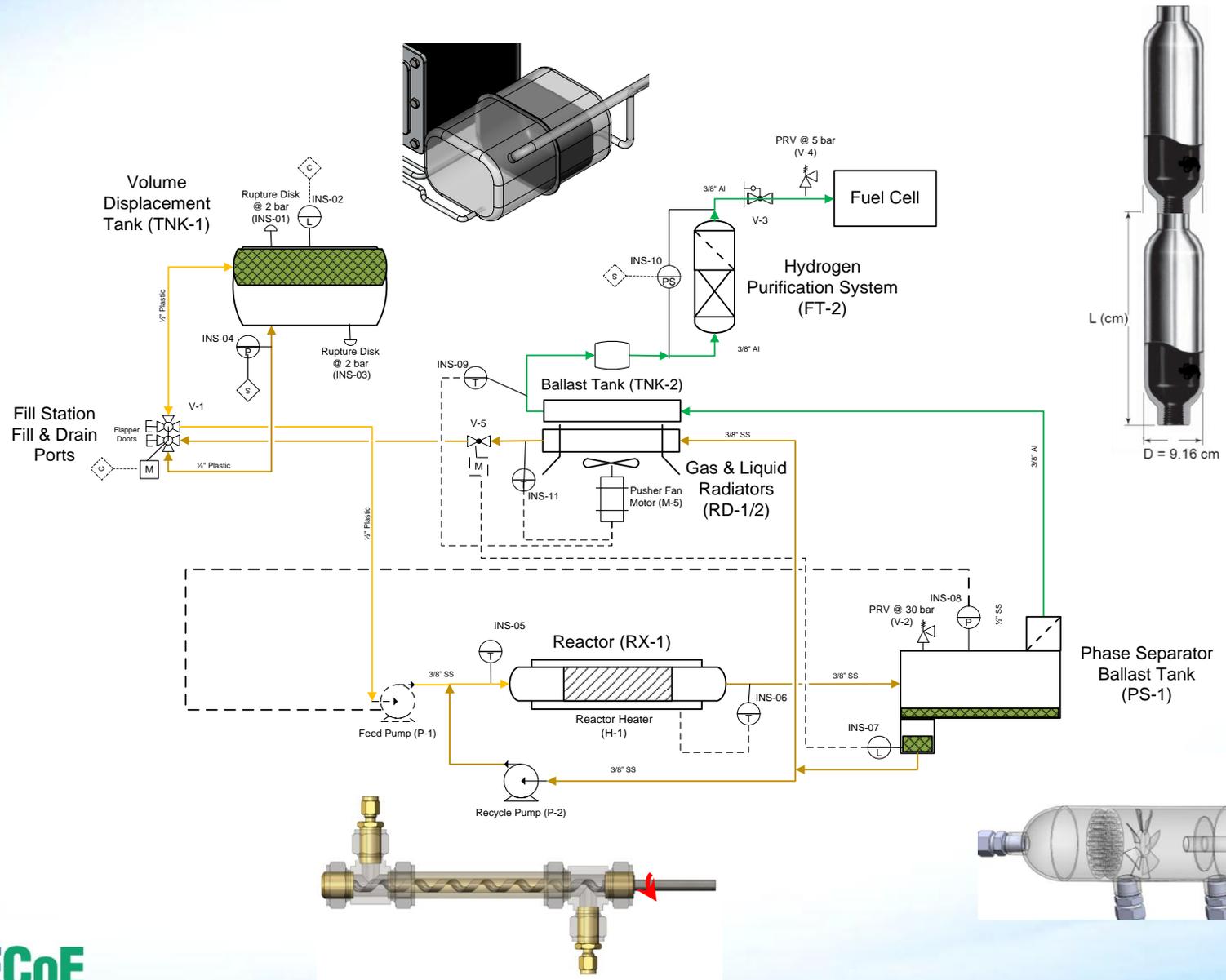
Filter caking after 20 slpm N<sub>2</sub> fluidized MOF-5



All filters reduce particle entrainment to below J2719 guidelines



# Chemical System Overview

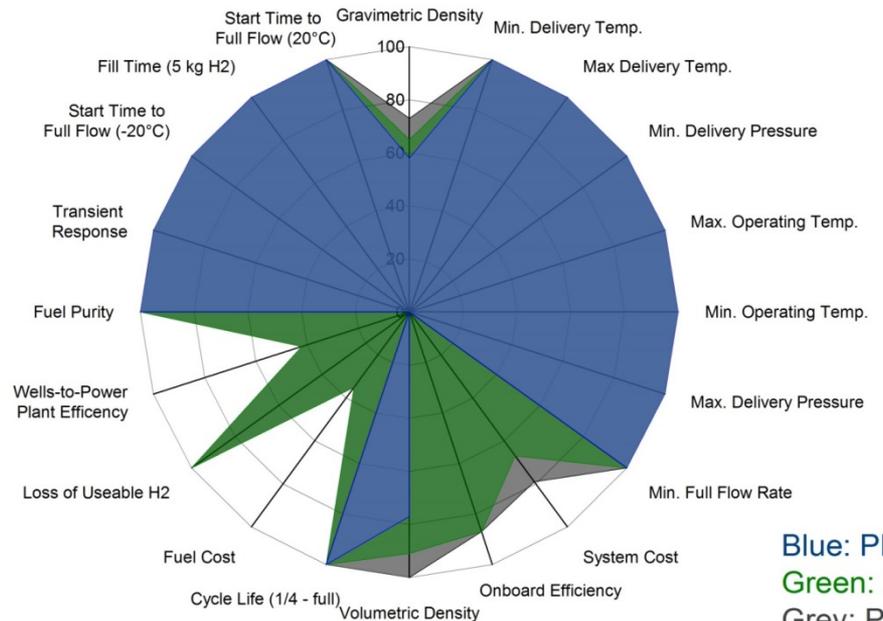
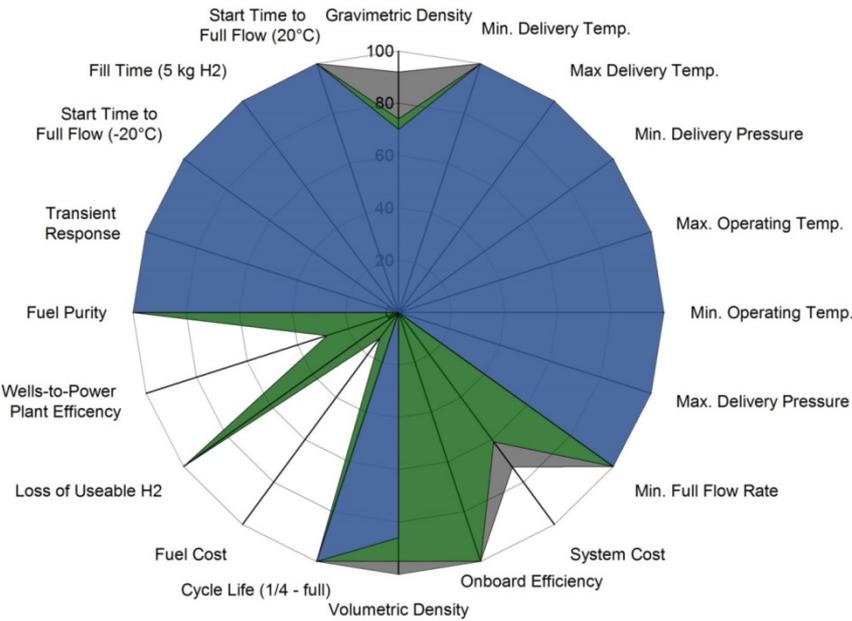


## Chemical System

50 wt.% slurries

### Ammonia Borane

### Alane



Blue: Phase 1  
 Green: Phase 2  
 Grey: Projected  
 (HSECoE Estimates)

#### Technical Hurdles:

Fuel Cost, System Cost, WTPP, Gravimetric Density

Fuel Cost, System Cost, WTPP, **On-board Efficiency**, Gravimetric Density

# Chemical Hydrogen Milestones

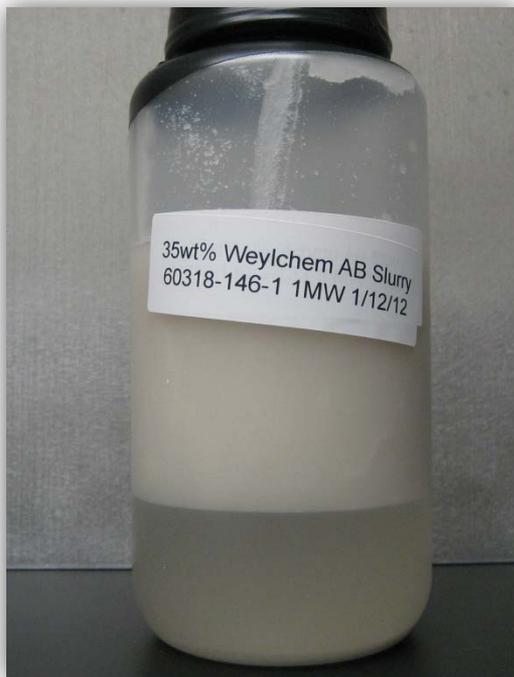
Chemical System						
Component	Partner	Proposed SMART Milestones	Due Date	Modified Date	Status	Reason
Materials Synthesis/Characterization	PNNL	Provide a total of 2 L of sonicated AB slurry (1L of 50wt% AB slurry and 1L of 35 wt. % AB slurry) to LANL. With material provided by LANL.	11/15/2013			Slurry Preparation Flow Through Reactor
Flow Through Reactor	LANL	Perform a minimum of 10 flow thorough reactor studies on 30 and 50 wt. % alane slurries and report space time yields, temperatures and gas compositions for modeling analysis.	12/31/2013			
Flow Through Reactor	LANL	Perform a minimum of 10 flow thorough reactor studies on 30 and 50 wt. % AB slurries and report space time yields, temperatures and gas compositions for modeling analysis.	12/31/2013			BoP Components
Gas liquid Separator	UTRC	Demonstrate a gas/liquid separator with a specific Souders-Brown velocity of >0.013 (m/s)/kg and >0.029 (m/s)/L.	12/31/2013			
Filter	UTRC	Demonstrate an ammonia filter cartridge with <27 kg/kgNH3 and <22 Liter/kg NH3 that enables a purified gas with <0.1 ppm NH3 (SAE J2719 guideline).	12/31/2013			System Modeling
System Modeling	NREL/PNNL/ LANL	Update the chemical system model with Phase 2 performance data, integrate into the framework; document and release models to the public.	3/31/2014			
System Modeling	NREL	Update the chemical system model with Phase 2 performance data, integrate into the framework; document and release models to the public.	3/31/2015			Reporting
Reporting	LANL/NREL/ PNNL/ SRNL	Prepare and submit final reports on research efforts related to chemcia hydrogoen storage systems.	3/31/2014			

Complete
On Schedule
Incomplete

# Chemical Hydrogen Media Preparation

Provide a total of 2 L of sonicated AB slurry (1L of 50wt% AB slurry and 1L of 35 wt. % AB slurry) to LANL. With material provided by LANL

One Liter  
35wt% AB in  
silicon oil



One Liter  
50wt% AB in  
silicon oil



60wt%  $\text{AlH}_3$  Slurry  
Successfully  
Demonstrated

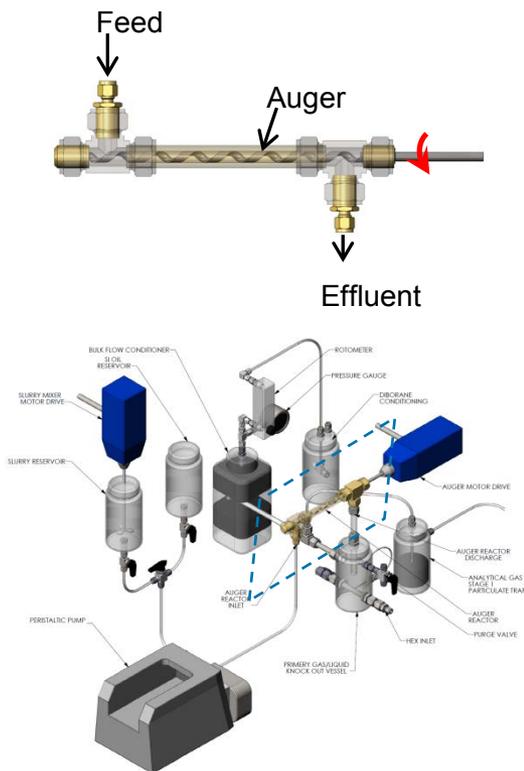


# Chemical Hydrogen Media Preparation

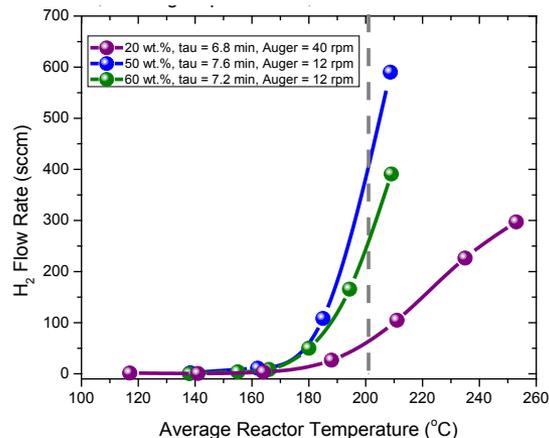
Perform a minimum of 10 flow through reactor studies on 30 and 50 wt. % alane slurries and report space time yields, temperatures and gas compositions for modeling analysis.

Perform a minimum of 10 flow through reactor studies on 30 and 50 wt. % AB slurries and report space time yields, temperatures and gas compositions for modeling analysis.

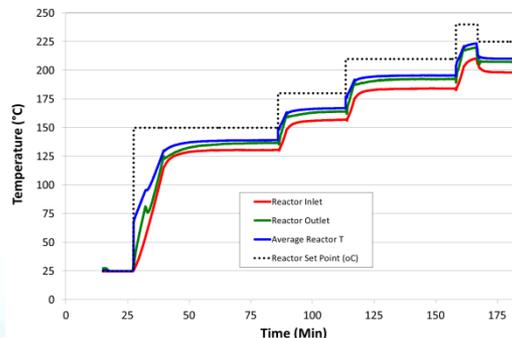
## Flow Through Reactor Experiments



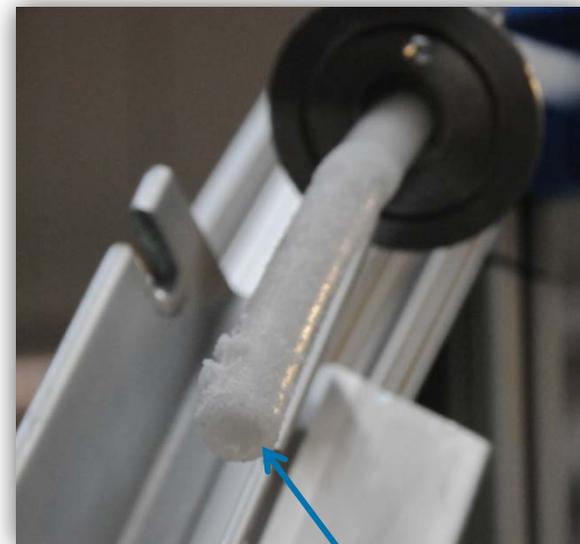
## 20-50 wt.% $\text{AlH}_3$ Successfully Slurries Tested



## 60 wt.% $\text{AlH}_3$ in MPF



## 50% AB Slurry Clogged in Pumps and Lines

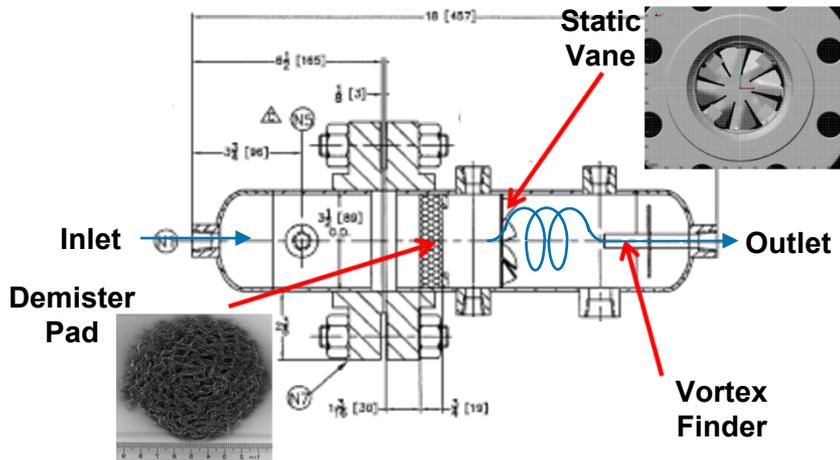


Viscous AB filled the 1/2 in Teflon tubing

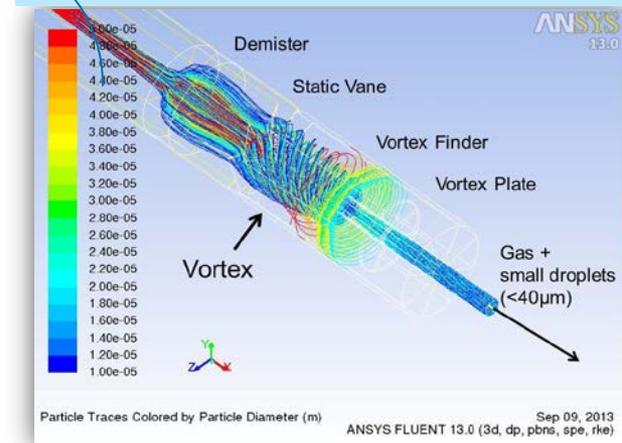
# Chemical Hydrogen BoP Components

Demonstrate a gas/liquid separator with a specific Souder-Brown velocity of  $>0.013 \text{ (m/s)/kg}$  and  $>0.029 \text{ (m/s)/L}$ .  
 Demonstrate an ammonia filter cartridge with  $<27 \text{ kg/kgNH}_3$  and  $<22 \text{ Liter/kg NH}_3$  that enables a purified gas with  $<0.1 \text{ ppm NH}_3$  (SAE J2719 guideline).

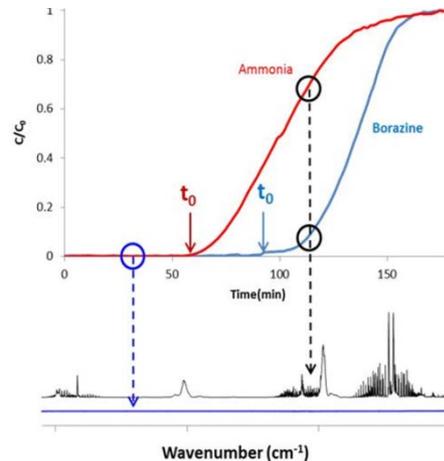
## GLS Designed and Evaluated



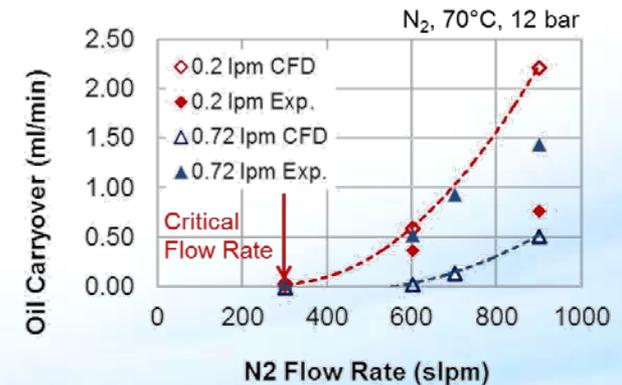
## Fluent model predicts droplet size and location



## Ammonia and Borazine Filters Effectively Eliminate Gas Contamination



## GLS shown to Effectively Eliminate oil Carryover Under Operational Conditions

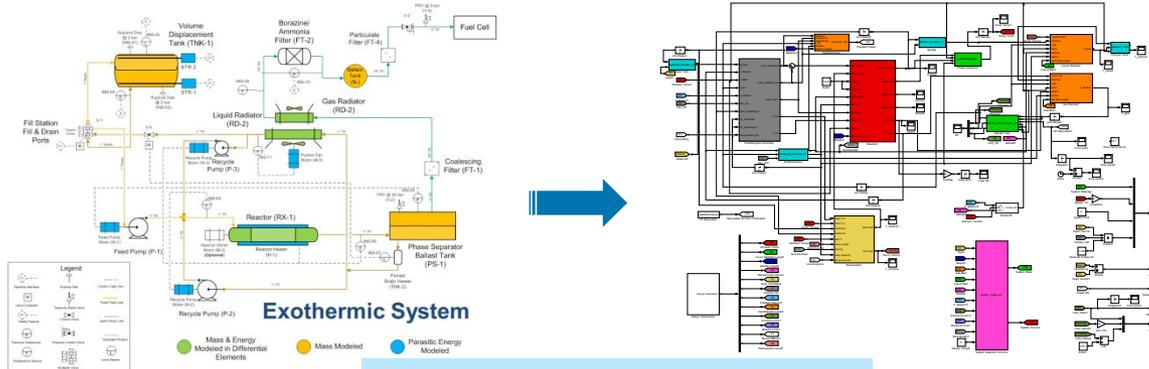




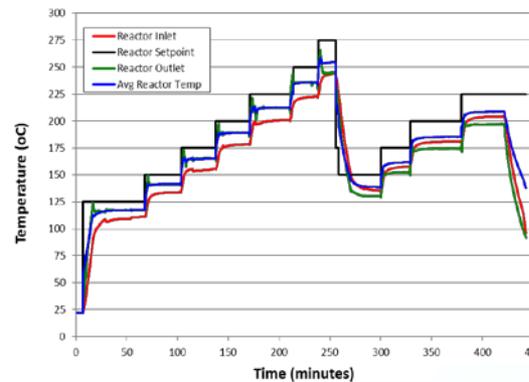
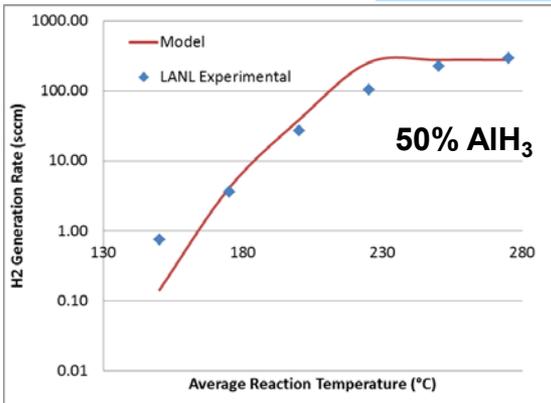
# Chemical Hydrogen System Modeling

Update the chemical system model with Phase 2 performance data, integrate into the framework; document and release models to the public.

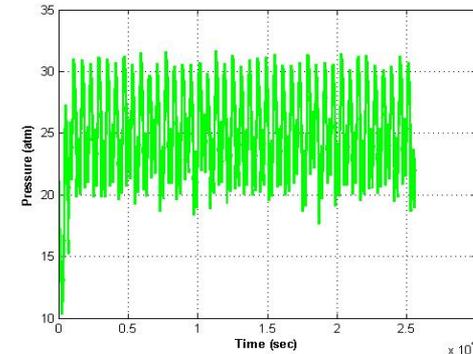
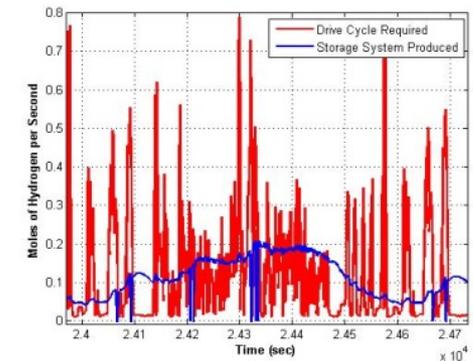
## P&ID Translated to Simulink



## Thermal Models Match to Experimental Results

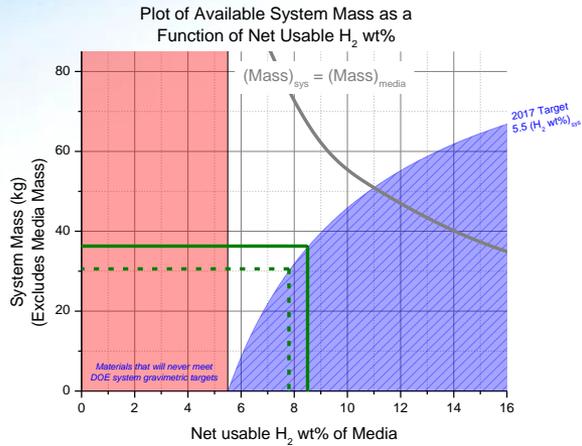


## System Models Show Continuous Hydrogen Feed from Ballast Tank

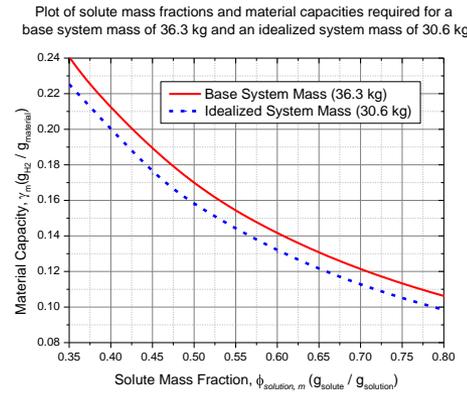


# Chemical Hydrogen Material Properties

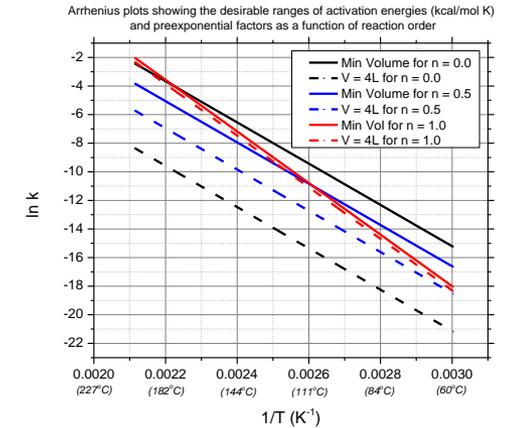
## Media Gravimetric Density



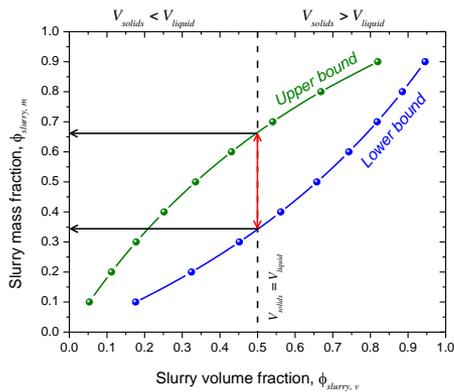
## Slurry Gravimetric Density



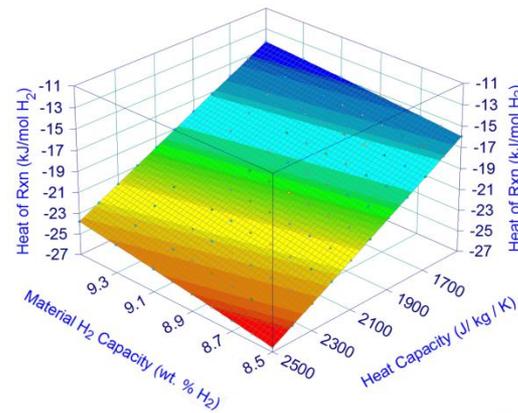
## Slurry Kinetics



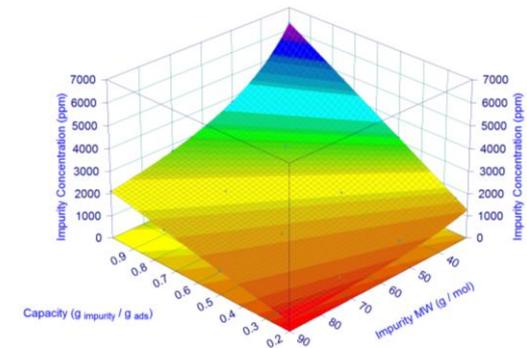
## Slurry Mass/Volume Fraction



## Enthalpy of Reaction



## Impurities



# Required Materials Properties

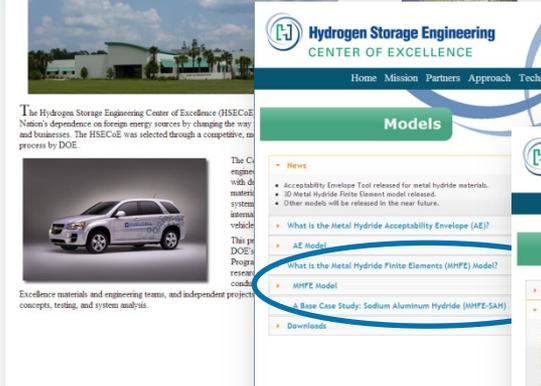
Parameter	Symbol	Units	Range*	Influence
Minimum Material capacity (liquids)	$\gamma_{mat}$	$g_{H_2} / g_{material}$	$\sim 0.078 (0.085)^\dagger$	System
Minimum Material capacity (solutions)	$\gamma_{mat}$	$g_{H_2} / g_{material}$	$\sim 0.098 (0.106)^\dagger$	System
Minimum Material capacity (slurries)	$\gamma_{mat}$	$g_{H_2} / g_{material}$	$\sim 0.112 (0.121)^\dagger$	System
Kinetics: Activation Energy	$E_a$	kcal / mol	28–36	Reactor and Shelf life
Kinetics: Preexponential Factor	A		$4 \times 10^9 - 1 \times 10^{16}$	
Endothermic Heat of Reaction	$\Delta H_{rxn}$	kJ / mol $H_2$	$\leq +17 (15)^\dagger$	On-board efficiency
Exothermic Heat of Reaction	$\Delta H_{rxn}$	kJ / mol $H_2$	$\leq -27$	
Maximum Reactor Outlet Temperature	$T_{outlet}$	$^\circ C$	250	Heat Exchanger
Impurities Concentration	$y_i$	ppm	No <i>a priori</i> estimates can be quantified	Purification
Media $H_2$ Density	$(\gamma_{mat})(\phi_m)(\rho_{mat})$	kg $H_2$ / L	$\geq 0.07$	Tank size System
Regen Efficiency	$\eta_{regen}$	%	$\geq 66.6\%$	Well-to-Power Plant Efficiency
Viscosity	$\eta$	cP	$\leq 1500$	Fill time Pump size On-board efficiency

# WEB Site Models Added



List of Models Available

www.HSECoE.org



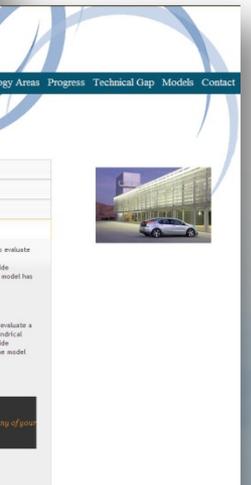
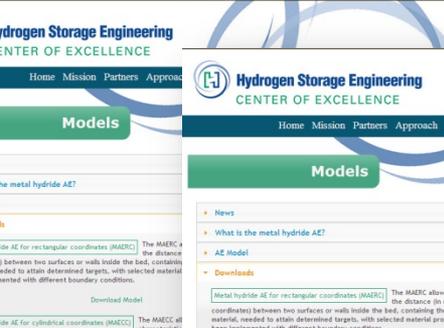
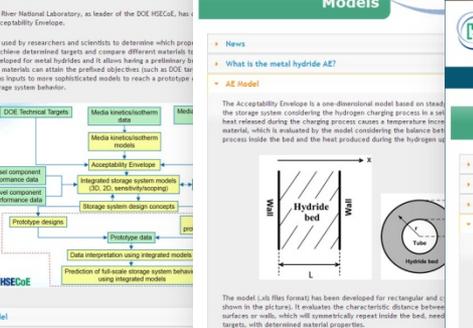
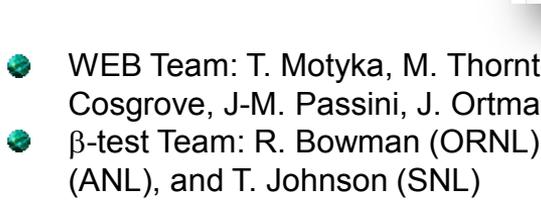
Description of Model

Outline of Analysis



Model Download

Identification of User



 WEB Team: T. Motyka, M. Thornton, J. Cosgrove, J-M. Passini, J. Ortman  
  $\beta$ -test Team: R. Bowman (ORNL), D. Papadias (ANL), and T. Johnson (SNL)



## WEB Site Models Added



[www.HSECoE.org](http://www.HSECoE.org)

Type 4 Tank sizing code	units	Green = input fields	
Input parameters			Notes
Operating Temperature	C	na	Room Temperature analysis, assumed valid for all temperatures
Operating Pressure	Bar	250	When pressure varies by cycle, use max pressure
Tank Material	-		No choice: Carbon Fiber Composite
Liner Material	-		No choice: HDPE
Liner Thickness [t]	cm	0.4	Liner thickness set by functional requirements, not load bearing
Fiber Transition Efficiency	%	80%	Practical difference between stress analysis and actual burst test. 100% = no difference
Primary Geometry Specification: Internal			
Tank Length (Internal) [L-d]	cm		Only 2 of these 3 are independent. Input 0 if variable is free
Tank Radius (Internal) [R <sub>0</sub> ]	cm	22.5	Only 2 of these 3 are independent. Input 0 if variable is free
Tank Volume Goal (Internal) [V <sub>g</sub> ]	com	105.000	Only 2 of these 3 are independent. Input nonzero guess if variable is free
Tank Geometry Calculation			
Tank Internal Length (cm) [L <sub>i</sub> ]	cm	81.0	31.99757018
Tank Internal Radius (cm) [R <sub>i</sub> ]	cm	22.5	
Tank Internal Volume Actual (com) [V <sub>i</sub> ]	com	105.000	Hemispherical end caps assumed, always calculated from L and R
Volume goal attainment	%	100.0%	To get a closer match, specify Tank Radius [R <sub>0</sub> ] directly
Wall Thickness Calculation			
Tank Material strength at operating temp	Bar	153.06	Room temperature 2.1 hoop axial fiber orientation, 60% fiber if
Safety Factor (Design Basis)	-	2.25	may be adjustable: 2.25 and 2.35 have been considered
Wall Radius = R+t	cm	22.9	
Tank Wall thickness (total)	cm	1.051977166	includes transition efficiency. Does not account for discrete layers
Layer thickness increment	cm	0.09144	thickness of each carbon fiber layer
# layers	cm	12	
Rounded up thickness	cm	1.09728	
Minimum layer thickness	cm	0.27432	3 layers minimum
Final wall thickness	cm	1.09728	
Maximum safety factor		2.35	Safety Factor x (Final Wall Thickness / Ideal Wall Thickness)
Estimated maximum burst pressure	Bar	586.7	indication of potential conservatism, using even number of lamina thicknesses
Tank External Geometry Calculation			
Tank External Length	cm	84.0	
Tank External Radius	cm	24.0	
Tank External Volume	com	123.051	
L/D Ratio (External)	-	1.8	
Liner Geometry and Mass Calculation			
Total volume of liner material	com	3327.2	
Liner material density	kg/com	9.5E-04	HDPE
Liner mass	kg	3.1	
Tank Wall Material Calculation			
Total volume of tank wall material	com	1.472E+04	
Tank Wall material density	kg/com	1.61E-03	Carbon fiber composite (T700S)
Tank wall mass	kg	23.7	
Summary			
Liner Mass	kg	3.1	
Composite mass	kg	23.7	
Total mass	kg	26.9	Total Tank Mass
Tank Efficiency			
Gravimetric	L/kg	3.91	Note this value does not include hydrogen, adsorption material, balance of plant, etc.
Tank Cost			
HDPE material cost	\$/kg	2.06	Raw material cost estimate based on representative 2007 prices
Carbon fiber composite material cost	\$/kg	30.65	Raw material cost estimate based on representative 2007 prices
liner cost	\$/	6.48	
composite cost	\$/	727.04	
total tank cost	\$/	733.52	Total of composite and HDPE only, manufacturing and all other costs not included

- WEB Team: T. Motyka, M. Thornton, J. Cosgrove, J-M. Passini, J. Ortman
- β-test Team: R. Bowman (ORNL), D. Papadias (ANL), and T. Johnson (SNL)

## Models on the WEB Schedule

<b>MH Acceptability Envelope</b>	<b>Hardy/SRNL</b>	<b>complete</b>
<b>MH Finite Element Model</b>	<b>Hardy/SRNL</b>	<b>complete</b>
<b>Tank Volume/Cost Model</b>	<b>Simmons/PNNL</b>	<b>complete</b>
<b>MH Framework Model</b>	<b>Pasini/UTRC</b>	<b>complete</b>
<b>CH Framework Model</b>	<b>Brooks/PNNL</b>	<b>6/2014</b>
<b>AD Framework Model</b>	<b>Tamburello/SRNL</b>	<b>9/2014</b>
<b>AD Finite Element Model</b>	<b>Hardy/SRNL</b>	<b>3/2015</b>

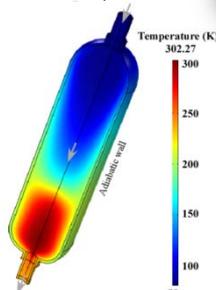
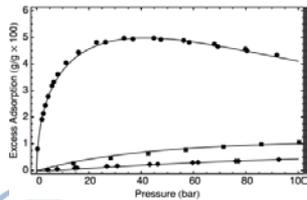
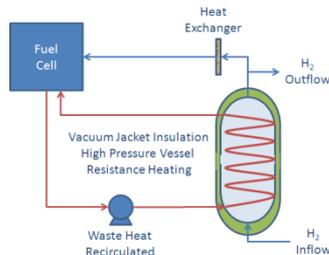
# Where are we going in Phase 3: Technology Readiness Levels

## 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	



# Where are we going in Phase 3: Technology Readiness Levels

Materials Base for Aut

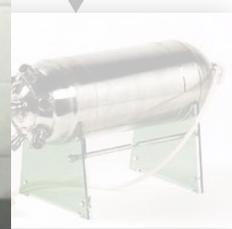
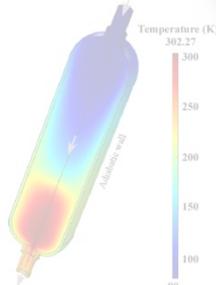
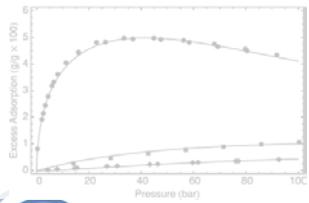
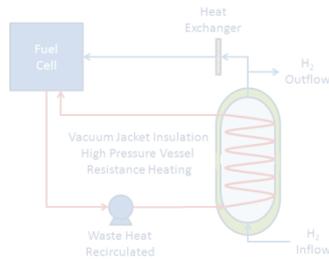
TRL 4 System Validation in Laboratory Environment

Storage Systems Applications

Materials CoEs

HSECoE

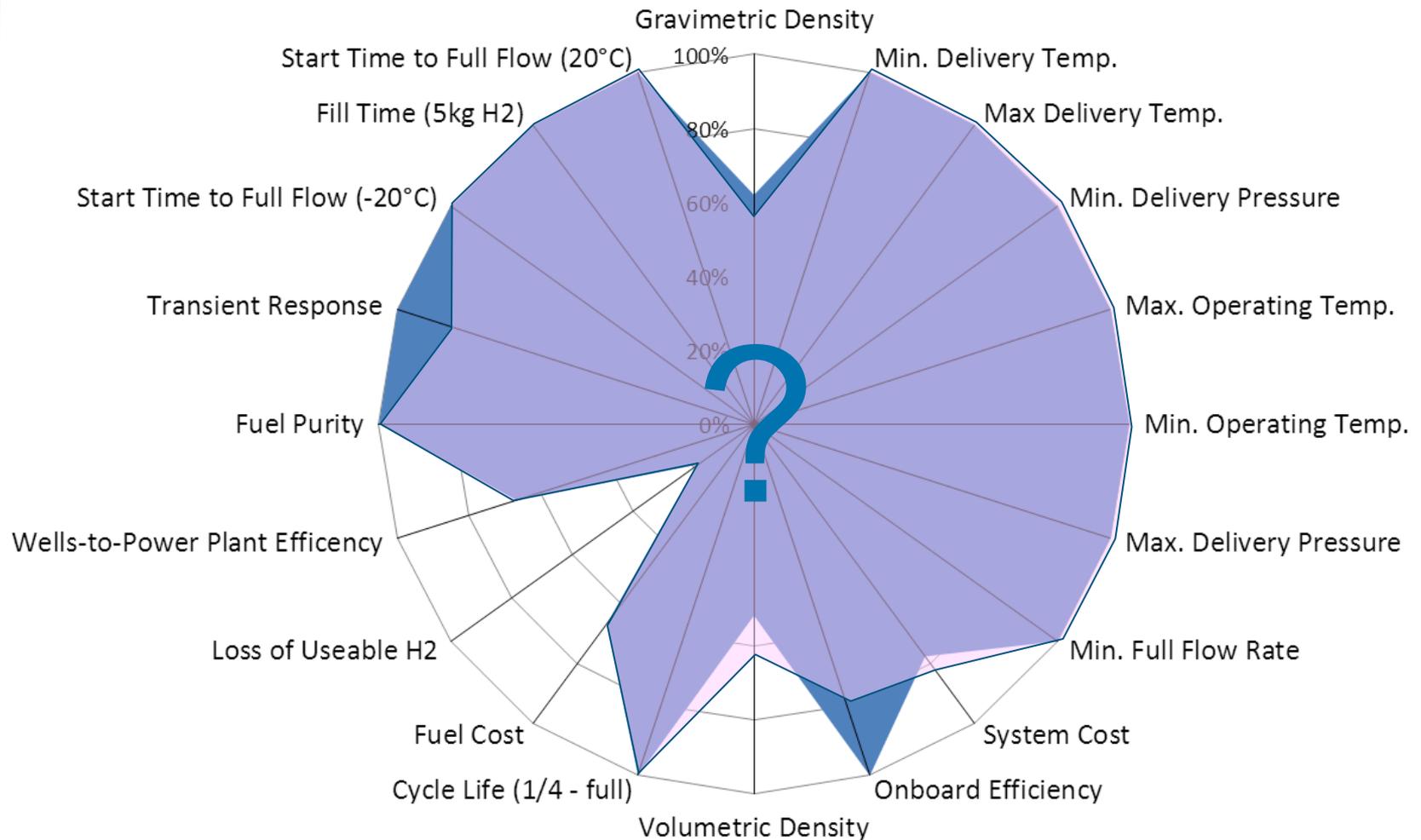
TRL 1	TRL 2	TRL 3	TRL 4	TRL 5	TRL 6	TRL 7	TRL 8	TRL 9
Basic Technology Research		Research to Prove Feasibility			Technology Demonstration	System Commissioning		System Operation
Basic Principals	Concept Formulation	Characteristic Proof of Concept	System Validation in Laboratory Environment	System Validation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



# Preliminary vs. Demonstrated Spider Chart

*Why Phase 3 demonstration is critical in model validation*

MATI Adsorbent Storage System (2012)



## **LANDMARK Innovations**

*What has the Center done to change the way we look at hydrogen storage?*

- **Overall**

- Technical target prioritization
- Development of models which integrate the storage system, fuel cell and vehicle drive cycles

- **Metal Hydrides**

- Acceptability envelope
- Microchannel catalytic burner

- **Chemical Hydrogen Storage**

- Storage material requirements
- Auger reactor for slurries and helical reactor for neat liquids
- Demonstrated 60wt.% alane slurry reactor

- **Adsorbents**

- LN2 tank cooling strategy
- Low cost HX Flow Through Design
- Combined MOF Compaction/ Augmentation
- Microchannel HX in compacted media design

## Technical Lessons Learned

### *Metal Hydride System: End of Phase 1*

- ❖ **Parallel materials development effort needed**
- ❖ **Less effort should have been spent on evaluating and down selecting candidate materials during Phase 1**
- ❖ **Efforts should have been focused on radically improve the efficiency and design of heat exchangers and other BoP components.**

### *Adsorbent System*

- ❖ **Heat and mass transfer modeling necessary to understand system**
- ❖ **Model validation necessary to fine tune models and gain confidence in model accuracy**
- ❖ **Forecourt concerns which impact fuel cost are important, and should have been included in analyses**
- ❖ **Prioritizing technical targets important in evaluating approaches to their mitigation**

## Technical Lessons Learned

### *Chemical Hydrogen Storage*

- ❖ **System volumetric capacity is a key benefit with chemical hydrogen storage materials.**
- ❖ **AB slurries are unusable in a silicon oil due to coagulating of AB**
- ❖ **Neat liquid phase chemical hydrogen storage materials around 8 wt. % hydrogen required to meet DoE 2017 targets.**
- ❖ **Solid or slurry phase chemical hydrogen materials requiring off-board regeneration are unlikely commercial candidates without innovations in materials handling and system durability.**
- ❖ **Compact and inexpensive reactor designs accommodating gas evolution two phase flow will require additional development.**
- ❖ **It is very difficult to validated chemical hydrogen storage system models because the complexity of the physical phenomena.**

## Lessons Learned Programmatically

- ❖ **Organize the team functionally to distribute responsibility and gain ownership by the members.**
  - ❖ Assignment of Technology Area Leads to lead model development in Phase 1
  - ❖ Assignment of System Architects to move system concept forward into Phase 2
- ❖ **Set up clear communications networks to facilitate data and information flow.**
  - ❖ IP Agreement
  - ❖ F2F Meetings
  - ❖ SharePoint Site
  - ❖ Monthly Telecons
  - ❖ Safety and risk issues discussed regularly

## Lessons Learned Programmatically (cont.)

### ❖ Milestones

- ❖ Negotiate clear milestones with partners for each individual tasks needing to be accomplished and track milestone accomplishment.
- ❖ **Facilitate discussion and face to face meetings early after identifying milestone may be in jeopardy to correct situation**
- ❖ Down select from multiple technical approaches as soon as possible
- ❖ Readjust partner responsibility after down select decisions
- ❖ **Perform FMEA early and often to stimulate nonlinear thinking**
- ❖ **Disseminate findings in a manner that the stakeholders can understand and use.**
- ❖ **Judiciously evaluate and selectively implement stakeholder guidance**

# Reviewers Comments

*“This is a very successful and well run project that should not end in 2014.”*

*“If the DOE Hydrogen and Fuel Cells Program is going to keep funding research on hydrogen storage, it should consider a “reinvention” of the HSECoE into a new entity that keeps the core HSECoE capabilities intact”*

- **The program has been extended to run through fiscal year 2015 with current funding.**

*“DOE and the Center should carefully discuss the scope of Phase III activities.”*

- **Phase III planning and consultation with DoE was extensive with the ultimate decision made to focus efforts on the adsorption system utilizing the two heat exchanger systems which show the most promise and diversity in approaching the technical targets.**

*“A clear and detailed statement of the specific technical challenges and plans for addressing those challenges should be included in the plans for the Phase III effort.”*

- **A clearer and more concise description of the technical hurdles and approaches has been given in this and the following partner contributions.**

*“The signature problem that may ultimately limit overall project success is that no single material that meets all of the DOE targets has been identified. Consequently, engineering systems based on sub-optimal materials are being developed.”*

- **It is the objective of the HSECoE to model, design and build the best systems with the materials available and to project what materials characteristics are needed to achieve the all of the DoE technical targets.**

# Summary

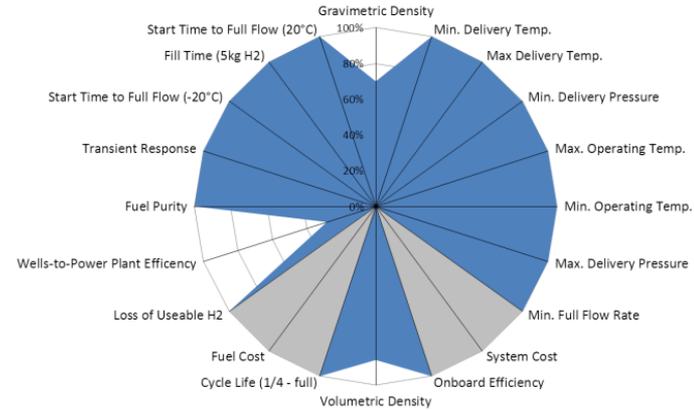
## • Chemical Systems

- Limited in gravimetric density and efficiency due to materials limitations.
- AB Slurry could not be pumped while Alane slurry was successfully demonstrated using a auger flow through reactor.
- High fuel cost resulting from recycle inefficiencies limits potential for Chemical Hydrogen Storage materials.

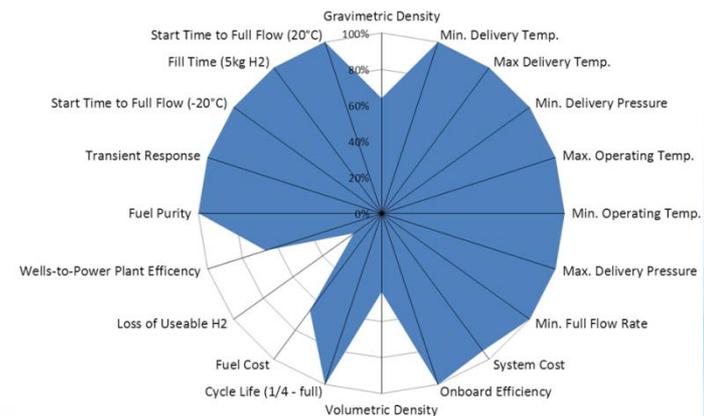
## • Adsorption Systems

- Volumetric density addressed with microchannel MATI HX Design
- Charge time addressed with flow through cooling and independent LN2 tank cooling
- Low pressure adsorption systems hold best opportunity to meet DoE Technical Targets.

## Chemical System



## Adsorbent System





# **Technical Back-Up Slides**

# System Test Matrixes

Phase 3 ideas for testing specific t  
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-H <sub>2</sub> /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	Estimated costs of lab scale system to actual cost of lab scale system	Amount of LN2 and H2 consumed during refill	External temperature

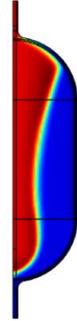
# System Component Specification

Component	Assumed Validation in Phase II			Responsible Design Organization	What can be validated with modeling rather than experimental work?
Internal Heat Exchanger: <b>HexCell Resistance Heater with Flow-Through Cooling</b>	Modeling and partial experimental validation of individual components/capabilities			SRNL / UQTR	1 <sup>st</sup> -order thermal behavior (already completed).  Simple, low-cost design; Verify capability for rapid cooling: dynamic behavior (such as channeling) can only be evaluated experimentally
Cryo-Adsorbent Material: <b>Powder MOF-5</b>	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

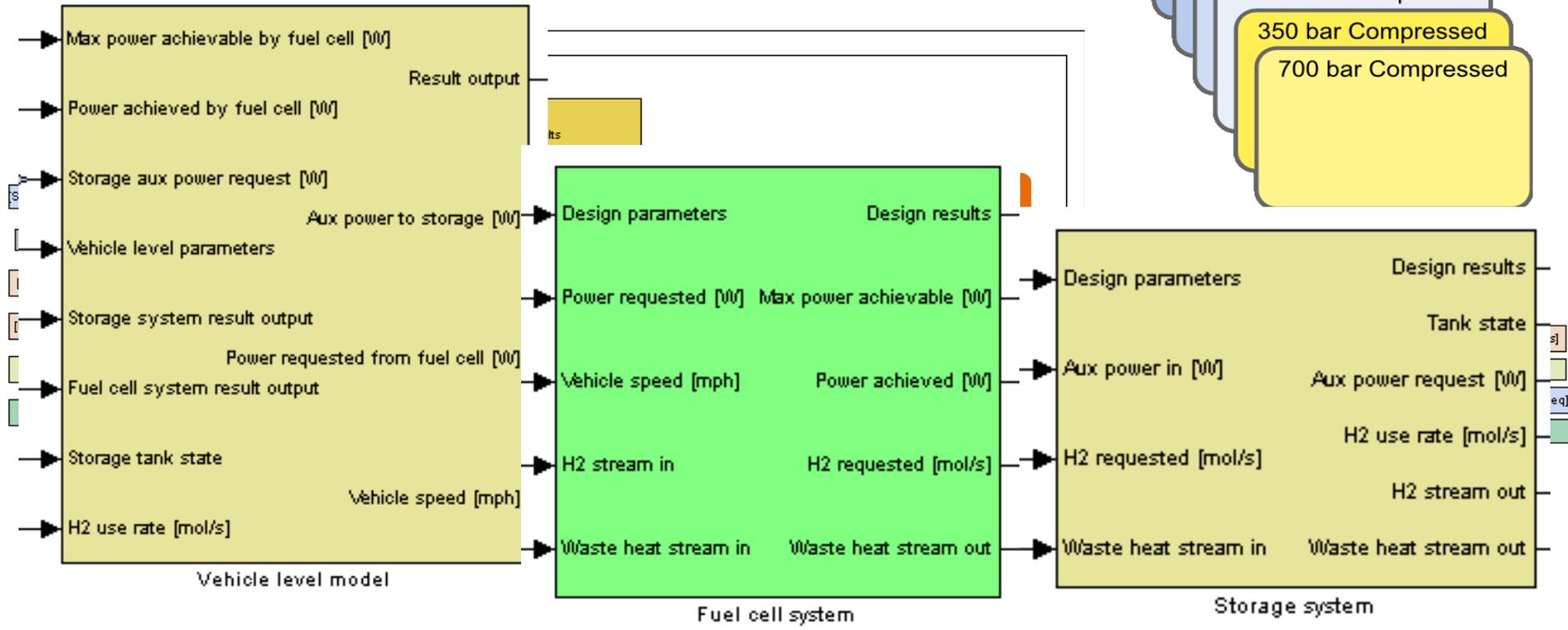
# Integrated Model Framework

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



SRNL 200 bar  
AX-21  
Flow-Through

- UTRC NaAlH<sub>4</sub> Powder  
H<sub>2</sub> requested H<sub>2</sub> stream out
- UTRC NaAlH<sub>4</sub> Pellets
- UTRC/SRNL 1:1 Li-Mg-N-H
- GM NaAlH<sub>4</sub>
- GM/SRNL/JPL AX-21
- PNNL Solid AB
- PNNL/LANL Liquid AB
- 350 bar Compressed
- 700 bar Compressed



# Addressing DOE's Technical Targets

Target	2017 Value	Units	Measurement	Additional Measurements
Gravimetric Capacity	0.055	$g_{H_2} / g_{sys}$	Total Mass of Gas Stored	Total Mass of System (all equipment, tubing, tank, etc.)
Volumetric Capacity	40	$g_{H_2} / L_{sys}$	Total Mass of Gas Stored	Total Volume of System (all equipment, tubing, tank, etc.)
System Cost	12	\$/kWh	Total Mass of Gas Stored	Total cost of the full experimental set-up
Fuel Cost	2-6	\$/gge	Not Measured at SRNL/OSU	
Ambient Temperature	-40 - 60 (sun)	°C	Room Temperature	
Min/Max Delivery Temperature	-40 - 85	°C	H <sub>2</sub> Outlet Temperature	
Operational cycle life (1/4 tank to full)	1500	cycles	Not Measured at SRNL/OSU	
Min/Max Delivery Pressure	5 / 12 bar	bar	H <sub>2</sub> Outlet Pressure	
On-board efficiency	90	%	Energy used to release the hydrogen (converted into H <sub>2</sub> )	
Wells-to-Power Plant Efficiency	60	%	Energy used to refuel / reload the hydrogen (converted into H <sub>2</sub> )	
System Fill Rate	1.5	kg <sub>H<sub>2</sub></sub> / min	Time to completely fill the tank (function of operating conditions)	Scaling this to our 2-Liter tank, it would only be a 4 second fill for the ~100 grams of H <sub>2</sub>
Min Full Flow Rate	0.02	(g/s)/kW	Not Measured at SRNL/OSU	
Start time to full flow rate (20 °C)	5	s	H <sub>2</sub> Flow Rate?	Time to achieve full flow rate at start-up (no "hold time" listed)
Start time to full flow rate (-20 °C)	15	s	Not Measured at SRNL/OSU	
Transient Response (10%-90% & 90%-0%)	0.75	s	H <sub>2</sub> Flow Rate?	Time to achieve desired response in flow rate ("driving" response to rapidly accelerate and stop)
Fuel Purity (SAE J2719 & ISO/PDTS 14687-2)	99.97	%H <sub>2</sub>	Gas composition (via mass spec or RGA)	
Permeation & Leakage		Scch/h	Not Measured at SRNL/OSU	
Toxicity			Not Measured at SRNL/OSU	Dust cloud ignition at BASF and/or UTRC
Safety			Not Measured	Design for applicable safety standards
Loss of usable H <sub>2</sub>	0.05	(g/h)/kg <sub>H<sub>2</sub>,stored</sub>	Not Measured at SRNL/OSU	Simplified thermos bottle + MLVI system TBD