

Donald L. Anton Director Theodore Motyka Assistant Director

Savannah River National Laboratory

June 18, 2014



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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

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Barriers

- **B. System Cost**
- C. Efficiency
- D. Durability
- G. Materials of Construction

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

Partners



HSECoE Technical Objectives

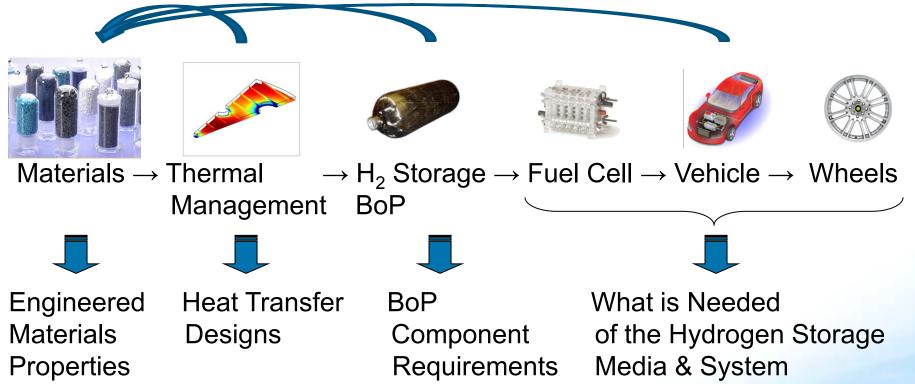
Using systems engineering concepts, design innovative material-based hydrogen storage system architectures with the potential to meet DOE performance and cost targets.

- 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.

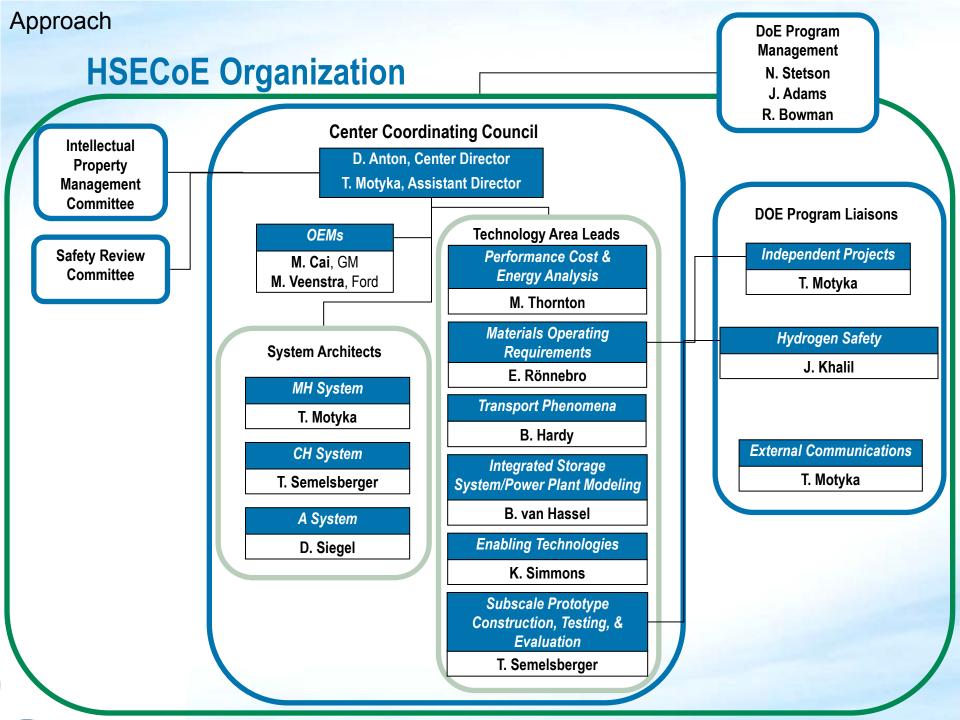


Why Perform Materials Development and System Engineering in Parallel?

continuous feedback with system design through the integrated model identifying materials requirements







(H)

Technical Matrix

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

Internal Communications

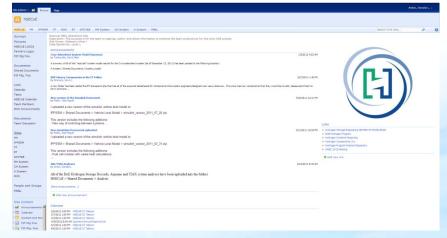




- **AMR Pre-Meeting (May-June)**
- Tech Team Review F2F Meeting (Feb.-March)
- **Monthly System Architect Telecoms**
- **Monthly Coordinating Council Telecoms**
- Semi-monthly technical team telecoms
- SharePoint Site used extensively to share documents and data



HSECoE



Phased Approach



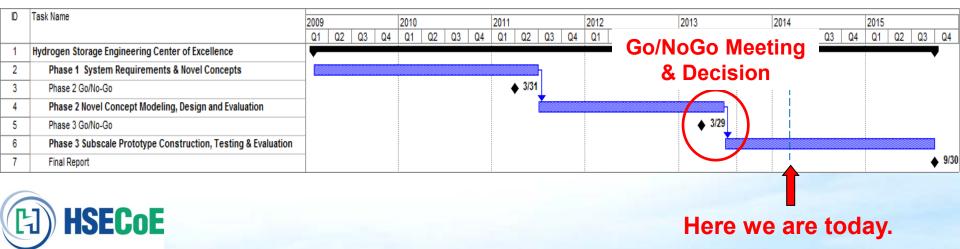
- Where were we and where can we get to?
 - Model
 Development
 - Benchmarking
 - Gap Identification
 - Projecting advances

- 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



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

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- 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



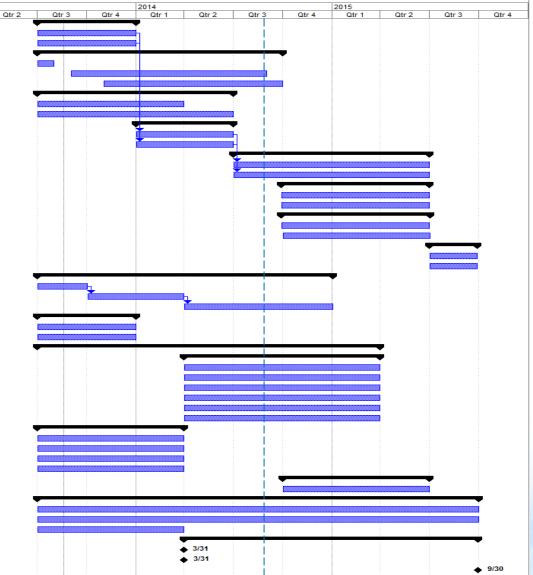
- Evaluate prototype & assess performance
- Compare to and refine models
- Modify test apparatus/prototype
- 8.0 Decommission prototypes
- 9.0 Thermos bottle testing
- **10.0** Chemical system completion
- 11.0 Performance/cost model updates
- **12.0** Materials' requirements refinement
- **13.0 Project management**
- 14.0 Final Reports

Phase 3 Gantt Chart

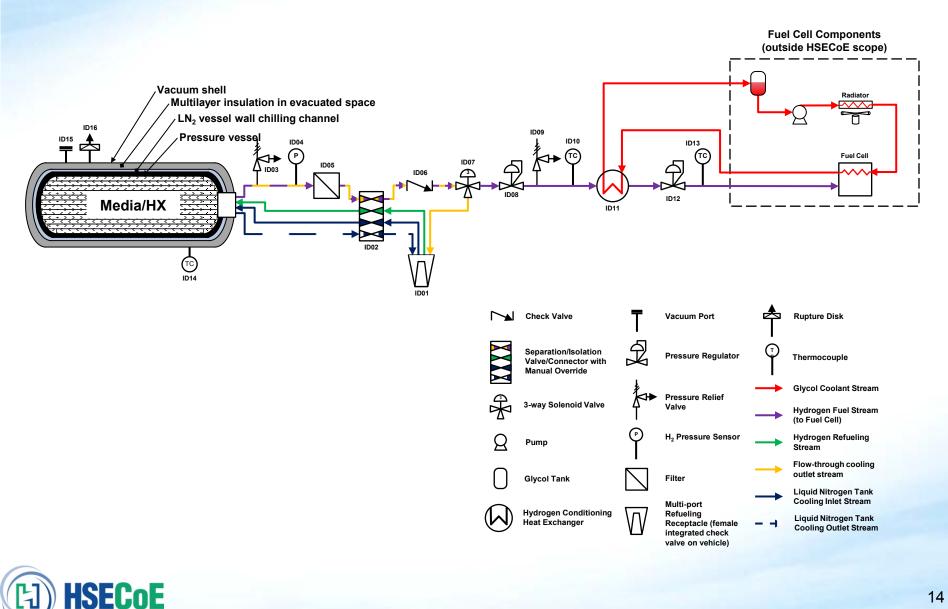
Γ	ID	WBS	Task Name
	1	1.0	Design subscale prototype systems
	2	1.1	Design 2L HexCell
	3	1.2	Design 2L MATI
	4	2.0	Synthesize/Modify Materials
	5	2.1	Scale MOF-5 Mfg.
	6	2.2	Cyclic Degradation of MOF 5
	7	2.3	Characterize Scaled-up Conductivity
	8	3.0	Complete test facilities
	9	3.1	HexCell Test Rig
	10	3.2	MATI Test Rig
	11	4.0	Fabricate/assemble prototype system
	12	4.1	HexCell
	13	4.2	MATI
	14	5.0	Evaluate prototype & assess performance
	15	5.1	HexCell Ssytem
	16	5.2	MATI System
	17	6.0	Compare to and refine models
	18	6.1	HexCell Design
	19	6.2	MATI Design
	20	7.0	Modify test apparatus/prototype
	21	7.1	HexCell
	22	7.2	MATI
	23	8.0	Decommission Prototypes
	24	8.1	HexCell
	25	8.2	MATI
	26	9.0	Thermos Bottle Testing
	27	9.1	Design Full Scale Thermos Bottle Tank
	28	9.2	Mfg Thermos Bottle Test Rig Pressure Vessel
╞	29	9.3	Test and Evaluate Full Scale Thermos Bottle Tank
+	30	10.0	Chemical System Testing
+	31 32	10.1	AB Evaluations Alane Evaluations
╞	33	10.2	
╞	34	11.0	Performance/Cost Model Updates
╞	35	11.1	Adsorbent Adsorbent Tank to Wheels Efficency
┢	36	11.1.2	-
┢	37	11.1.2	Provide Cost Model for Adsorbent System Reduce Part Count of Adsorbent System to 20
╞	38	11.1.3	Complete FMEA on Adsorbent System
┢	39	11.1.4	Design monolithic Type 1 & 3 tanks
ŀ	40	11.1.6	Post updated adsorbent Models on the WEB
┢	40	11.2	Chemical
ŀ	42	11.2.1	Chemical Tank to Wheels Efficency
ŀ	43	11.2.2	System Modeling
┢	43	11.2.2	Cost Modeling
ŀ	45	11.2.4	Post Updated Chemical Models on the WEB
ŀ	46	12.0	Materials' Requirements Refinement
ŀ	47	12.1	Adsorbent
ŀ	48	13.0	Project Management
ŀ	49	13.1	Center
ŀ	50	13.2	Adsorbent
┢	51	13.3	Chemical
┟	52	14.1	Final Reports
┟	53	14.1	Metal Hydride Report
+	54	14.2	Chemical Report
ł	55	14.3	Adsorbent Repfort
L	~~		

HSECoE

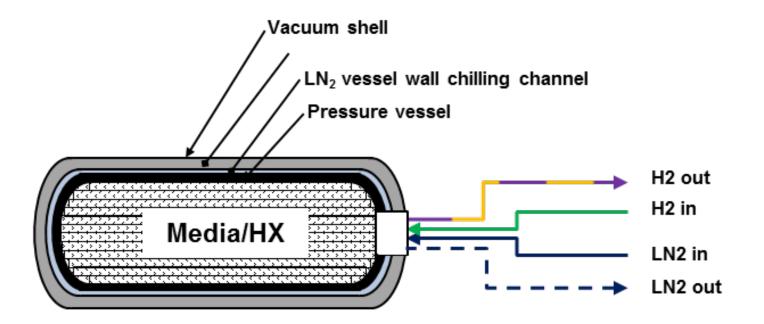
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Adsorbent System Overview



Adsorbent System Overview

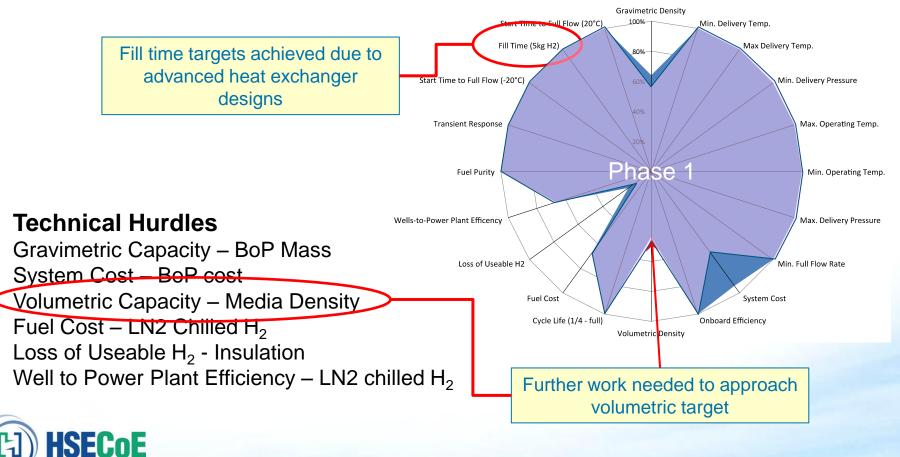




Adsorbent System

Media: MOF-5 P: 5-60 bar – Type I Al Pressure Vessel T: 80-160K - MLVI

HexCell Heat Exchanger

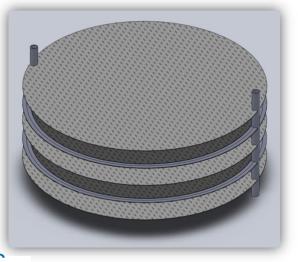


Adsorbent Heat Exchanger Types

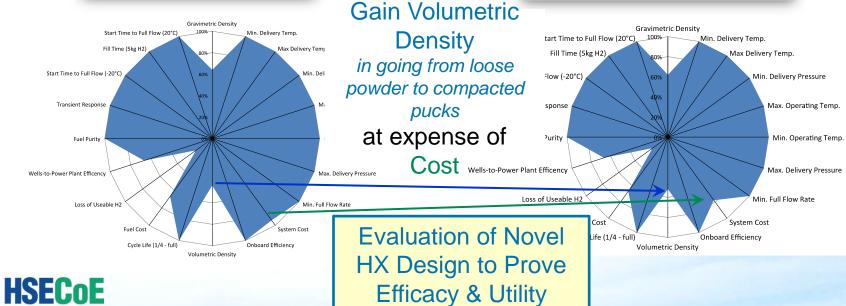
HexCell



MATI



17



Approach HSECoE Adsorbent System S*M*A*R*T Milestones

	-	Addsorbent 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.	12/31/201	
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%.	9/30/2014	Adsorbent Media
Adsorbent Media	LANL	Perform a minimum of 10 heat capacity or thermal conductivity measurments at temperatures ranging from 70-200K on compacted MOF-5 samples preapred by Ford and to support validating system models and system level designs.	9/30/2014	
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.	12/31/201	
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.	9/30/2014	
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.	6/30/201!	MATI System
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.	9/30/201!	
HexCell HX	SRNL/UQTR	Design a 2L adsorbent subscale prototype utilizing a HexCell heat exchanger having 46g avialable hydrogen, internal densities of 0.13g/g gravimetric, and 23.4g/L volumetric.	12/31/2013	
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 avialable hydrogen, internal densities of 0.13g/g gravimetric, and 23.4g/L volumetric.	6/30/2015	HexCell System
Pressure Vessel	Hexagon-Lincoln	Design and manufacture a baseline, separable Type 1 tank 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 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
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	
Particualte Filter	UTRC	Demonstrate a particulate filter for a cryo-adsorbent bed passing less than 1mg/L and 10mm diameter (SAE J2719 guideline).	3/31/2014	Particulate Filter
System Modeling	NREL	Prepare a report on the impact of system design changes on the tank to wheels efficincy and document progress relative to a 300 mile range for adsorbent systems.	9/30/2014	
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
System Modeling	GM	Attend Center F2F meetings and submit a letter memo indicatingtechnical or programitic areas the Center should be pursuing with more emphasis. Actively participate in Center Coordinting Coucnil Telecoms. 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



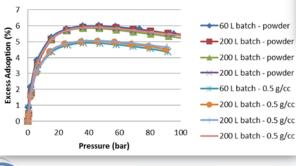
Conduct a scale-up of the MOF-5 manufacturing process to deliver > 9 kg of material while maintaining performance, as measured by surface area and particle size, to within 10% of lab-scale procedure.

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 measurments at temperatures ranging from 70-200K on compacted MOF-5 samples preapred by Ford and to support validating system models and system level designs.

10 kg of MOF-5 Received and Characterized





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Hydrogen Impurity Concentrations Selected

	J2719 SPEC PPM	Airgas Research Grade Hydrogen	OPTION A Airgas Proposal PPM	
Watera	5	.06 to .2	5 to 10 (H2)	
Total Hydrocarbons ^b (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	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 halogenatesd	0.05	< .05 (MDL)	1 (N)	

MATI Half-Pucks Fabricated



Cryogenic thermal conductivity apparatus upgraded for Powder Testing



MATI Heat Exchanger & Test Systems

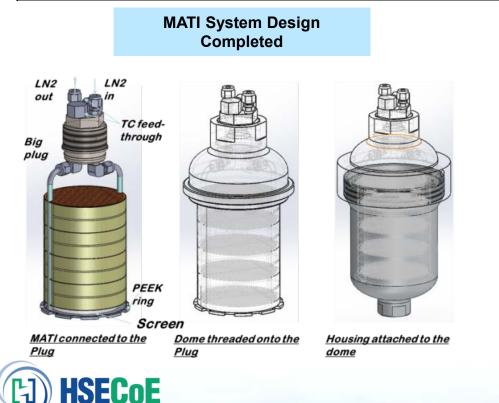


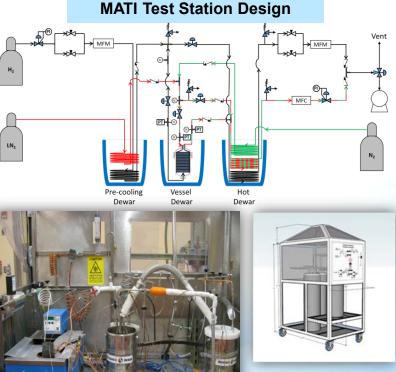
Design a 2L adsorbent subscale prototype utilizing a MATI thermal management system having 54 g available hydrogen, internal densities of 0.10g/g gravimetric, and 27g/L volumetric.

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.





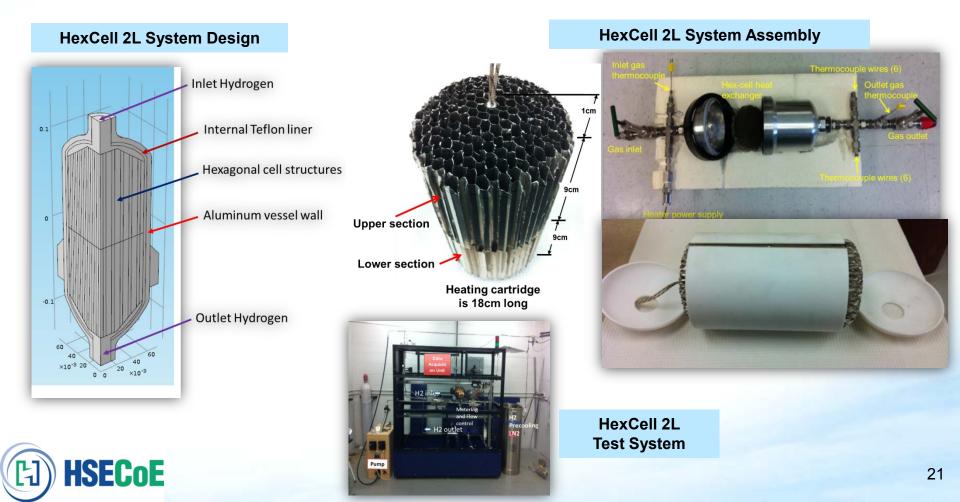
HexCell Heat Exchanger & Test System





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

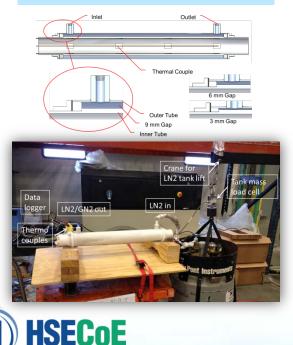


Pressure Vessel Demonstration

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 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.

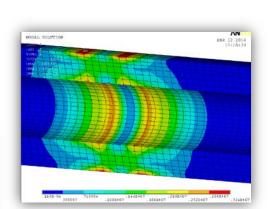
Design alternate tank configurations, such as monolithic Type 1, Type 3 with suitable cryogenic liner, and Type 4 with suitable cryogenic liner, that can operate at 100 bar service pressure, at temperatures of 80K – 160K, and offer a further 10% reduction in weight compared with the Phase 3 baseline 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 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.

Tank Cooling Design and Test Apparatus

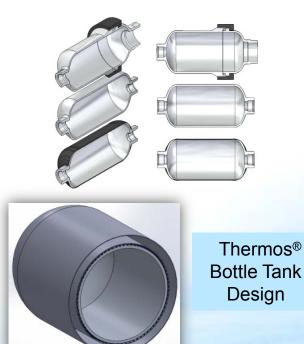


Thermal and Fatigue Stress Calculated

Alternate Tank Configurations



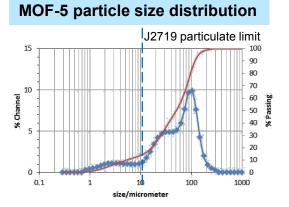
Peak thermal stress is 3.2 MPa (von Mises). Fatigue strength of 100 MPa is required for 5000 cycle life.





Particle Filter Demonstration

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



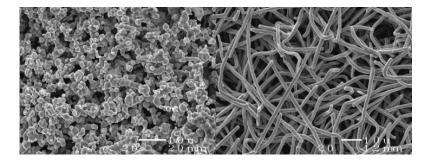
All filters survive LN2 thermal shock testing



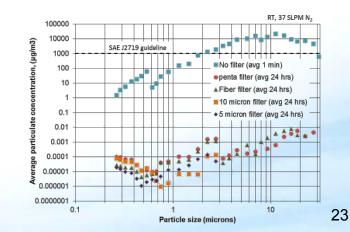
Filter caking after 20 slpm N₂ fluidized MOF-5



Both particle and fiber filters evaluated

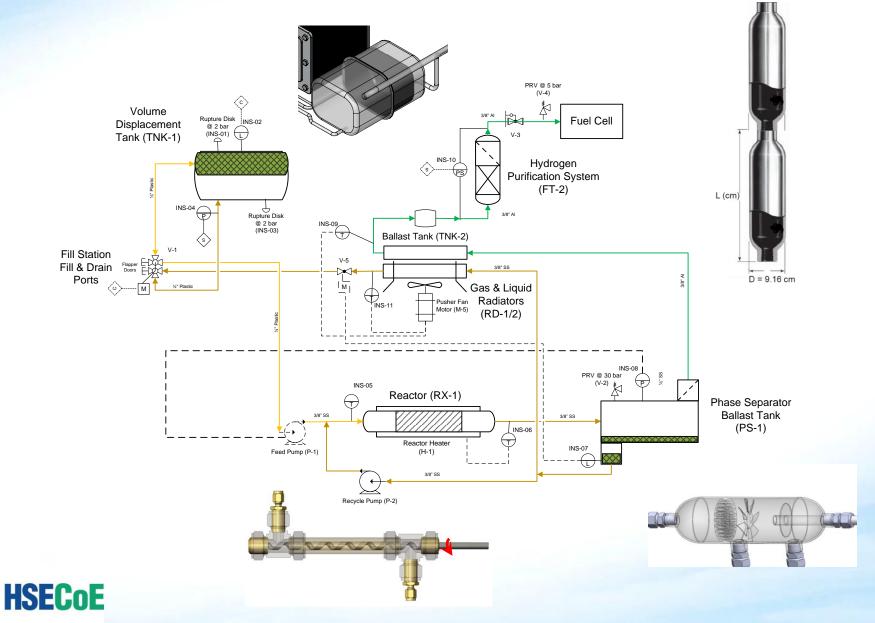


All filters reduce particle entrainment to below J2719 guidelines



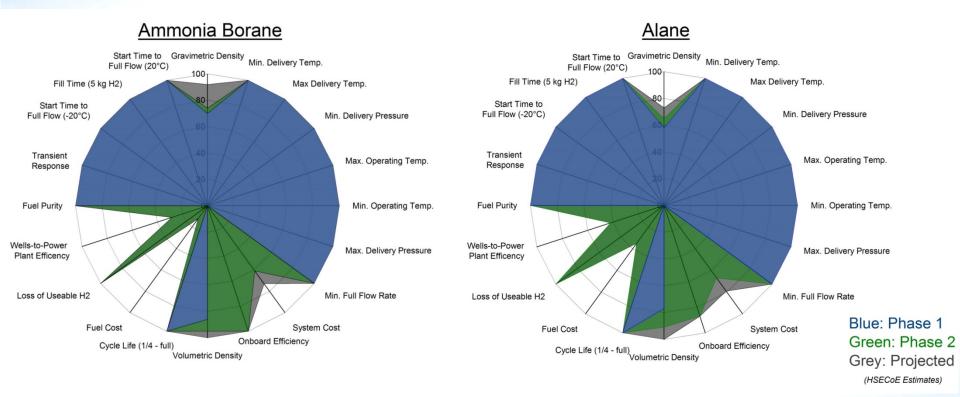
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Chemical System Overview



Chemical System

50 wt.% slurries



<u>Technical Hurdles:</u> Fuel Cost, System Cost, WTPP, Gravimetric Density

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



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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 F	reparation
Flow Through Reactor	LANL	Perform a minimum of 10 flow thorugh reactor studies on 30 and 50 wt. % alane slurries and report space time yields, temperatures and gas compositions for modeling analysis.	12/31/201	Flow	Through
Flow Through Reactor	LANL	Perform a minimum of 10 flow thorugh reactore reactor studies on 30 and 50 wt. % AB slurries and report space time yields, temperatures and gas compositions for modeling analysis.	12/31/201	Re	actor
Gas liquid Seperator	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	BoP Co	mponents
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	Sustam	Madalina
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	System	Modeling
Reporting	LANL/NREL / PNNL / SRNL	Prepare and submit final reports on research efforts related to chemcia hydrgoen storage systems.	3/31/2014	Rep	oorting

Complete
On Schedule
Incomplete



Chemical Hydrogen Media Preparation



LOS Alamos

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





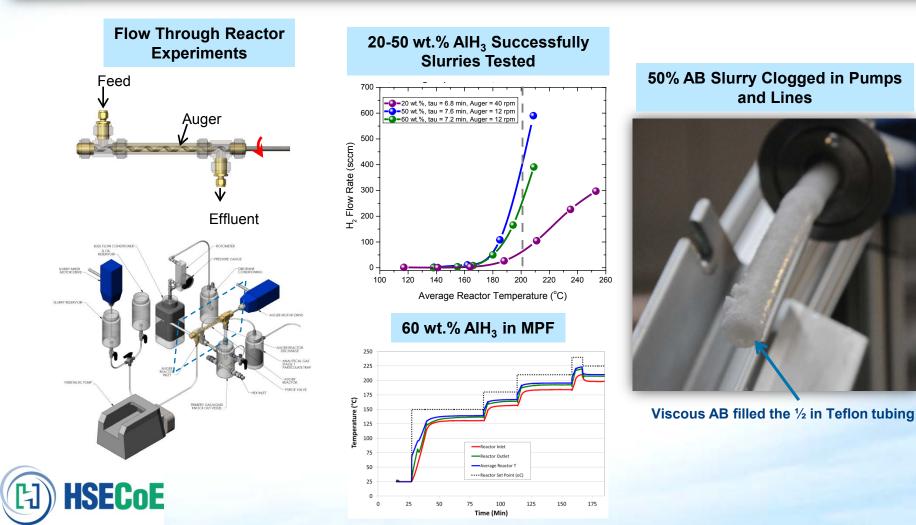
Chemical Hydrogen Media Preparation



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

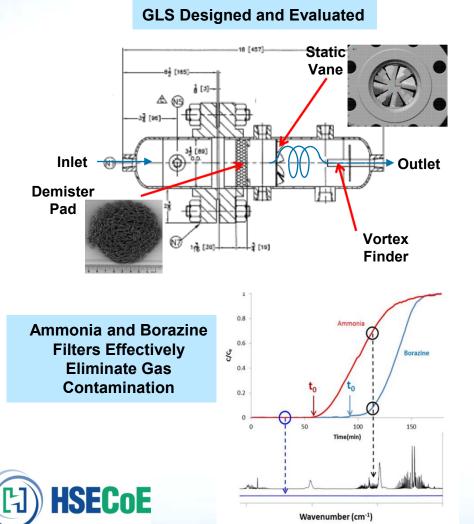


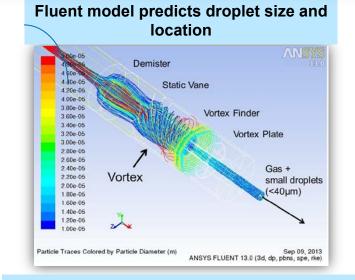


Chemical Hydrogen BoP Components

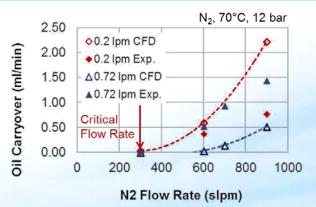
Demonstrate a gas/liquid separator with a specific Souders-Brown velocity of >0.013 (m/s)/kg and >0.029 (m/s)/L.

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).





GLS shown to Effectively Eliminate oil Carryover Under Operational Conditions



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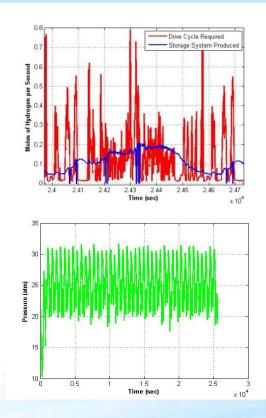
Chemical Hydrogen System Modeling

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

b-d ₽ 한 번 번 번 번 번 번 번 **Exothermic System** 0 Parasitic Energy Modeled 闘 **Thermal Models Match to Experimental Results** 1000.00 300 -Model Reactor Inle 275 LANL Experimental Reactor Setpoint 100.00 250 Reactor Outlet Avg Reactor Tem H2 Generation Rate (sccm) 225 50% AIH₃ 200 Temperature (oC) 10.00 175 150 125 1.00 180 230 280 100 130 75 0.10 50 25 0.01 100 150 250 300 350 400 450 Average Reaction Temperature (°C) Time (minutes)

P&ID Translated to Simulink

System Models Show Continuous Hydrogen Feed from Ballast Tank



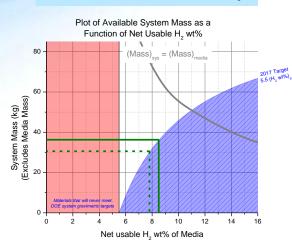


Pacific Northwest

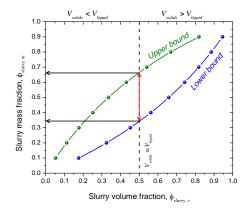
Accomplishment Chemical Hydrogen Material Properties



Media Gravimetric Density



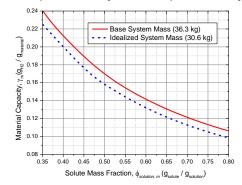
Slurry Mass/Volume Fraction



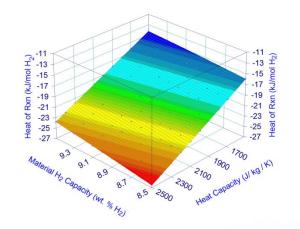
HSECoE

Slurry Gravimetric Density

Plot of solute mass fractions and material capacities required for a base system mass of 36.3 kg and an idealized system mass of 30.6 kg

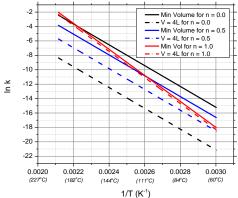


Enthalpy of Reaction

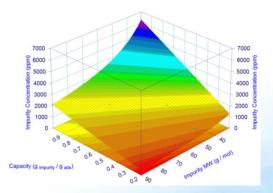


Slurry Kinetics

Arrhenius plots showing the desirable ranges of activation energies (kcal/mol K) and preexponential factors as a function of reaction order



Impurities





Required Materials Properties

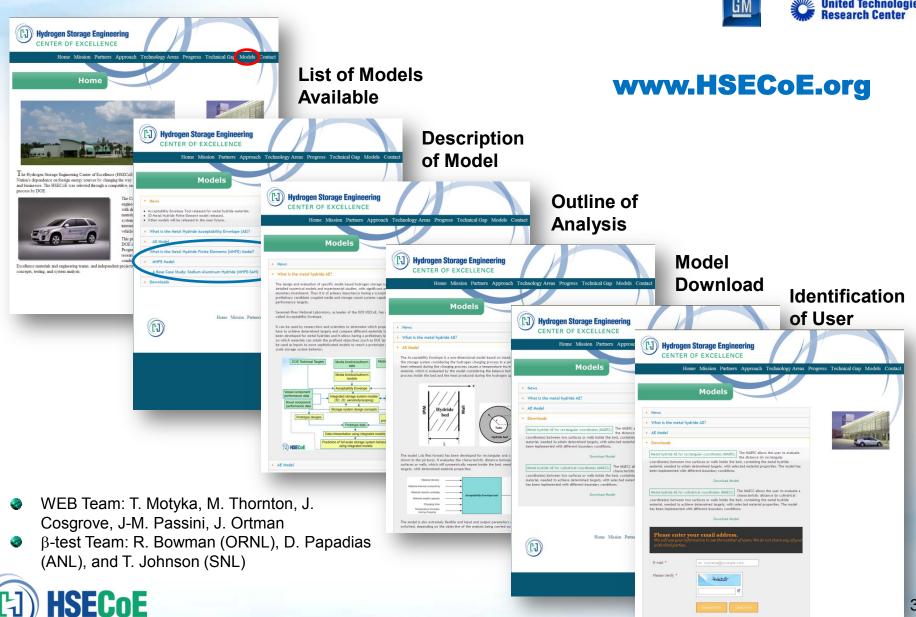
Parameter	Symbol	Units	Range*	Influence	
Minimum Material capacity (liquids)	γmat	g _{H2} / g _{material}	~ 0.078 (<i>0.085</i>) [†]	System	
Minimum Material capacity (solutions)	γmat	g _{H2} / g _{material}	~ 0.098 (<i>0.106</i>) [†]	System	
Minimum Material capacity (slurries)	γmat	g _{H2} / g _{material}	~ 0.112 (<i>0.121</i>) [†]	System	
Kinetics: Activation Energy	Ea	kcal / mol	28–36	Reactor and	
Kinetics: Preexponential Factor	А		4 x 10 ⁹ – 1 x 10 ¹⁶	Shelf life	
Endothermic Heat of Reaction	ΔH _{rxn}	kJ / mol H₂	≤ +17 (<i>15</i>) [†]	On-board efficiency	
Exothermic Heat of Reaction	∆H _{rxn}	kJ / mol H₂	≤ -27		
Maximum Reactor Outlet Temperature	Toutlet	°C	250	Heat Exchanger	
Impurities Concentration	уі	ppm	No <i>a priori</i> estimates can be quantified	Purification	
Media H ₂ Density	Density (γ _{mat}) (φ _m)(ρ _{mat}) kg H₂ / L ≥ 0.07		≥ 0.07	Tank size System	
Regen Efficiency	ηregen	%	≥ 66.6%	Well-to-Power Plant Efficiency	
Viscosity	η	сР	≤ 1500	Fill time Pump size On-board efficiency	





United Technologies

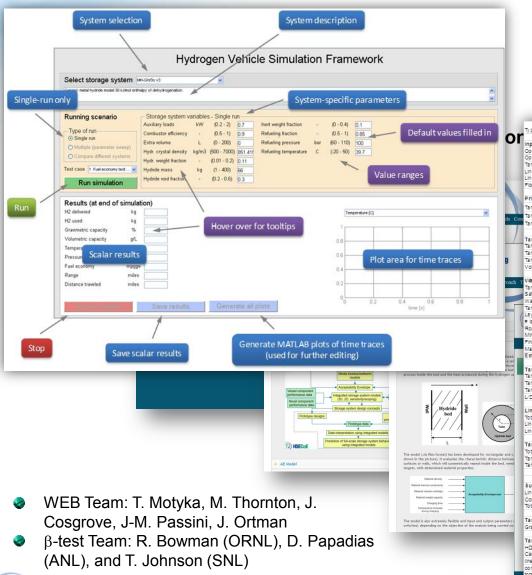
WEB Site Models Added



HSECoE

4

WEB Site Models Added







www.HSECoE.org

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	30.65 6.44 727.0	

Models on the WEB Schedule

MH Acceptability Envelope MH Finite Element Model Tank Volume/Cost Model MH Framework Model CH Framework Model AD Framework Model AD Finite Element Model

Hardy/SRNL	complete
Hardy/SRNL	complete
Simmons/PNNL	complete
Pasini/UTRC	complete
Brooks/PNNL	6/2014
Tamburello/SRNL	9/2014
Hardy/SRNL	3/2015

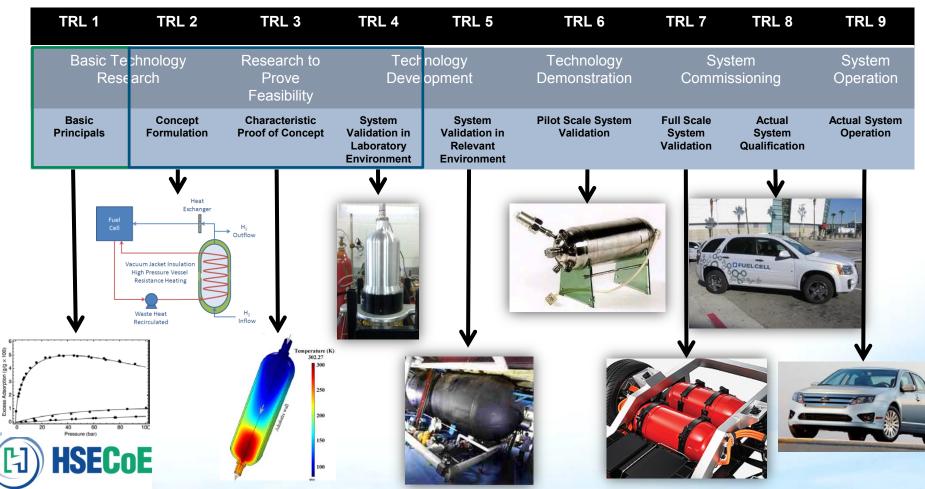


Where are we going in Phase 3: Technology Readiness Levels

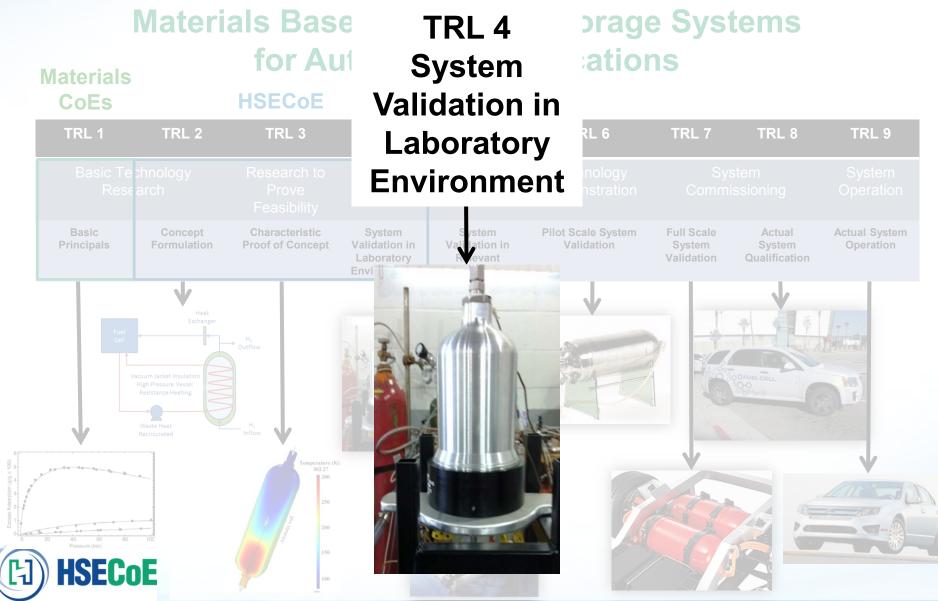
HSECoE

Materials Based Hydrogen Storage Systems for Automotive Applications

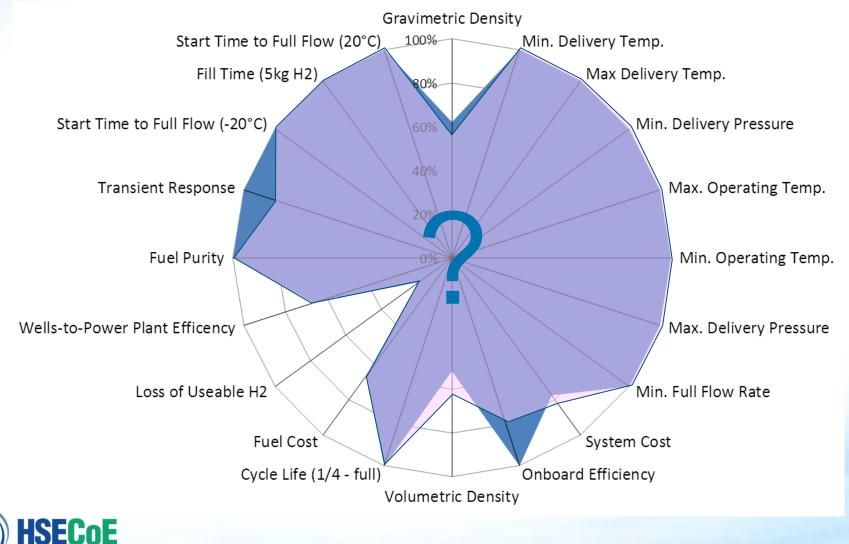
Materials CoEs



Where are we going in Phase 3: Technology Readiness Levels



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

HSEC₀E

- 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

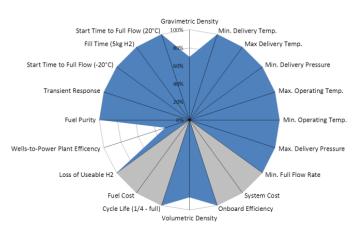
- Limited in gravimetric density and efficiency due to materials limitations.
- AB Slurry could not be pumped while Alane slurry was successfully demonstrated using a auger flow through reactor.
- High fuel cost resulting from recycle inefficiencies limits potential for Chemical Hydrogen Storage materials.

Adsorption Systems

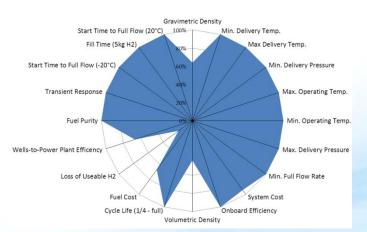
HSEC_DE

- 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

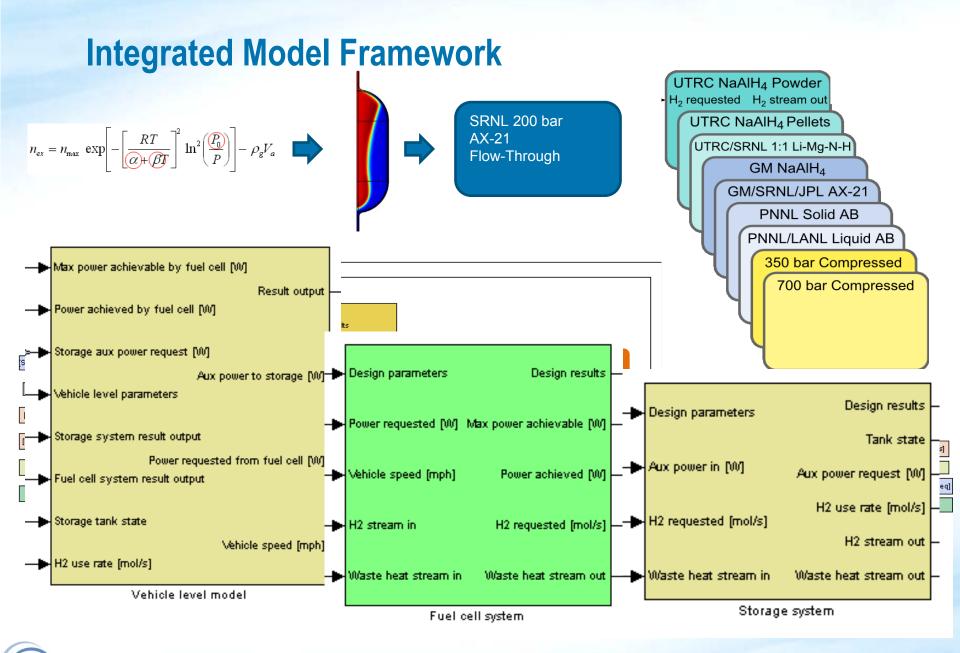
	Target	Gravimetric capacity	Volumetric capacity	System cost	Fuel cost	Ambient temperature	
	Unit	wt%	g-H ₂ /L	\$/kWh net	\$/gge at pump	°C	
Phase 3 ideas for testing specific t Phase 3 goal for this system: System/material form: powder/compacted	2017 Ultimate	5.5 7.5	40 70		2-6 2-3	-40 - 60 (sun) -40 - 60 (sun)	
Will this target be		Yes-Partial	ves-Partial	Maybe	No	Indirect via modeling	
What is the test or	What is the test or model approach?		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 temperatur	
What exactly should be measured in this test to verify the target or model?		system 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	

HSECoE

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System Component Specification

Component	Assumed Validation in Phase II				De	onsible sign ization	What can be validated with modeling rather than experimental wor			
Internal Heat Exchanger: HexCell Resistance Heater with Flow- Through Cooling	Modeling and partial experimental validation of individual components/capabilities		SRNL /	UQTR	1 st -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: Powder MOF-5		Modeling and experimental validation		SRNL / L Ford (E		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 validatio Multi-layer vacuum insulation Modeling of heating rate/dormancy performance		LC	Part	volume, and cost validate proje tial dormancy Validate dorm		rt of system; capacity actions mancy model; vel stability; is of design	Cryo-burst testing No supplier (JPL work scope reduction)		N/A N/A	Yes



HSECoE

Addressing DOE's Technical Targets

HSECoE

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Target	2017 Value	Units	Measurement	Additional_Measurements
Gravimetric Capacity	0.055	g _{H2} / g _{sys}	Total Mass of Gas Stored	Total Mass of System (all equipment, tubing, tank, etc.)
Volumetric Capacity	40	g _{H2} / 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 ₂ 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 ₂ Outlet Pressure	
On-board efficiency	90	%	Energy used to release the hydrogen (converted into H ₂)	
Wells-to-Power Plant Efficiency	60	%	Energy used to refuel / reload the hydrogen (converted into H ₂)	
System Fill Rate	1.5	kg _{H2} / 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 H2
Min Full Flow Rate	0.02	(g/s)/kW	Not Measured at SRNL/OSU	
Start time to full flow rate (20 ^o C)	5	S	H ₂ 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 ₂ 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 ₂	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 ₂	0.05	(g/h)/kg _{H2,stored}	Not Measured at SRNL/OSU	Simplified thermos bottle + MLVI system TBD