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Savannah River National Laboratory

May 14, 2013



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Project ID# ST004

### **Overview**

### Timeline

•Start: February 1, 2009

•End: June 30, 2014

•70% Complete (as of 3/31/13)

### **Budget**

•Total Center Funding:

- DOE Share: \$ 36,232,765
- Contractor Share: \$3,591,709
- FY '12 Funding: \$ 5,930,000
- FY '13 Funding: \$ 5,150,000

Prog. Mgmt. Funding

- FY '12: \$ 400,000
- FY '13: \$ 300,000

HSECoE

### **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.



Relevance

# Why Perform Materials Development and System Engineering in Parallel?

continuous feedback with system design identifying materials requirements







### **Technical Matrix**

		System A	Architects
		Adsorbent System Siegel	Chemical Hydride System Semelsberg
	Performance Modeling & CostAnalysis ThorntonContemporation	Thornton WeimarCONNEL CONNEL Pacific Northwest MICHALLAGONION	Thornton Weimar
	Integrated Power Plant & Storage System Modeling van Hassel	Tamburello	Brooks
Techn	Transport Phenomena Hardy	Hardy <b>SRNL</b> Corgnali, Sulic Ortman, Drost	Brooks Semelsberger
Technology Areas	Materials Operating Requirements Rönnebro	Veenstra Chahine Simpson	Rönnebro Semelsberger
as	Enabling Technologies Simmons	Simmons Newhouse Reiter Reiter	van Hassel Holladay Simmons Semelsberger
	Subscale Prototype Demonstrations	Chahine Hardy SRNL	Semelsberger

### **Phased Approach**



- Where are we and where can we get to?
  - Model
     development
  - Benchmarking
  - Gap Identification
  - Projecting advances

- How do we get there (closing the gaps) and how much further can we go?
  - Component development
  - Concept validation
  - Integration testing
  - System design
  - Materials requirements

- Put it all together and confirm claims.
  - System integration
  - System assessments
  - Model validation
  - Gap analysis
  - Performance projections

### **Important Dates Phase 2**

- Duration: 5.5 years
  - Phase 1 Start: Feb. 1, 2009
  - Phase 1-2 Transition: March 31, 2011
  - Phase 1 End: June 30, 2011
  - Phase 2 Start: July 1, 2011
  - Phase 3 Go/No-Go Determination: March 31,2013
  - Phase 2 End: June 30, 2013
  - Phase 3 Start: July 1, 2013

### Completion Date: June 30, 2014 $\Rightarrow$ 3/31/15?



**HSECoE** 

### Phase 1-2 State-of-the-Art

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

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



**HSECoE** 

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### **HSECoE** Phase 2 Go/NoGo Milestones

Chemical Hydrides				3/31/2011			3/31/2013	
						Phase	2 HSECoE Go	/No-Go
							Targets	
			Phase 1 H	SECoE Base	line (System)		(full scale)	
			Phase 1	Phase 1	Phase 1	Phase 2	Phase 2	Phase 2
		2015 DOE	HSECoE	HSECoE	HSECoE	HSECoE	HSECoE	HSECoE
		Goal	Baseline	Basline	Baseline	Actuals	Actuals	Actuals
Target	Units	(System)	(Material)	(BOP only)	(System)	(Material)	(BOP only)	(System)
Gravametric Capacity	kg H2/kg system	0.055	0.076	0.092	0.042	0.076	0.109	0.045
mass	liters	102			133			124
Volumetric Capacity	kg H2/L system	0.04	0.074	0.077	0.039	0.074	0.102	0.043
volume	kg	140			144			130
System Cost *	\$/kWh net	6		25.6	25.6		25.6	25.6
	\$	480						
Fuel Cost	\$/gge at pump	2-6						
Min Operating Temp	°C	-40			?			0
Max Operating Temp	°C	60			50			50
Min Delivery Temp	°C	-40			-40			-40
Max Delivery Temp	°C	85			85			85
Cycle Life	cycles	1500			1000			1000
Min Delivery Pressure	bar	5			5			5
Max Delivery Pressure	bar	12			12			12
Onboard Efficiency	%	90			97			97
Well to Power Plant Efficiency	%	60			37			37
System Fill Time	min	3.3			2.7			2.7
Min Full Flow Rate	(q/s/kW)	0.02			0.02			0.02
	(g/s/(tv)) a/s	1.6			1.6			1.6
Start Time to Full Flow (20°C)	sec	5			1			1.0
Start Time to Full Flow (-20°C)		15			1			1
Transient Response	sec	0.75			0.49			0.49
Fuel Purity	%H2	99.97			99.97			99.99
	/0112	Meets or			00.01			00.00
Permeation, Toxicity, Safety	Scc/h	Exceeds			s			s
	000/11	Standards			Ũ			U
Loss of Useable Hydrogen	(g/h)/kg H2 stored				0.1			0.1
	(g/H//Kg HZ otorod	0.00			0.1			0.1
Responsible Organization	Component		3/31/2011			3/31/2013		
LANL, PNNL			Fluid AB a	t 50w#%		Fluid AB at 6	5w#%	
PNNL			Bladder Ta			Bladder Tank		
	Reactor			gh Reactor		Flow Through		
	System Design			grincedetoi		now mough	Reactor	
FININL	BoP							
PNNL	Pumps		Feed/Recy	cle/Transfer F	Pumps	Feed/Recycle	e/Transfer Pum	ine
UTRC	Heat Exchanger		r eeu/rtecy		umpa		ger mass and	
UTRC	GLS		Gas\Liquid	Separator		Gas\Liquid S		
UTRC	Purification		Purification				rification mass	and volume
UIRC	Funication		runication	1		nyurugen Pu		



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### **HSECoE** Phase 2 Go/NoGo Milestones

Chemical Hydrides				3/31/2011			3/31/2013	
						Phase	2 HSECoE Go	/No-Go
							Targets	
			Phase 1 H	SECoE Base	line (System)		(full scale)	
			Phase 1	Phase 1	Phase 1	Phase 2	Phase 2	Phase 2
		2015 DOE	HSECoE	HSECoE	HSECoE	HSECoE	HSECoE	HSECoE
		Goal	Baseline	Basline	Baseline	Actuals	Actuals	Actuals
Target	Units	(System)	(Material)	(BOP only)	(System)	(Material)	(BOP only)	(System)
Gravametric Capacity	kg H2/kg system	0.055	0.076	0.092	0.042	0.076	0.109	0.045
mass	liters	102			133			124
Volumetric Capacity	kg H2/L system	0.04	0.074	0.077	0.039	0.074	0.102	0.043
volume	kg	140			144			130
System Cost *	\$/kWh net	6		25.6	25.6		25.6	25.6
	\$	480						
Fuel Cost	\$/gge at pump	2-6						
Min Operating Temp	°C	-40			?			C
Max Operating Temp	°C	60			50			50
Min Delivery Temp	°C	-40			-40			-40
Max Delivery Temp	°C	85			85			85
Cycle Life	cycles	1500			1000			1000
Min Delivery Pressure	bar	5			5			5
Max Delivery Pressure	bar	12			12			12
Onboard Efficiency	%	90			97			97
Well to Power Plant Efficiency	%	60			37			37
System Fill Time	min	3.3			2.7			2.7
Min Full Flow Rate	(q/s/kW)	0.02			0.02			0.02
	g/s	1.6			1.6			1.6
Start Time to Full Flow (20°C)	sec	5			1			1
Start Time to Full Flow (-20°C)		15			1			1
Transient Response	sec	0.75			0.49			0.49
Fuel Purity	%H2	99.97			99.97			99.99
-		Meets or						
Permeation, Toxicity, Safety	Scc/h	Exceeds			S			s
		Standards						
Loss of Useable Hydrogen	(g/h)/kg H2 stored	0.05			0.1			0.1
Responsible Organization	Component		3/31/2011			3/31/2013		
LANL, PNNL			Fluid AB a	t 50wt%		Fluid AB at 6	5wt%	
PNNL	Tark		Bladder Ta	nk		Bladder Tank		
LANL	Reactor		Flow Throu	gh Reactor		Flow Through	Reactor	
PNNL	System Design					_		
	BoP							
PNNL	Pumps		Feed/Recy	cle/Transfer F	Pumps	Feed/Recycle	e/Transfer Pum	ips
UTRC	Heat Exchanger		Í		-		ger mass and	•
UTRC	GLS		Gas\Liquid	Seperator		Gas\Liquid S		
UTRC	Purification		Purification				rification mass	and volume

**HSECoE** 

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### **HSECoE** Phase 2 Go/NoGo Milestones

	Chemic	al Hydrides				3/31/2011			3/31/2013		
					Phase 1 H	SECoE Base	line (System)	Phase 2	2 HSECoE Go Targets (full scale)	o/No-Go	
				2015 DOE	Phase 1	Phase 1 HSECoE	Phase 1 HSECoE	Phase 2 HSECoE	Phase 2 HSECoE	Phase 2 HSECoE	
				Goal	Baseline	Basline	Baseline	Actuals	Actuals	Actuals	
	Creation at a	Target	Units	(System)		(BOP only)		(Material)	(BOP only)	(System)	
	Gravametri	ic Capacity mass	kg H2/kg system liters	0.055 102	0.076	0.092	0.042 133	0.076	0.109	0.045 124	
	Volumetric		kg H2/L system	0.04	0.074	0.077	0.039	0.074	0.102	0.043	
	Volumotine	volume	kg	140	0.071	0.011	144	0.07 1	0.102	130	
	System Co	ost *	\$/kWh net	6		25.6	25.6		25.6	25.6	
			\$	480							
	Fuel Cost		\$/gge at pump	2-6							
	Min Opera	0	°C	-40			?			0	
	Max Opera Min Delive	ating Temp	℃ ℃	60 -40			<u>50</u> -40			50 -40	
	Max Delive		°C	-40			-40			-40	
	- · · · ·		· · ·	1		1				1	
Responsible Organiz	ation	Component		3/3	31/2011				3/31/201	13	
LANL	, PNNL	Media		FI	uid AB a	at 50wt%			Fluid AE	3 at 65wt9	6
	PNNL	Tank		BI	adder Ta	ank			Bladder	Tank	
	LANL	Reactor		FI	ow Throu	ugh Read	tor		Flow Th	rough Rea	actor
		System Des	ian			0				0	
	BoP PNNL Pu										
				E	Feed/Recycle/Transfer Pumps				Eood/De	ovolo/Tra	nofor Dumpo
					eu/Rec			μs		•	insfer Pumps
	UTRC	Heat Excha	anger						Heat Ex	changer r	mass and volume c
	UTRC		GLS	Ga	as\Liquio	d Seperat	tor		Gas\Liquid Seperator		
	UTRC	Purific	ation		Purification				Hydrogen Purification mass and volu		
					-				.,		
	D	ble Organization	0 +		3/31/2011			3/31/2013			

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

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### **Phase 2** Adsorbent System Milestones

Component Materials Development	Ford	S*M*A*R*T Milestone Report on ability to develop compacted MOF-5 adsorbent media having a total hydrogen material density of greater than or equal to 0.3 g/t. 42 density of 11 wt. % and 33 g/liter and thermal	Status 10/1/12 H2 grav. density of the MCF-5 material >11% is possible with .3 g/cc. (w/o ENG) at P = 60-5 bar and T = 80-160K with 60% packing efficiency. H2 vol. density of the MOF-5 material >33 gl is possible with .5 g/cc (+5% ENG) at P = 60-5 bar and T = 80-160K with 100% packing efficiency. Thermal conductivity of 5 W/m-K is possible with .3 g/cc to	
Materials Development	Ford/UM/ BASF	conductivity of 0.5 W/m-K at P = 60-5 bar and T = 80-160K. Report on ability to demonstrate a composite MOF-5 adsorbent monoliths having H2 effective kinetics equivalent to 5.6 kg usable H2 over 3 minutes and permeation in packed and powder particle beds with flow rate of 1 m/s superficial velocity and pressure drop of 5 bar.		metrics. Met Metric The kinetic response of the MOF-5 mat the desired response while the permeat be a challenge with densities greater th
Materials Development	SRNL/ UQTR	Report on ability to develop a compacted MOF-5 adsorbent media bed having a total hydrogen density of: 11 % g H2/(g MOF) and 33 g H2/(liter MOF) at P = 60 - 5 bar and T = 80 - 160 K	Lealuation of isothems provided by Ford for initial & final states gives: 180kg/m² (uncompacted) GC=0.15 VC=26.5 missing the VC metric 322kg/m² GC=0.10 VC=33.0 missing the GC metric 520g/m² GC=0.07 VC=33.7 missing the GC metric	Alternative compaction methods will be to identify higher volumetric density mor meeting the metrics.
Structured Bed	GM	Report on ability to develop MOF-5 powder bed having a total hydrogen density of: 15 wt. % g H2/(g MOF) and 20 g H2/(liter MOF) at P = 60 - 5 bar and T = 80 - 160 K.	Based on the modified DubiningsAsthakov adsorption model, at 60 - 5 bar and 80 - 160 K the 3 liter test vessel contains 18.6% total deliverable g H2/(g MOF) and 30.5% g H2/(liter MOF) surpassing the metric.	Exceeded metric These results will be validated with lab e
Composite Tank	JPL	Report on ability to develop testing capability to burst test Type 4 composite and Type 1 (metal) tanks at 40K and demonstrate tanks meeting minimally 2.5x nominal operating burst pressure.	Design and fabrication of a cryogenic pressure test/burst system capable of testing at 77K has been completed. Safety oversight and documentation is currently 75% complete. Operating this system at 40 K is not feasible. The capability to perform cryogenic cycling has also been implimented.	Safety documentation will be completed of Type 4 COPVs, pressure testing of Ty be performed at 77K and adding the cap cryogenic cycoic testing capability <b>exce</b> <b>metrics</b> at his temperature.
Composite Tank	Lincoln	Report on ability to develop Type 4 (composite) and Type 1 (metal) tanks capable of use between 40 and 160K meeting ASME pressure vessel code for use at 60 bar having a mass less than 10 kg and a volume less than 120 liters.	Type 1 tanks have been designed and manufactured having a mass of 2.44 kg and a volume of 2.0 lites. These tanks were designed to operate at 100 bar with a minimum burst ratio of 2.25 (225 bar). The actual burst achieved during RI testing was 686 bar. Type 4 tanks have been designed and manufactured having a mass of 3.7 kg and a volume of 5.68 liters. These tanks were designed to operate at 100 bar with a minimum burst ratio of 2.25 (225 bar). The actual burst achieved during RI burst achieved during RT testing was 370 bar. anks have been suppied to JPL to brust testing at 7K to entry low temperature burst pressures. These tanks were appropriately designed having safety factors equivalent to current DOI MTRSA standards for compressed gas bull containers.	Based on these resutts single piece 120 Type 4 tanks will be designed and and and calculated. It is anticipated that the Type meet hte mass target while the <b>Type</b> 4
Composite Tank	PNNL	Report on ability to identify Type IV tank liner materials suitable for 40K operation having a mass less than 8 kg and a volume less than 3 liters (2.55 mm thickness).	After evaluating 8 different materials it was occuluded that the liner separates from the shell when the pressure is decreased below 35bar with a liner thickness of 2.55mm. With current materials this <b>metric is not feasible</b> and either a Type 1 or 3 tank design is necessary.	Metric not achievable
MLVI	JPL	Report on ability to develop a thermal insulation design having less than a 5 W heat leak at 40K having a mass less than 11 kg and volume less than 35 liters.	Detailed modeling and coupon-scale validation experiments have been completed showing that the thermal isolation system composed of a 60-layer MLI blanket composed of VDA mylar and dacron separators within a vacuum of at least 16+1 Grr, reduces parasitic heat load to 2V for a voceding the metric.	25% scale experimental verification has preliminary results are being analyzed w exceeding of metric.
Internal MATI HX	OSU	Report on ability to develop and demonstrate a Modular Adsorption Tank Insert capable of allowing less than 3 min. refueling time and H2 release rate of 0.02 g H2/(sec. kW) with a mass less than 9.4 kg and a volume less than 4.2 liters.	Current MATI designs exceed the metric for weight and volume, similulation demonstrates that these designs can provide the required discharge performance.	Exceeded metric Laboratory testing is being used to confi and manufacturing studies have confirme can be used for this component.
Internal non-MATI HX	UTRC- SRNL	Report on ability to develop and demonstrate an isolated heat- exchanging loop capable of allowing less than 3 min. refueling time and $HZ$ release rate of 0.02 g $HZ$ (sec. KW) with a mass less than 6.5 kg and a volume less than 6 liters.	The efficacy of an isotated-dop internal heat exchanger was examined. Computational analyses showed that four externally heated hydrogen (fuel cell radiator heated) through isolated heating channels of a fin-and-tube HX within the adsorbent would NOT provide enough heat for the minimum drive cycle requirements. An H2 combustor should be able to raise the H2 temperature high enough, however the fin-and-tube HX has higher mass and volume than a comparable MATI.	This metric was suspended as not viab
Internal flow through HX	SRNL/ UQTR	Report on ability to develop and demonstrate an internal flow through HX system based on compacted medic acpable of allowing less than 3 min. scaled refueling time and H2 release rate of 0.02 g H2(sec. kW) with a mass less than 6.5 kg and a volume less than 6 liters.	Models for 6mm 322kg/m3 pellets indicate that, relative to 130kg/m3 powder, flow through cooling requires a significantly larger mass of exhaust hydrogen and a longer time to cool. <b>Compacted MOF will not meet the metric</b> . It appears that <u>180kg/m3 MOF-5 powder in an aluminum honeycomb</u> will meet the metric.	Met metric Experiments to validate the models and concept are in progress at UQTR. Pellet loaded into hex mesh.
Internal flow through HX	GM	Report on ability to develop and demonstrate an internal flow through cooling system based on powder media capable of allowing less than 3 min. scaled refueling time, and an internal heating system for scaled H2 release rate of 0.20 g H2/(sec. kW) with a mass less than 6.5 kg and a volume less than 6 liters.	Model of charging process predicts that for a 60bar system, a 10.3 liter, 27.7 kg heat exchanger is required to successfully discharges 5.6 kg /H2 at lulicacle. For a 200 bar system, a 5.5 liter 15 kg aluminum helical coil HX is capable of meeting discharge target. The current experimental stainless steel sheathed coils have higher density. Neither HX meets the mass metric.	It is not anticipated that the mass me achieved. Bypass line and pressure tra added to the test system in order to con and initial bed temperature at conditions through cooling experiment. The model p determined experimentally.
External HX	JPL	Report on ability to develop and demonstrate FC radiator capable of heating 80K hydrogen stream to 233K flowing at 1.6g/sec with no icing at 50%RH with a mass increase of less than 2.5 kg and a volume less than 1.5 liters.	performance metrics at all but -40°C ambient conditions. An auxiliary heater may be required for such conditions.	Met metrics. Changes in funding and sc demonstration, and no experimental valid conducted.
Catalytic Combustor	OSU	Report on ability to develop and demonstrate a 1 kW catalytic combustor to augment partial H2 preconditioning by an existing FC radiator with >85% efficiency having a mass less than 0.6 kg and volume less than 0.5 liters.	Validated simulation results demonstrate that the microchannel combustor has an efficency >95% meeting the metric.	Metric exceeded A small prototype with 7 to 10 unit cells validate models and estimate the mass a
ВоР	PNNL	Report on ability to identify BoP materials (excluding internal HX, external HX, and combustor) suitable for 60 bar cryogenic adsorbert system having mass less than 17 kg and a volume less than 18.5 liters.	The BOP mass is significantly reduced with the lower pressure from 200bar to 69bar. The mass of the 69 bar solenoid operated values are 1/10th the weight of the 200 bar values with an overall mass and volume of 0.81kg and 0.63L respectively. The final BOP mass and volume without the internal tank heat exchanger, the fuel cell, H2 gas warm up loop, and the tank is 6.7kg and 8.5L <b>far exceeding the metric</b> .	Metric exceeded
System Design	SRNL	Report on ability to identify a system design having a mass less than 137 kg and a volume less than 279 liters meeting the all of the HSECoE drive cycles	Several system designs exceeding metricss: - 200 bar, 80 K, Powder MOF-5, FT Cooling + HexCell HX Type 3 Tank (System mass = 110 kg, System volume = 219 L) - 100 bar, 70 K, Powder MOF-5, FT Cooling + HexCell HX Type 1 Al Tank (System mass = 127 kg, System volume = 258 L) - 80 bar, 80 K, 80 % MPD 0.322 g/cc Compacted MOF-5, MATI, Type 3 Tank (System mass = 120 kg, System volume = 25 L)	Metric exceeded
Efficiency Analysis	NREL	Calculate and model the well-to-powerplant (WTPP) efficiency for two adsorbent storage system designs and compare results relative to the 60% technical target.	In progress	Will complete by 12/31/12

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### **Phase 2** Adsorbent System Milestones

	Adsorbent System Component	Partner		S*M*A*R*T Milestone	Status 10/1/12		Projected Outcome
	Materials Development	Ford	having a tota to 0.3 g/L, H	ility to develop compacted MOF-5 adsorbent media I hydrogen material density of greater than or equal 2 density of 11 wt. % and 33 g/liter and thermal of 0.5 W/m-K at P = 60-5 bar and T = 80-160K.	H2 grav. density of the MOF-5 material >11% is possible with .3 g/cc (w/o ENG) at $P = 60.5$ with 60% packing efficiency. H2 vol. density of the MOF-5 material >33 g/l is possible with .60-5 bar and T = 80-160K with 100% packing efficiency. Thermal conductivity of .5 W/m-K is .5 g/cc + 10% ENG with temperatures > 100-120 K.	The capability of achieving specific metrics with a given configuration is possible, investigations will be continue to devise a media morphology which will <b>meet all of the metrics</b> .	
	Materials Development	Ford/UM/ BASF	monoliths ha H2 over 3 mi	ility to demonstrate a composite MOF-5 adsorbent ving H2 effective kinetics equivalent to 5.6 kg usable nutes and permeation in packed and powder particle w rate of 1 m/s superficial velocity and pressure drop	kinetics is planned. Permeation testing has been conducted for various temperatures and de extrapolation of permiation test data at 0.12 m/s, the 5bar pressure drop milestone is possib uncompressed darcy) at a media density of 0.3 g/cc but will be a significant challenge beyon the metric.	sities. Based on the e (initial assessment of	Met Metric The kinetic response of the MOF-5 material will achieve the desired response while the permeation will continue to be a challenge with densities greater than 0.3 g/cc.
	Materials Development	SRNL/ UQTR	media bed ha	ility to develop a compacted MOF-5 adsorbent aving a total hydrogen density of: 11 % g H2/(g g gH2/(liter MOF) at P = 60 - 5 bar and T = 80 - 16	Evaluation of isothems provided by Ford for initial & final states gives: 1806g/m <sup>2</sup> (uncompacted) GC=0.15 VC=26.5 missing the VC metric 322kg/m <sup>2</sup> GC=0.10 VC=33.0 missing the GC metric 520g/m <sup>3</sup> GC=0.07 VC=38.7 missing the GC metric		Alternative compaction methods will be pursued with Ford to identify higher volumetric density morphologies meeting the metrics.
	Structured Bed	GM	hydrogen der	ility to develop MOF-5 powder bed having a total nsity of: 15 wt. % g H2/(g MOF) and 20 g H2/(liter 60 - 5 bar and T = 80 - 160 K.	Based on the modified Dubinin-Asthakov adsorption model, at 60 - 5 bar and 80 - 160 K the 5 18.6% total deliverable g H2/(g MOF) and 30.5% g H2/(liter MOF) surpassing the metric.	liter test vessel contains	Exceeded metric These results will be validated with lab experiments.
	Composite Tank	JPL		ility to develop testing capability to burst test Type 4 d Type 1 (metal) tanks at 40K and demonstrate	Design and fabrication of a cryogenic pressure test/burst system capable of testing at 77K h Safety oversight and documentation is currently 75% complete. Operating this system at 40 capability to perform couponic currently has also been implemented.		Safety documentation will be completed and burst testing of Type 4 COPVs, pressure testing of Type 1 tanks will be performed at 77K and adding the capability of concepting events fasting capability according the
Report on abili	ty to identify	Tune	<u> </u>	After evaluating 8 d	ifferent materials it was concluded		
•	• •	• •		that the liner separate	ates from the shell when the		
ank liner mate					sed below 35bar with a liner		
operation havir kg and a volum	•			1'	m. With current materials this	Metric	not achievable
•		, iiie	13	metric is not feasi	<b>ble</b> and either a Type 1 or 3 tank		
(2.55 mm thick	(ness).			design is necessar	у.		
	Internal MATI HX	OSU		lity to develop and demonstrate a Modular ank Insert capable of allowing less than 3 min.	Current MATI designs exceed the metric for weight and volume, similulation demonstrates t	nat these designs can	Exceeded metric Laboratory testing is being used to confirm simulations
			mass less th	e and H2 release rate of 0.02 g H2/(sec. kW) with a an 9.4 kg and a volume less than 4.2 liters.	provide the required discharge performance. The efficacy of an isolated-loop internal heat exchanger was examined. Computational analy	on abound that former	and manufacturing studies have confirmed that aluminum can be used for this component.
	Internal non-MATI HX	UTRC- SRNL	exchanging I time and H2 less than 6.5	ility to develop and demonstrate an isolated heat- oop capable of allowing less than 3 min. refueling release rate of 0.02 g H2/(sec. kW) with a mass is g and a volume less than 6 liters.	The emcacy or an isolateo-loop internal neat exchanger was examined. Computational analy externally headed hydrogen (tude call radiator heade) through isolated heating channels of a f adsorbert would NOT provide enough heat for the minimum drive cycle requirements. An H2 able to raise the H2 temperature high enough, however the fin-and-tube HX has higher mass a comparable MATI.	n-and-tube HX within the combustor should be	This metric was suspended as not viable.
	Internal flow through HX	SRNL/ UQTR	through HX s allowing less rate of 0.02 g	ility to develop and demonstrate an internal flow ystem based on compacted media capable of than 3 min. scaled refueling time and H2 release y H2/(sec. kW) with a mass less than 6.5 kg and a than 6 litres	Models for 6mm 322kg/m3 pellets indicate that, relative to 130kg/m3 powder, flow through c significantly larger mass of exhaust hydrogen and a longer time to cool. Compacted MOF metric. It appears that <u>180kg/m3 MOF-5 powder in an aluminum honeycomb</u> will meet the	vill not meet the	Met metric Experiments to validate the models and demonstrate the concept are in progress at UQTR. Pellets have been loaded into hex mesh.
	Internal flow through HX	GM	volume less than 6 liters. Report on ability to develop and demonstrate an internal flow through cooling system based on powder media capable of allowing less than 3 min. scaled refueling time, and an internal heating system for scaled H2 release rate of 0.02 g H2/(sec. kW) with a mass less than 5.5 kg and a volume less than 6 liters.		Model of charging process predicts that for a 60bar system, a 10.3 liter, 27.7 kg heat exchar successfully discharges 5.6 kg H2 at full-scale. For a 200 bar system, a 5.5 liter 15 kg alumi capable of meeting discharge target. The current experimental stainless steel sheathed coils Neither HX meets the mass metric.	num helical coil HX is	It is not anticipated that the mass metric can be exhered. Bypass line and pressure transducer will be added to the test system in order to control the inite! H2 and initial bed temperature at conditions needed for flow- through cooling experiment. The model predictions will be determined experimentally.
	External HX	JPL	of heating 80 no icing at 50 a volume less	ility to develop and demonstrate FC radiator capable K hydrogen stream to 233K flowing at 1.6g/sec with 9%RH with a mass increase of less than 2.5 kg and s than 1.5 liters.	performance metrics at all but -40°C ambient conditions. An auxiliary heater may be required	Met metrics. Changes in funding and scope have exluded demonstration, and no experimental validation will be conducted.	
	Catalytic Combustor	OSU	combustor to FC radiator v	ility to develop and demonstrate a 1 kW catalytic b augment partial H2 preconditioning by an existing with >85% efficiency having a mass less than 0.6 kg ess than 0.5 liters.	Validated simulation results demonstrate that the microchannel combustor has an efficency >95% meeting the		Metric exceeded A small prototype with 7 to 10 unit cells will be tested to validate models and estimate the mass and volume.
			Report on ability to identify BoP materials (excluding internal HX, external HX, and combustor) suitable for 60 bar cryogenic adsorbent system having mass less than 17 kg and a volume less than 18.5 liters.		The BOP mass is significantly reduced with the lower pressure from 200bar to 69bar. The mass of the 69 bar solenoi operated values are 1/10h the weight of the 200 bar values with an overall mass and volume of 0.81kg and 0.63L respectively. The final BoP mass and volume without the internal tank heat exchanger, the fuel cell, H2 gas warm up loop, and the tank is 6.7kg and 8.5L <b>far exceeding the metric</b> .		Metric exceeded
	ВоР	PNNL	external HX, adsorbent sy	stem having mass less than 17 kg and a volume	loop, and the tank is 6.7kg and 8.5L far exceeding the metric.		
	BoP System Design	PNNL	external HX, adsorbent sy less than 18. Report on ab than 137 kg	stem having mass less than 17 kg and a volume	loop, and the tank is 6.7kg and 8.5L far exceeding the metric.	200 bar, 80 K, Powder 19 L) 127 kg, System volume	Metric exceeded

**HSECoE** 

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two adsorbent storage system designs and compare results relative to the 60% technical target.

Exceeded

Met

Continuing

# Phase 2 Adsorbent System Milestones

	Adsorbent System	Partner		S*M*A*R*T Milestone	Status 10/1/12		Projected Outcome
	Materials Development	Ford	having a tota to 0.3 g/L, H	ility to develop compacted MOF-5 adsorbent media I hydrogen material density of greater than or equal 2 density of 11 wt. % and 33 g/liter and thermal of 0.5 W/m-K at P = 60-5 bar and T = 80-160K.		/cc (+5% ENG) at P =	The capability of achieving specific metrics with a given configuration is possible, investigations will be continue to
	Materials Development	Ford/UM/ BASF	monoliths ha H2 over 3 mi		H2 effective kinetics have been conducted and proven over 240 cycles for MOF-5 powder. The m kinetics is planned. Permeation testing has been conducted for various temperatures and densi extrapolation of permitation test data at 0.12 m/s. the 5bar pressure drop milestone is possible ( uncompressed darcy) at a media density of 0.3 g/cc but will be a significant challenge beyond ti <b>the metric</b> .	ies. Based on the nitial assessment of	Met Metric The kinetic response of the MOF-5 material will achieve the desired response while the permeation will continue to be a challenge with densities greater than 0.3 g/cc.
	Materials Development	SRNL/ UQTR	media bed ha	ility to develop a compacted MOF-5 adsorbent aving a total hydrogen density of: 11 % g H2/(g g H2/(liter MOF) at P = 60 - 5 bar and T = 80 - 160	Evaluation of isotherms provided by Ford for initial & final states gives: 160kg/m <sup>2</sup> (uncompacted) GC=0.15 VC=26.5 missing the VC metric 322kg/m <sup>2</sup> GC=0.10 VC=33.0 missing the GC metric 520g/m <sup>2</sup> GC=0.07 VC=35.7 missing the GC metric		Alternative compaction methods will be pursued with Ford to identify higher volumetric density morphologies meeting the metrics.
	Structured Bed	GM	hydrogen der	ility to develop MOF-5 powder bed having a total nsity of: 15 wt. % g H2/(g MOF) and 20 g H2/(liter 60 - 5 bar and T = 80 - 160 K.	Based on the modified Dubinin-Asthakov adsorption model, at 60 - 5 bar and 80 - 160 K the 3 lit 18.6% total deliverable g H2/(g MOF) and 30.5% g H2/(liter MOF) surpassing the metric.	er test vessel contains	Exceeded metric These results will be validated with lab experiments.
	Composite Tank	JPL		ility to develop testing capability to burst test Type 4 nd Type 1 (metal) tanks at 40K and demonstrate	Design and fabrication of a cryogenic pressure test/burst system capable of testing at 77K has Safety oversight and documentation is currently 75% complete. Operating this system at 40 K is exploited to the system of the system at each provide the system of the system.		Safety documentation will be completed and burst testing of Type 4 COPVs, pressure testing of Type 1 tanks will be performed at 77K and adding the capability of excession excession testing accessibility.
Report on abilit ank liner mate operation having kg and a volum	rials suitable g a mass les	for 4	40K an 8	that the liner separa pressure is decreas	ifferent materials it was concluded ates from the shell when the sed below 35bar with a liner m. With current materials this	Metric I	not achievable
(2.55 mm thick			15	metric is not feasi design is necessar	<b>ble</b> and either a Type 1 or 3 tank		
	Internal MATI HX	OSU	refueling time	ank Insert capable of allowing less than 3 min. e and H2 release rate of 0.02 g H2/(sec. kW) with a an 9.4 kg and a volume less than 4.2 liters.	Current MATI designs exceed the metric for weight and volume, similulation demonstrates that provide the required discharge performance.	these designs can	Laboratory testing is being used to confirm simulations and manufacturing studies have confirmed that aluminum can be used for this component.
	Internal non-MATI HX	UTRC- SRNL	Report on ab exchanging I time and H2	ity to develop and demonstrate an isolated heat- oop capable of allowing less than 3 min. refueling release rate of 0.02 g H2/(sec. kW) with a mass i kg and a volume less than 6 liters.	The efficacy of an isolated-loop internal heat exchanger was examined. Computational analyse externally heated hydrogen (fuel cell radiator heated) through isolated heating channels of a fin- adsorbent would NOT provide enough heat for the minimum dine cycle requirements. An H2 con able to raise the H2 temperature high enough, however the fin-and-tube HX has higher mass and comparable MATI.	ind-tube HX within the nbustor should be	This <b>metric was suspended</b> as not vlable.
	Internal flow through HX	SRNL/ UQTR	through HX s allowing less	ility to develop and demonstrate an internal flow ystem based on compacted media capable of than 3 min. scaled refueling time and H2 release J H2/(sec. kW) with a mass less than 6.5 kg and a han 6 liters.	Models for 6mm 322kg/m3 pellets indicate that, relative to 130kg/m3 powder, flow through cool significantly larger mass of exhaust hydrogen and a longer time to cool. <b>Compacted MOF will</b> metric. It appears that <u>180kg/m3 MOF-S powder in an aluminum honeycomb</u> will meet the m	not meet the	Met metric Experiments to validate the models and demonstrate the concept are in progress at UQTR. Pellets have been loaded into hex mesh.
Report on abilit Insulation desig 5 W heat leak a less than 11 kg 35 liters.	n having les at 40K having	s tha g a n	an a nass	experiments have b thermal isolation sy blanket composed within a vacuum of a	and coupon-scale validation een completed showing that the stem composed of a 60-layer MLI of VDA mylar and dacron separators at least 1e-4 Torr, reduces parasitic <b>r exceeding the metric.</b>	been sta being ar	ale experimental verification arted, and preliminary resunal nalyzed which should provi <b>ing of metric</b> .
_				•		00 bar, 80 K, Powder	
	System Design	SRNL	than 137 kg	ility to identify a system design having a mass less and a volume less than 279 liters meeting the all of drive cycles	MOF-5, FT Cooling + HexCell HX, Type 3 Tank (System mass = 110 kg, System volume = 219 - 100 bar, 70 K, Powder MOF-5, FT Cooling + HexCell HX, Type 1 Al Tank (System mass = 12 = 258 L) - 80 bar, 80 K, 80% MPD 0.322 g/cc Compacted MOF-5, (System mass = 120 kg, System volume = 259 L)	7 kg, System volume	Metric exceeded
	Efficiency Analysis	NREL	two adsorber	d model the well-to-powerplant (WTPP) efficiency for t storage system designs and compare results a 60% technical target	In progress		Will complete by 12/31/12

Suspended

Not Met

### **Chemical Hydride System Projection** End of Phase 1 Fuel Cell

#### 2017 Targets

Media: Fluid Phase Ammonia Borane: 50wt.% AB in BMIMCI (1-n-butyl-3-methylimidazolium chloride)

- 12 Components:
  - **Bladder Tank**
  - **Flow Through Reactor**
  - Gas Liquid Separator/Ballast Tank
  - Radiator

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Hydrogen Purification

H<sub>2</sub> Purity

**HSECoE** 



**HSECoE** 

### **Chemical Hydride: Slurry Development**

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



#### Ammonia Borane Slurry Development



H-

release

13

release

## **Chemical Hydride: Reactor**



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



14

260 280

### **Chemical Hydride: BoP-Gas/Liquid Separator**





# **Chemical Hydride: BoP-Gas Purification**



United Technologies Research Center

Milestone		Metric Outcome
Report on ability to <b>develop a borazine s</b> minimum replacment interval of 1800 miles in a minimum outlet borazine concentration concentration = 4,000 ppm) having a maxin kg and maximum volume less of 3.6 liters.	of driving resulting of 0.1 ppm (inlet	achieved but volume metric missed. of adsorbent media could be conducted to meet etric but emphasis will be placed on reactor
Report on ability to <b>develop an ammonia</b> minimum replacment interval of 1800 miles in a minimum ammonia outlet concentration concentration = 500 ppm )having a maximu and a maximum volume of 1.6 liters.	of driving resulting n of 0.1 ppm (inlet Met Metric	
0.05 0.00001 0.0001 0.001 0.01 0.1 1 PNH3/bar	20C model 20C 50C model 50C 77C model 77C UTRC	Ammonia $t_0$
15% 10% 5% 6% 1 2 2 disorption/desorption cycle number [-] 7 80 wt% Mrci2 on IRH-33 5% 6% 10% 10% 10% 10% 10% 10% 10% 10	B C D 60 psig, 0 % RH	Wavenumber (cm <sup>-1</sup> )
HSECoE		

**HSECoE** 

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### **Chemical Hydride: System Design**



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



### **Chemical Hydride: BoP-Displacement Tank**





One liter volume displacement tank designed/built/tested

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



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



Viton is a registered trademark of DuPont Performance 18 Elastomers L.L.C.



### **Chemical Hydride System Waterfall Charts**



#### Volume Target



# Chemical Hydride System Projection End of Phase 2

2017 Targets

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





# **Chemical Hydride System Projection** End of Phase 2

2017 Targets

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

**Gravimetric Density** 

**On-Board Efficiency** 

**System Cost** 

H<sub>2</sub> Purity

- Gas Liquid Separator/Ballast Tank
- Radiator
- Purification



Volumetric Density

Onboard Efficiency

Cycle Life (1/4 - full)



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### Adsorbent System Projection End of Phase 1 2017 Targets



Multilayer insulation

Evel cell components (outs)

### **Adsorbent System: Media Engineering**



Milestone	Metric Outcome
Report on ability to <b>develop compacted MOF-5 adsorbent media</b> having a total hydrogen material density of greater than or equal to 0.3 g/L, H2 density of 11 wt. % and 33 g/liter and thermal conductivity of 0.5 W/m-K at P = 60-5 bar and T = 80-160K.	The capability of achieving individual metrics with a given configuration has been demonstrated. No one structure has been identified achieving all of the metrics.
	<b>Met Metric</b> The kinetic response of the MOF-5 material will achieve the desired response while the permeation will continue to be a challenge with densities greater than 0.3 g/cc.



# **Adsorbent System: BoP-Composite Tank**



#### Cryo-burst test facility competed



**HSECoE** 





#### Segmented AI tank design



#### Composite tank design



#### **Cryogenic Tank Testing**







HEXAGON



**HSECoE** 

### **Adsorbent System: BoP-Insulation Development**



	Milestone	м	etric Outcome
	evelop a thermal insulation design having less than K having a mass less than 11 kg and volume less	25% scale experimental vernic	cation has been started, and preliminary hich should prove <b>exceeding of metric</b> .
Bell Jar	<image/>	Image: Sector	
		2.7	○ Experiment: 30 Layers

2.5 C

5.0E-05

1.0E-04

P [Torr]

1.5E-04

2.0E-04

### **Adsorbent System: BoP-Internal Heat Exchange**



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

### Modular Adsorption Tank Insert (MATI)

#### System Concept



Cross-flow HX

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

**HSECoE** 



MATI v1 – Combined LN2 cooling and H2 distribution









### **Adsorbent System: BoP-Internal Heat Exchange**



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

#### Powder & Pellet HexCell HX



### **Adsorbent System: System Design**



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

Internal heat exchanges (al cobons) (x45) Thank types (x6) Low, internal (x6) Hermitighand (x7) Heat and types (x7) (x7) (x7) Mastar appeel (x7) (x7) (x7) Mastar appeel (x7) Mastar appeel (x7) Heat and types (x7) Heat and types (x7) Personal (x7) Heat and types (x7) Heat and types (x7) Personal (x7) Heat and types (x7) Heat			(x2)	x87)	Eliminate unrealizable system options and combinations of options 22 Million Reasonable System Combinations: - Immer Neat econges ( Ja option; ( Jal) - There ( yes ( G) - Uebo Tation ( G) - Meening Next ( Jal) - Meening Next				
Option #1	<u> </u>	Option #	s	Option N	Full tank pressure (x12)     Full tank pressure (x12)     Full tank temperature (x6)     Empty tank temperature (x8)				
1	1	1		1					
2	1	1		1	Filter the				
					Results				
N.	1	1		1	Final 4 Systems:				
1	2	1		1	<ul> <li>Three flow-through cooling with resistance HX options:</li> </ul>				
2	2	1		1	1. HexCell with powder MOF-5				
	i. Ne	No		Ne	2. HexCell with 0.32 g/cc compacted MOF-5 pellets				
N									

**HSECoE** 

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



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0151	All sealed by pro-	10.00		18.00	1.00			610	1.00				Procey Edit and enables and enabled
011-	Insulation	12.00	73.00	18.2	1.00	53	8.00	<b>E1X</b>	100	0.180	1.00	347	insulation should with F23 (assumed to be 3) size of residence system service
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0.38	And Parker Dr.	100.00	73.00	100.00	1.00.00	85.0	6.00	80.00	10.0				Defrex.



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**HSECoE** 

### **HexCell Adsorbent System Projection** End of Phase 2 2017 Targets HexCel

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



### **HexCell Adsorbent System Projection** End of Phase 2 2017 Targets HexCel

MOF-5, no thermal enhancement, 80 K initial fill XXXX ٠ aration/Isolati Pressure Regula Valve/Connector with Manual Override Type 1 Al pressure vessel, 100 bar • Pressure Relief o Fuel Cell) Double-wall 60-layer MLVI jacket design, 5W heat leak @ 80 K . drogen Refueling low-through coo Adsorption: Porous-bed "flow-through" cooling/fueling Glycol Tank utlet stream • ouid Nitrogen Tan Multi-port Refu oling Inlet Stream vdrogen Cond **Desorption: Electrical resistance heater/honeycomb HX 140K** Receptacle (fem iquid Nitrogen Tanl integrated chee Heat Exchange ooling Outlet Stre TBD Gravimetric Density HSECoE Estimates Start Time to Full Flow (20°C) 100% Min. Delivery Temp. Max Delivery Temp. Fill Time (5kg H2) Start Time to Full Flow (-20°C) Min. Delivery Pressure Gravimetric Density-1. Volumetric Density 2. Transient Response Max. Operating Temp. 3. System Cost Loss of Usable H<sub>2</sub> 4. Phase Euel Purity Min. Operating Temp. Wells-to-Power Plant Efficency Max. Delivery Pressure Loss of Useable H2 Min. Full Flow Rate Fuel Cost System Cost Cycle Life (1/4 - full) Onboard Efficiency **HSECoE** Volumetric Density

1013 (TC)

### **MATI Adsorbent System Projection** End of Phase 2 2017 Targets MATI

- Compacted MOF-5, no thermal enhancement, 80 K initial fill •
- •
- •
- Adsorption: LN2 chilled plates
- Desorption: BoP heated H2/140K



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### **MATI Adsorbent System Projection** End of Phase 2 2017 Targets MATI

- Compacted MOF-5, no thermal enhancement, 80 K initial fill •
- Type 1 AI pressure vessel, 100 bar •



tinos O

Valve/Connector with

Manual Overrid

Runture Disk
# Waterfall Charts for 80 K, 100 bar HexCell System





### Adsorbent System FMEA Updated Failure Modes and Effects Analysis

Highest risk items identified from initial FMEA

#### Corrective actions taken

#### Example actions during phase 2 for reducing the Risk Priority Number (RPN)

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



### **Wells-to-Power Plant Analyses**

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

#### **Drive Cycles**



#### **Energy Efficiency**

**HSECoE** 

4



#### **Integrated System Modeling**



#### **GHG Emissions**



# **Technical Target Prioritization**

- ٠
- All targets must still be met simultaneously All Prioritization identifies performance must-have vs. design choice targets
- Guides design trade-offs to optimize overall ۲ system/vehicle performance to meet customer expectations
- QFD approach originally taken

#### Method for the refined analysis ۲

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

### **Refined Analysis**

HSECOE

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

#### **Original Target Ranking**







### **WEB Site Models Added**



### **WEB Site Models Added**



(C1) Hydrogen Storage Engine

### **WEB Site Models Added**



Home Mission Partners Approach Technology Areas I

Models

- News
- What is the Metal Hydride Acceptability Envelope (AE)?
- AE Model
- What is the Metal Hydride Finite Elements (MHFE) Model?

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

The Savannah River National Laboratory, as the leader of the HSECoE, developed a new detailed 30 model (MHFE) based on a Finite Element approach. The model is valid for general metal hydride vessels.

The approach followed in developing the model is summarized here:

- 1. Three simplified scoping models (for kinetics, scaling (geometry) and heat removal) have been set up (not currently available in the download section) in order to assess preliminary system designs prior to invoking the detailed 3D finite element analysis. Such simplified models can be used, along with the Acceptability Envelope (AE) model analysis, to perform and a quick assessment of storage systems and identify those capable of achieving determined performance targets. The kinetics scoping model can be used to evaluate the effect of temperature and pressure on the loading and discharge kinetics, determining the optimum achievable loading. The geometry acoping tool can be used to evaluate the size of the system, the optimal placement of heat transfer equipment and the gravimetric capacities for the geometry conjunt and the maximum achievable for the context configuration and the system. Me optimal placement of heat transfer equipment and the gravimetric capacities for the geometry conjing model to achie use to calculate the state of the system (increases over the length of the cooling channels. More details about the scoping models available in *heavy*, *j. Hardy&Actum* 1.
- 2. The MHFE model has been set up including energy (with heat and pressure work exchange), momentum and mass balances, along with chemical kinetics. To do that, the data available from the scoping models can be used as inputs to the detailed 30 model. In particular? (1) the output from the geometry scoping tool can be used as inputs for the model geometry, or, alternatively, available data about bed dimensions can be directly used as inputs for the energy balance equation or, alternatively data wailable about the used as inputs for the energy balance equation or, alternatively data wailable about the scope of the start of the scope of the scope

### R. Bowman and T. Jo test models

**HSECoE** 



Models

News

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

One of the most promising metal hydride materials, studied all around the world, is Sodium Aluminum Hydride (SAH). A detailed 30 model for SAH based on the Finite Element approach has been implemented in COMSCO Multiphysics Version 4.2a platform. Kinetics data were collecter from the experiments previously carried out by United Technologies Research Center<sup>®</sup> (UTRC) for their SAH prototypes (see <u>Masher I</u>) and the COMSOL® model has been applied to one of the UTRC prototype designs.

#### SHELL AND FINNED TUBE HYDRIDE VESSEL [PROTOTYPE]





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

#### HYDRIDE BED CROSS SECTION SCHEMATIC



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





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## **Metal Hydride FEM Model**



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3D_NaAlH4_Loading_2012.mph (root)	▼ Parameters				A statistics
Pi Parameters	Name	Expression	Value	Description	
a= Variables 1	Pref	101325	101325	Reference Pressure (Pa), Atmospheric Pressure	
- Therpolation 1 (A)	Uref	0.1	0.10000	Reference Speed (0.1 m/s)	
. Interpolation 3 (Bz.	Lref	0.1	0.10000	Reference Length (m) - Bed Radius	
S. Interpolation 4 (Cz.	Cref	Pref/(R*Tref)	40.624	Reference Concentration (mol/m^3)	
Ny Interpolation 5 (Dz.	Tref	300	300.00	Reference Temperature (K)	
Interpolation 6 (Ah	rho_ref	M_H2*Cref	0.081898	Reference H2 Density (kg/m^3)	
Interpolation 7 (Bh)	co	P0/(R*T0)	32.674	Initial H2 Concentration (mol/m^3)	
Interpolation 8 (C) (Linterpolation 9 (Jh)	Dp	3E-7	3.0000e-07	Bed Particle Diameter	
S. Interpolation 1 (Ak)	epsilon	.5	0.50000	Bed Void Fraction	
S. Interpolatic , 1 S./	M_NaAlH4	54/1000	0.054000	g-molecular weight of NaAlH4 (Kg/mol)	
wation 12 (c')	M_H2	2.016/1000	0.0020160	g-molecular weight of H2 (Kg/mol)	
Interpolation 13 (Dk,	R	8.314	8.3140	Gas Constant [J/mol-K]	
Interpolation 14 (Ek)	PO	101325	101325	Initial Pressure (Pa)	
Interpolation 15 (Fk)	TO	373	373.00	Initial Bed Temperature (K)	
Interpolation 17 (Bv)	Tinj	373	373.00	Temperature of Injected H2 (K)	
Interpolation 18 (Cv)	Vinj	14	14.000	Velocity of Injected H2 in Feed Tube (m/s)	0.1
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## **Metal Hydride FEM Model**



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# **Metal Hydride FEM Model**





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# **Metal Hydride FEM Model**





295 MB | 315 MB

### Accomplishment/Future Work

# **HSECoE Website Status/Plan**

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



# 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

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### **System Test Matrixes**

Phase 3 ideas for testing s hase 3 goal for this system:	· · ·																					
ystem/material form: powder/a	compacted? Flo Target	Gravimetric capacity	Volumetric capacity	System cost	Fuel cost	Ambient temperature	Min/max delivery temperature	Operational cycle life (1/4 tank to full)	Min delivery pressure to FC	Max delivery pressure to FC	On-board efficiency	Well to power plant efficiency	System fill rate	Min full flow rate	Start time to full flow (20°C)	Start time to full flow (-20°C)	Transient response (10%-90% & 90%- 0%)	Fuel purity (SAE J2719 & ISO/PDTS 14687-2)	Permeation & leakage	Toxicity	Safety	Loss of usable
-	Unit 2017 Ultimate	wt% 5.5 7.5	g-H <sub>2</sub> /L 40 70	\$/kWh net	\$/gge at pump 2-6 2-3	*C -40 - 60 (sun) -40 - 60 (sun)	°C -40/85 -40/85	cycles 1500 1500	bar (abs) 5 3	bar (abs) 12 12	%	%	kg-H <sub>2</sub> /min 1.5 2	(g/s)/kW 0.02 0.02	s 5 5	s 15 15	s 0.75 0.75	%H <sub>2</sub> 99.97 99.97	Scch/h See note See note	- See note See note	- See note See note	(g/h)/kg-H2 stor 0.05 0.05
ill this target be tested?		Yes-Partial	Yes-Partial	Maybe	No	Indirect via modeling	Indirect via modeling	Yes-Partial	Yes	Yes	Yes	Indirect via modeling	Yes	Indirect via modeling	Yes	Indirect via modeling	Yes	Yes	No	Yes-Partial	Yes	Yes
that 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	room temperature	delivery temperature Separate	Stress models ASME. Limited material cycling test (possibly 500 cycles?) + extrapolation	Test both 3 and 5 bar.	regulation to 12 bar functions over specified operating	warm system to	Modeling: Thornton, Hardy	Detailed model car estimate what flow rates / sorbent/ minimum temperature and what pressure?	Modeling:	Experiments: Chahine	Modeling: Tamburello & Hardy	Modeling: Hardy; Experiments: Chahine	H2 purity from	Reiter and	Dust cloud ignition	Design should be robust and testing procedures should be vetted in advance for possible risks	
what exactly should be measured in his test to verify the target or model?		Usable capacity. Include 5 bar & 3 bar operating pressure as test matrix and see effect on gravimetric	Usable capacity	Estaimated costs of lab scale system to actual cost of lab scale system			H2 outlet temperature	Fatigue behavior. Structure of tank internals before/after cycling (tomography?). H2 purity before/after	at a function of charge state and discharge rate	H2 outlet pressure at a function of charge state and discharge rate	Energy input to tank to induce H2 release	Cost and energy inputs during refill	Time to complete fill as a function of tank starting temperature and state of charge	H2 outlet flow as a function of state of charge and "drive cycle"	full flow	Time to achieve full flow. Consider extrapolating 20 C data to -20 C.		desorbed gas using	through liner.	N/A. BASF and/or UTRC will conduct dust cloud tests?		Temperature of tank vs time. Vacuum level in insulated jacket.
that is the reference test or model nare	i refers to experiments; 'M' efers to models	Test 4.4 - System Delivery Test E:	4.3 - System Fill Test 4.4 - System Delivery Test E: Chahine M: Tamburello	Sytem Cost Projections M: Weimar & Veenstra	WTW Efficiency Projections M: Thornton	<insert model<br="">name&gt;M: Tamburello</insert>	name> M:	Cycle Tests; E: Chahine and Simmons		r 4.4 System Delivery Test; E: Chahine				Test and 4.6 System	4.5 - System start- up test; E: Chahine	up test; M:			Buithers and	Dust cloud test; E: Khalil and/or BASF	Safety Protocols; E Chahine	: Insulation Test; Reiter
oes the test involve possible scaling? Will the system size be varied in hase 3 to examine finite-size ffects?)		No. Only one size will be tested	No. Only one size will be tested	volume manufacturing will	scale to account for economies of scale (large number of			No. Only one size will be tested	No. Only one size will be tested	No. Only one size will be tested	No. Only one size will be tested	No. Only one size will be tested	Possibly. Should detemine how fill time varies with state of charge and initital temperature	No. Only one size will be tested			No. Only one size will be tested		Consider for Phase 2 at JPL	N/A	N/A	Yes, examine different amour of insulation
modeling required to justify scaling? should modeling be used to etermine the size of the system or ragnitude of effect to be tested?)		between finite- size effects and the size of system which can	Yes. Need to quantify tradeoff between finite- size of fects and the size of system which can realistically be tested.	° Yes	Yes	No	No	No	No	No	Yes	No	Yes. Need to quantify tradeoff between finite- size effects and the size of system which can realistically be tested.	Yes	No	No	Yes	No	No	No	No	Yes
there any contraints to the test set- p (i.e. test facility limits, materials vailability, etc.) ?		See UQTR limits below		N/A	N/A	Unlikely that heating or cooling system to these temperatures will be possible.	Chahine	Cycle test is limited by time to complete a cycle and consumables (H2, N2)	No	No	No	N/A	Note limitations or UQTR cooling rate of compressed H2		No? Chahine	N/A	Chahine	Test rig should be designed to enable sampling of H2 purity	Reiter	N/A	Chahine	Availability of M is a concern. JPL address

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## **System Test Matrixes**

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		Т	arge	et			metri acity	с		olume capaci			Syste	em co:	st		Fuel c	cost			nbien perati	
			Unit	t		w	٬t%			g-H <sub>2</sub> /	'L		\$/kV	Wh ne	t	\$/{	gge at	pump	)		°C	
Phase 3 ideas for testing spec Phase 3 goal for this system: System/material form: powder/comp			2017				5.5			40							2-6				60 (si	
	Target	capacity	lltima capacity	te	70ELCOX	7	7.5	IIIC [1/4 tank to	pressure to FC	70 pressure to FC	efficiency	1	System ini rate	MILLION FACE	flow (20*C)	flow (-20°C)	2-3	<u>}</u>		-40 -	60 (si	un)
	Unit	wt%	g-H <sub>2</sub> /L	\$/kWh net	\$/gge at pump	*C	°C	full) cycles	bar (abs)	bar (abs)	efficiency %	plant efficiency %	kg-H <sub>2</sub> /min	(g/s)/kW	s	5	0%) s	14687-2) %H <sub>2</sub>	leakage Scch/h			(g/h)/kg-H2 sto
	2017 Ultimate	5.5 7.5 Yes-Partial	40 70 Yes-Partial	Maybe	2-6 2-3 No	-40 - 60 (sun) -40 - 60 (sun) Indirect via modeling	-40/85 -40/85 Indirect via modeling	1500 1500 Yes-Partial	5 3 Yes	12 12 Yes	90 Yes	60 Indirect via modeling	1.5 2 Yes	0.02 0.02 Indirect via modeling	5 5 Yes	15 15 Indirect via modeling	0.75 0.75 Yes	99.97 99.97 Yes	See note See note No	See note See note Yes-Partial	See note See note Yes	0.05 0.05 Yes
hat is the test or model approach?	in: lis In: an to		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		Test will be at room temperature	Will measure H2 delivery temperature Separate component test	Stress models ASME. Limited material cycling test (possibly 500 cycles?) + extrapolation	Test both 3 and 5 bar.	regulation to 12 bar	warm system to	Modeling: Thornton, Hardy			Experiments: Chahine	Modeling: Tamburello & Hardy	Modeling: Hardy; Experiments: Chahine	H2 purity from		Dust cloud ignition	Design should be robust and testing procedures should be vetted in advance for possible risks	g Clarify whethe
hat exactly should be measured in is test to verify the target or model?	ini ba pr mi ef	sable capacity. clude 5 bar & 3 ar operating ressure as test atrix and see ifect on ravimetric	Usable capacity	actual cost of lab	Amount of LN2 and H2 consumed during refill	External temperature	H2 outlet temperature	Fatigue behavior. Structure of tank internals before/after cycling (tomography?). H2 purity before/after	at a function of charge state and			Cost and energy inputs during refill	tank starting	H2 outlet flow as a function of state of charge and "drive cycle"	Time to achieve	extrapolating 20.C	Time to achieve desired response in flow rate	Composition of desorbed gas using Mass spectrometer or RGA.	Transport of H2 through liner. Other?	N/A. BASF and/or UTRC will conduct dust cloud tests?	Meets appicable safety standards	Temperature ( tank vs time. Vacuum level insulated jack
E refe hat is the reference test or model nar experi refers t	ers to iments; 'M' to models	est 4 - System elivery Test E: hahine M:	4.3 - System Fill Test 4.4 - System Delivery Test E: Chahine M: Tamburello	Sytem Cost Projections M: Weimar & Veenstra		<insert model<br="">name&gt; M: Tamburello</insert>	≺Insert model name> M: Tamburello	Cycle Tests; E: Chahine and Simmons			/ 4.4 System Delivery Test; E: Chahine	4.3 System Fill test, M: Thornton, Hardy	4.3 System Fill Test; E: Chahine, M: Hardy &	4.4 System Deliver Test and 4.6 System Dynamic Test; M: Pasini, Tamburello, Hardy; E: Chahine	4.5 - System start-	4.5 - System start- up test; M: Tamburello and Hardy	4.6 System Dynamic Test; E: Chahine		Permeation Test: E Reither and Simmons	Dust cloud test; E: Khalil and/or BASF	Safety Protocols; E Chahine	E: Insulation Tes Reiter
oes the test involve possible scaling? Vill the system size be varied in vare 3 to examine finite-size fects?)			No. Only one size will be tested			No. Only one size will be tested	No. Only one size will be tested	No. Only one size will be tested	No. Only one size will be tested	No. Only one size will be tested		No. Only one size will be tested	Possibly. Should detemine how fill time varies with state of charge and initital temperature		No. Only one size will be tested		No. Only one size will be tested	N/A	Consider for Phase 2 at JPL	N/A	N/A	Yes, examine different amo of insulation
modeling required to justify scaling? hould modeling be used to termine the size of the system or agnitude of effect to be tested?)	qu be siz siz vil	uantify tradeoff etween finite- ze effects and the ze of system hich can	Yes. Need to quantify tradeoff between finite- size of system which can realistically be tested.	e Yes	Yes	No	No	No	No	No	Yes	No	Yes. Need to quantify tradeoff between finite- size effects and the size of system which can realistically be tested.	Yes	No	No	Yes	No	No	No	No	Yes
there any contraints to the test set- p (i.e. test facility limits, materials valiability, etc.) ?			See UQTR limits below	N/A	N/A	Unlikely that heating or cooling system to these temperatures will be possible.	Chahine	Cycle test is limited by time to complete a cycle and consumables (H2, N2)		No	No	N/A	Note limitations on UQTR cooling rate of compressed H2		No? Chahine	N/A	Chahine	Test rig should be designed to enable sampling of H2 purity	Reiter	N/A	Chahine	Availability of is a concern. J address

### **System Test Matrixes**

	Target		Gravi cap	metri acity	с		olume capaci			Syste	em cos	st		Fuel o	cost			nbien perati	
	Unit		w	't%			g-H <sub>2</sub> /	′L		\$/k\	Vh ne	t	\$/{	gge at	pump	)		°C	
Phase 3 ideas for testing specific ta Phase 3 goal for this system:	2017		5	5.5			40							2-6	5		-40 -	60 (si	un)
System/material form: powder/compacted	Ultimate	bercost	7	7.5	ine (1/4 tank to		<b>70</b>	efficiency		System ini rate	WIII TON HOW Face	flow (20°C)	flow (-20°C)	2-3	22/19/8/130/P0/13	leakage	-40 -	60 (su	un)
Will this target be t	tested?	3e at pump 2-6 2-3	*C -40 - 60 (sun) -40 - 60 (sun) Indirect via	°C -40/85 -40/85 Indirect via	full) cycles 1500 1500 Yes-Partial	pressure to FC bar (abs) 5 3 Yes	bar (abs) 12 12 Yes	90 Yes	plant efficiency % 60 Indirect via	kg-H2/min 1.5 2 Yes	(g/s)/kW 0.02 0.02 Indirect via	s 5 5 Yes	s 15 15 Indirect via	0%) s 0.75 0.75 Yes	14687-2) %H <sub>2</sub> 99.97 99.97 99.97 Yes	Scch/h See note See note	See note See note Yes-Partial	See note See note Yes	(g/h)/kg-H2 stored 0.05 0.05 Yes
		o refuel will imated by and ion	Test will be at room temperature	modeling Will measure H2 delivery temperature Separate component test	Stress models ASME. Limited material cycling	Test both 3 and 5 bar.	Verify pressure regulation to 12 ban functions over specified operating conditions	warm system to	Modeling: Thornton, Hardy		modeling: Tamburello & Hardy, Pasini	Experiments: Chahine	modeling: Modeling: Tamburello & Hardy	Modeling: Hardy; Experiments: Chahine	H2 purity from		Dust cloud ignition	Design should be robust and testing procedures should be vetted in advance for possible risks	
		nt of LN2 an isumed ;refill	d External temperature	H2 outlet temperature	Fatigue behavior. Structure of tank internals before/after cycling (tomography?). H2 purity before/after	at a function of charge state and discharge rate	H2 outlet pressure at a function of charge state and discharge rate	Energy input to tank to induce H2 release	Cost and energy inputs during refil	Time to complete fill as a function of	H2 outlet flow as a function of state of charge and "drive cycle"		Time to achieve full flow. Consider extrapolating 20 C data to -20 C.	Time to achieve desired response in flow rate	Composition of desorbed gas using Mass spectrometer or RGA.	Transport of H2 through liner. Other?	N/A. BASF and/or UTRC will conduct dust cloud tests?	Meets appicable safety standards	Temperature of tank vs time. Vacuum level in insulated jacket.
What is the test or	model approach?	Efficiency tions M: ton	≺insert model name> M: Tamburello	<insert model<br="">name&gt; M: Tamburello</insert>	Cycle Tests; E: Chahine and Simmons		y 4.4 System Delivery Test; E: Chahine			4.3 System Fill Test, t; E: Chahine, M: v Hardy &	4.4 System Delivery Test and 4.6 System Dynamic Test; Mc Pasini, Tamburello, Hardy; E: Chahine	4.5 - System start- up test; E: Chahine		4.6 System Dynamic Test; E: Chahine	H2 Purity Test: E: Veenstra, Siegel, and Chahine	Permeation Test: E: Reither and Simmons	Dust cloud test; E: Khalil and/or BASF	Safety Protocols; E Chahine	: Insulation Test; E: Reiter
		odels shoul o account for mies of scal number of es and g stations)	or le No. Only one size	No. Only one size will be tested	No. Only one size will be tested	No. Only one size will be tested	No. Only one size will be tested	No. Only one size will be tested	No. Only one size will be tested	Possibly. Should determine how fill time varies with state of charge and initital temperature	No. Only one size will be tested	No. Only one size will be tested	No. Only one size will be tested	No. Only one size will be tested	N/A	Consider for Phase 2 at JPL	N/A	N/A	Yes, examine different amounts of insulation
			No	No	No	No	No	Yes	No	Yes. Need to quantify tradeoff between finite- size effects and the size of system which can realistically be tested.	Yes	No	No	Yes	No	No	No	No	Yes
			Unlikely that heating or cooling system to these temperatures will be possible.	Chahine	Cycle test is limiter by time to complete a cycle and consumables (H2, N2)		No	No	N/A	Note limitations on UQTR cooling rate of compressed H2		No? Chahine	N/A	Chahine	Test rig should be designed to enable sampling of H2 purity	Reiter	N/A	Chahine	Availability of MLV is a concern. JPL to address

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

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# **System Test Matrixes**

	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
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	tested?	Yes-Partial	¥₂s-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	•	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 shou this test to verify t	ld be measured in he target or model?	Usable capacity. Include 5 bar & 3 bar operating pressure as test matrix and see effect on gravimetric capacity.	Usable capacity	Estaimated costs of lab scale system to actual cost of lab scale system	Amount of LN2 and H2 consumed during refill	External temperature

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Component	Component Assumed Validation in Component Design with modeling rather		What can be validated with modeling rather than experimental work?	Rationale for including/excluding from Phase III	Areas of Concern Requiring Testing	Limitations on Scaling	Include in Phase	
Internal Heat Exchanger: HexCell Resistance Heater with Flow-	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	Cool-down time; non- uniform temperature distribution; robustness of HX with respect to temperature/pressure cycling; efficiency	N/A	Yes	
Through Cooling				experimentally Integral part of system;	(energy consumed during fill)			
Cryo-Adsorbent Material: <b>Powder MOF-5</b>	Modeling and experimental validation	SRNL / UQTR / Ford (BASF)	Theoretical H2 uptake; heat transfer (partial)	validate capacity projections; Quantify effects due to bed inhomogeneities (non- uniform packing)	Packing density, heat transfer, and adsorption capacity	N/A	Yes	
Inter-Wall LN <sub>2</sub> Pre-chiller: <b>"Thermos Bottle"</b>	Modeling only; Constant wall temperature models to show the need/benefit	PNNL / Lincoln Composites	1 <sup>st</sup> -order thermal behavior can be modeled	Validate system thermal models; Phase-change within the channel must be evaluated experimentally	Choked flow due to LN2 phase change	Channel cross-section must remain intact	Yes – partially	
Internal Heat Exchanger: MATI with Isolated-H2 Heating and Isolated- LN2 Cooling	Modeling and partial experimental validation of individual components/capabilities	OSU	1 <sup>st</sup> -order thermal behavior has already been verified.	Quantify advantages in cooling rate and system volume; Verify rapid cooling capability and desorption performance	Welds, cycling, and verification of adsorption/desorption behavior, design complexity/robustness	N/A	Yes – partially	
Cryo-Adsorbent Material: Compacted MOF-5 "pucks" (0.32 g/cc)	Modeling and partial experimental validation	OSU / Ford (BASF)	Theoretical H2 uptake; heat transfer (partial)	Integral part of system; validate capacity and kinetic projections; Assess robustness and heat transfer limitations	Cracking/crumbling, heat transfer, and adsorbent behavior	N/A	Yes – partially	
Type 1 Aluminum pressure vessel	Design and partial experimental validation	LC	Mass, volume, and cost	Integral part of system; validate capacity projections	Cryo-burst testing	N/A	Yes	
Multi-layer vacuum insulation	Modeling of heating rate/dormancy performance	JPL	Partial dormancy performance	Validate dormancy model; vacuum level stability; robustness of design	No supplier (JPL work scope reduction)	N/A	No	

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Compone	۸ nt		d Validation	in	onsible sign	What can be validated with modeling rather				
		P	hase II		ization	than experim				
HexCell Resistance Heater with Flow- Through Cooling	experimental validation of individual components/capabilities	SRNL / UQTR	1 <sup>st</sup> -order thermal behavior (already completed).	cooling: dynamic behavior (such as channeling) can only be evaluated experimentally	of HX with respect to temperature/pressure cycling; efficiency (energy consumed during fill)	N/A	Yes			
Cryo-Adsorbent Material: Powder MOF-5	Modeling and experimental validation	SRNL / UQTR / Ford (BASF)	Theoretical H2 uptake; heat transfer (partial)	Integral part of system; validate capacity projections; Quantify effects due to bed inhomogeneities (non- uniform packing)	Packing density, heat transfer, and adsorption capacity	N/A	Yes			
Inter-Wall LN <sub>2</sub> Pre-chiller: <b>"Thermos Bottle"</b>	Modeling only; Constant wall temperature models to show the need/benefit	PNNL / Lincoln Composites	1 <sup>st</sup> -order thermal behavior can be modeled	Validate system thermal models; Phase-change within the channel must be evaluated experimentally	Choked flow due to LN2 phase change	Channel cross-section must remain intact	Yes – partially			
Internal Heat Exchanger: MATI with Isolated-H2 Heating and Isolated- LN2 Cooling	Modeling and partial experimental validation of individual components/capabilities	OSU	1 <sup>st</sup> -order thermal behavior has already been verified.	Quantify advantages in cooling rate and system volume; Verify rapid cooling capability and desorption performance	Welds, cycling, and verification of adsorption/desorption behavior, design complexity/robustness	N/A	Yes – partially			
Cryo-Adsorbent Material: Compacted MOF-5 "pucks" (0.32 g/cc)	Modeling and partial experimental validation	OSU / Ford (BASF)	Theoretical H2 uptake; heat transfer (partial)	Integral part of system; validate capacity and kinetic projections; Assess robustness and heat transfer limitations	Cracking/crumbling, heat transfer, and adsorbent behavior	N/A	Yes – partially			
Type 1 Aluminum pressure vessel	Design and partial experimental validation	LC	Mass, volume, and cost	Integral part of system; validate capacity projections	Cryo-burst testing	N/A	Yes			
Multi-layer vacuum insulation	Modeling of heating rate/dormancy performance	JPL	Partial dormancy performance	Validate dormancy model; vacuum level stability; robustness of design	No supplier (JPL work scope reduction)	N/A	No			

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Exchanger: HexCell Resistance Heater with Flow- Through Cooling "Thermos Bottle" Internal Heat Exchanger: MATI with Isolated-H2 Heating and Isolated- LN2 Cooling Cryo-Adsorbent Material: Modeling a	Modeling and xperimental va of individu omponents/caj	alidation ual	SRNL /	UQTR		er thermal behavic ady completed).	Verify ca	, low-cost design; apability for rapid dynamic behavior s channeling) can
"Thermos Bottle"     need/b       Internal Heat     Modeling a       Exchanger:     MATI       with Isolated-H2     of indix       Heating and Isolated-     components/       LN2 Cooling     Cryo-Adsorbent       Material:     Modeling a							-	v be evaluated perimentally
Internal HeatModeling aExchanger:MATIwith Isolated-H2of indixHeating and Isolated-components/LN2 CoolingCryo-AdsorbentMaterial:Modeling a	to show the Compo	sites can	be modeled		annel must be xperimentally	phase change	remain intact	,
Material: Modeling a	g and partial ntal validation dividual OSU ts/capabilities	1	r thermal behavior ady been verified.	Quantify ac cooling rate volume; V cooling ca	dvantages in e and system /erify rapid pability and performance	Welds, cycling, and verification of adsorption/desorption behavior, design complexity/robustness	N/A	Yes – partially
"pucks" (0.32 g/cc)	g and partial OSU / I ntal validation (BAS		etical H2 uptake; ransfer (partial)	validate ca kinetic proje robustnes	rt of system; apacity and ctions; Assess and heat limitations	Cracking/crumbling, heat transfer, and adsorbent behavior	N/A	Yes – partially
Type I Aluminum	and partial ntal validation LC	Mass, v	volume, and cost	validate	rt of system; capacity ections	Cryo-burst testing	N/A	Yes
	g of heating dormancy JPL		tial dormancy erformance	Validate dorr vacuum lev	mancy model; vel stability; ss of design	No supplier (JPL work scope reduction)	N/A	No

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Componer	nt P		d Val Phase	idation e II	in	De	onsible sign ization	What can be validate with modeling rathe than experimental wo			
Internal Heat Exchanger: HexCell Resistance Heater with Flow- Through Cooling	experime	ndividual	ation	SRNL /	UQTR		er thermal beh ady complete		Verify cap cooling: d (such as only b	ow-cost design; bability for rapid ynamic behavior channeling) can be evaluated erimentally	
Cryo-Adsorbent Material: <b>Powder MOF-5</b>	Moc experime	leling and ntal valid		SRNL / I Ford (I			retical H2 upta transfer (part		valid project effect inhomo	part of system; ate capacity ions; Quantify ts due to bed geneities (non- orm packing)	
Type 1 Aluminum pressure vessel	Design and partial experimental validation	LC	Mass, v	volume, and cost	validate proje	rt of system; e capacity ections	Cryo-burst testing		N/A	Yes	
Multi-layer vacuum insulation	Interview IPI			ial dormancy erformance	vacuum le	mancy model; vel stability; ss of design	No supplier (JPL work scope reduction)		N/A	No	

# **Adsorbent System Phase 3 Proposal**

Heat Exchange Systems



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

Containment



2 Liter Type 1 Segmented AI Tank





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

**HSECoE** 

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Type 1 SS Pressure Vessel



# **Chemical System Phase 3 Proposal**



### Phase 3 Approach

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

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## **Phase 3 Gantt Chart**

WBS	Task Name	Resource Names	Duration	Start	Finish	204.4					2004.5			
						Qtr 2	Qtr 3	Qtr 4	2014 Qtr 1	Qtr 2	Qttr 3	Qtr 4	2015 Qtr 1	Qtr 2
3.1	Design subscale prototype systems		66 days	Mon 7/1/13	Mon 9/30/13	100 2	V .	V	5861 1	1001 2	Sect O	100	1000	100 2
3.1.1	Adsorbent	SRNL/OSU	66 days	Mon 7/1/13	Mon 9/30/13			ĥ						
3.1.2	Chemical	LANL/PNNL	66 days	Mon 7/1/13	Mon 9/30/13			i i						
3.2	Synthesize/Modify Materials		326 days	Mon 7/1/13	Mon 9/29/14		-					÷.		
3.2.1	Adsorbent	FMC	111 days	Mon 7/1/13	Mon 9/29/14									
3.2.2	Chemical	PNNL	111 days	Mon 7/1/13	Mon 9/22/14			<b>.</b>						
3.3	Complete test facilities		196 days	Mon 7/1/13	Mon 3/31/14					÷.				
3.3.1	Adsorbent	UQTR/OSU	196 days	Mon 7/1/13	Mon 3/31/14				:	<b>1</b>				
3.3.2	Chemical	lani	196 days	Mon 7/1/13	Mon 3/31/14									
3.4	Acquire BoP/System Components		60 days	Wed 10/9/13	Tue 12/31/13				÷ –					
3.4.1	Adsorbent	UQTR/OSU/LC	60 days	Wed 10/9/13	Tue 12/31/13				h					
3.4.2	Chemical	LANL/UTRC	60 days	Wed 10/9/13	Tue 12/31/13				i-					
3.5	Fabricate/assemble prototype system		64 days	Wed 1/1/14	Mon 3/31/14			1						
3.5.1	Adsorbent	UQTR/OSU	64 days	Wed 1/1/14	Mon 3/31/14					<b>-</b>				
3.5.2	Chemical	LANL/UTRC	64 days	Wed 1/1/14	Mon 3/31/14				<u> </u>					
3.6	Evaluate prototype & assess performance		197 days	Tue 4/1/14	Wed 12/31/14					<u> </u>				
3.6.1	Adsorbent	UQTR/OSU	197 days	Tue 4/1/14	Wed 12/31/14					Ľ				
3.6.2	Chemical	lani	197 days	Tue 4/1/14	Wed 12/31/14					Ĭ.				
3.7	Compare to and refine models		197 days	Wed 4/2/14	Thu 1/1/15					<u> </u>				
3.7.1	Adsorbent	SRNL/OSU	197 days	Wed 4/2/14	Thu 1/1/15								İ	
3.7.2	Chemical	PNNL	197 days	Wed 4/2/14	Thu 1/1/15					1			ġ.	
3.8	Modify test apparatus/prototype		197 days	Tue 4/1/14	Wed 12/31/14					<u> </u>			•	
3.8.1	Adsorbent	SRNL/UQTR/OSU	197 days	Tue 4/1/14	Wed 12/31/14					Ľ.			h	
3.8.2	Chemical	lani	197 days	Tue 4/1/14	Wed 12/31/14								Ł	
3.9	Post updated models on WEB	SRNL/UTRC/PNNL/NREL	20 days	Thu 1/1/15	Wed 1/28/15								ř-	
3.10	Decommission prototypes as necessary		40 days	Thu 1/1/15	Wed 2/25/15									
3.10.1	Adsorbent	UQTR/OSU	40 days	Thu 1/1/15	Wed 2/25/15								Ľ	
3.10.2	Chemical	lani	40 days	Thu 1/1/15	Wed 2/25/15								Ľ.	
3.11	Performance/Cost Model Updates		164 days?	Fri 5/16/14	Wed 12/31/14					-				
3.11.1	Adsorbent	NREL, PNNL, UTRC, FMC	164 days?	Fri 5/16/14	Wed 12/31/14									
3.11.2	Chemical	NREL, PNNL, FMC, UTRC	164 days?	Fri 5/16/14	Wed 12/31/14									
3.12	Maaterials' Requirements Refinement		198 days?	Mon 3/31/14	Wed 12/31/14					-				
3.12.1	Adsorbent	FMC/SRNL	198 days?	Mon 3/31/14	Wed 12/31/14									
3.12.2	Chemical	LANL/PNNL	198 days?	Mon 3/31/14	Wed 12/31/14									
3.13	Project Management		457 days	Mon 7/1/13	Tue 3/31/15	I	•							•
3.13.1	Center	SRNL	457 days	Mon 7/1/13	Tue 3/31/15								:	
3.13.2	Adsorbent	UM	457 days	Mon 7/1/13	Tue 3/31/15									1
3.13.3	Chemical	lani	457 days	Mon 7/1/13	Tue 3/31/15								<u> </u>	
3.14	Write Final Report	All	66 days	Thu 1/1/15	Thu 4/2/15									•

(F1) HSECOE

### **Phase 3 Gantt Chart**

Luna					
WBS	Task Name	Resource Names D	Duration	Start Finish	2014 2015
24	Design autorials used at many surdayers		66 days	Base 7/4/42 Base 0/20/42	Gtr 2 Gtr 3 Gtr 4 Gtr 1 Gtr 2 Gtr 3 Gtr 4 Gtr 1 Gtr 2
3.1	Design subscale prototype systems		66 days	Mon 7/1/13   Mon 9/30/13	
3.1.1	Adsorbent		т млі	lactonac R	eing Developed for Each
3.1.2	Chemical		I IVII	ICSIONES D	
3.2	Synthesize/Modify Materials			Contributio	n in Decourace
3.2.1	Adsorbent			Johundanino	n in Resources
3.2.2	Chemical		_		
3.3	Complete test facilities		196 d	Mon 7/1/13 Mon 3/31/14	
3.3.1	Adsorbent	UQTR/OSU	196 c	Mon 7/1/13 Mon 3/31/14	
3.3.2	Chemical	lani	196	Mon 7/1/13 Mon 3/31/14	
3.4	Acquire BoP/System Components		"ýs	Wed 10/9/13 Tue 12/31/13	
3.4.1	Adsorbent	UQTR/OSU/LC	60 days	Wed 10/9/13 Tue 12/31/13	
3.4.2	Chemical	LANL/UTRC	60 days	Wed 10/9/13 Tue 12/31/13	
3.5	Fabricate/assemble prototype system		64 days	Wed 1/1/14 Mon 3/31/14	
3.5.1	Adsorbent	UQTR/OSU	64 days	Wed 1/1/14 Mon 3/31/14	
3.5.2	Chemical	LANL/UTRC	64 days	Wed 1/1/14 Mon 3/31/14	
3.6	Evaluate prototype & assess performance		197 days	Tue 4/1/14 Wed 12/31/14	
3.6.1	Adsorbent	UQTR/OSU	197 days	Tue 4/1/14 Wed 12/31/14	
3.6.2	Chemical	lani	197 days	Tue 4/1/14 Wed 12/31/14	
3.7	Compare to and refine models		197 days	Wed 4/2/14 Thu 1/1/15	••••••••••••••••••••••••••••••••••••••
3.7.1	Adsorbent	SRNL/OSU	197 days	Wed 4/2/14 Thu 1/1/15	
3.7.2	Chemical	PNNL	197 days	Wed 4/2/14 Thu 1/1/15	
3.8	Modify test apparatus/prototype		197 days	Tue 4/1/14 Wed 12/31/14	
3.8.1	Adsorbent	SRNL/UQTR/OSU	197 days	Tue 4/1/14 Wed 12/31/14	
3.8.2	Chemical	lani	197 days	Tue 4/1/14 Wed 12/31/14	
3.9	Post updated models on WEB	SRNLAUTRCAPNNLANREL	20 days	Thu 1/1/15 Wed 1/28/15	
3.10	Decommission prototypes as necessary		40 days	Thu 1/1/15 Wed 2/25/15	
3.10.1	Adsorbent	UQTR/OSU	40 days	Thu 1/1/15 Wed 2/25/15	
3.10.2	Chemical	lani	40 days	Thu 1/1/15 Wed 2/25/15	
3.11	Performance/Cost Model Updates	1	164 days?	Fri 5/16/14 Wed 12/31/14	
3.11.1	Adsorbent	NREL,PNNL,UTRC,FMC	164 days?	Fri 5/16/14 Wed 12/31/14	
3.11.2	Chemical	NREL,PNNL,FMC,UTRC	164 days?	Fri 5/16/14 Wed 12/31/14	
3.12	Maaterials' Requirements Refinement		198 days?	Mon 3/31/14 Wed 12/31/14	
3.12.1	Adsorbent		198 days?	Mon 3/31/14 Wed 12/31/14	
3.12.2	Chemical		198 days?	Mon 3/31/14 Wed 12/31/14	
3.13	Project Management		457 days	Mon 7/1/13 Tue 3/31/15	
3.13.1	Center	SRNL	457 days	Mon 7/1/13 Tue 3/31/15	
3.13.2	Adsorbent	UM	457 days	Mon 7/1/13 Tue 3/31/15	
3.13.3	Chemical		457 days	Mon 7/1/13 Tue 3/31/15	
3.14	Write Final Report	All	66 days	Thu 1/1/15 Thu 4/2/15	
1					

### Preliminary vs. Demonstrated Spider Chart Why Phase 3 demonstration is critical in model validation Chemical Hydrogen Storage System (2012)



### Preliminary vs. Demonstrated Spider Chart Why Phase 3 demonstration is critical in model validation Chemical Hydrogen Storage System (2012)



### **Technology Readiness Levels**

### Materials Based Hydrogen Storage Systems for Automotive Applications

#### Materials CoEs

#### HSECoE



### Summary

### Adsorption Systems

- Limited in volumetric density and dormancy at ~77K due to materials
- Temperature assisted PSA using a Type I tank at 60 bar is proposed for subscale prototype demonstration.

### Chemical Systems

HSECOE

- Limited in gravimetric density and efficiency due to materials.
- Liquid/Slurry flow through reactors with GLS and purification is proposed for subscale prototype demonstration.
- Phase 3 Go/NoGo meetings held with DoE with results forthcoming.

### Adsorbent System



### Chemical System







## **Technical Back-Up Slides**



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#### 49



Fuel cell system

**HSECoE** 





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