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Savannah River National Laboratory

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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 Semelsbergenes
	Performance Modeling & CostAnalysis Thornton	Thornton Weimar	Thornton Weimar
	Integrated Power Plant & Storage System Modeling van Hassel	Tamburello	Brooks
Techr	Transport Phenomena Hardy	Hardy ( SRNL Corgnali, Sulic Ortman, Drost	Brooks Semelsberger
Nology Areas	Materials Operating Requirements Rönnebro	Veenstra Chahine Simpson	Rönnebro Semelsberger
	Enabling Technologies Simmons	Simmons Newhouse 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	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	(g/s/kW)	0.02			0.02			0.02
	g/s	1.6			1.6			1.6
Start Time to Full Flow (20°C)	sec	5			1			1
Start Time to Full Flow (-20°C)	sec	15			1			1
Transient Response	sec	0.75			0.49			0.49
Fuel Purity	%H2	99.97			99.97			99.99
		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	Media		Fluid AB at	t 50wt%		Fluid AB at 6	5wt%	
PNNL	Tank		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/Transfer Pumps		
UTRC	Heat Exchanger					Heat Exchang	ger mass and	volume cut
UTRC	GLS		Gas\Liquid	Seperator		Gas\Liquid So	eperator	
UTRC	Purification		Purification	1		Hydrogen Pu	rification mass	and volume



**HSECoE** 

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

Chemical Hydrides				3/31/2011			3/31/2013	
						Phase 2	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	(g/s/kW)	0.02			0.02			0.02
	g/s	1.6			1.6			1.6
Start Time to Full Flow (20°C)	sec	5			1			1
Start Time to Full Flow (-20°C)	sec	15			1			1
Transient Response	sec	0.75			0.49			0.49
Fuel Purity	%H2	99.97			99.97			99.99
		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	Media		Fluid AB at	t 50wt%		Fluid AB at 6	5wt%	
PNNL	Tai k		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	nps
UTRC	Heat Exchanger					Heat Exchang	ger mass and	volume cut
UTRC	GLS		Gas\Liquid	Seperator		Gas\Liquid So	eperator	
UTRC	Purification		Purification			Hydrogen Pu	rification mass	and volume

**HSECoE** 

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

	Chemical Hydrides		3/31/2011				3/31/2013				
				Phase 1 HS	SECoE Base	line (System)	Phase 2	2 HSECoE Go. Targets (full scale)	/No-Go		
			2015 DOE	Phase 1 HSECoE Baseline	Phase 1 HSECoE Basline	Phase 1 HSECoE Baseline	Phase 2 HSECoE Actuals	Phase 2 HSECoE Actuals	Phase 2 HSECoE 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		05.0	144		05.0	130		
		\$/KVVN net	480		25.0	25.0		25.0	25.0		
	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		
Responsible Organiza	ation Component		3/3	31/2011				3/31/201	3		
LANL	, PNNL Media		Flu	uid AB a	t 50wt%			Fluid AB	at 65wt%	/ 0	
	PNNL Tank		Bla	Bladder Tank					Bladder Tank		
	LANL Reactor		Flo	Flow Through Reactor				Flow Through Reactor			
	PNNL System Des	ign			-				-		
	BoP	0									
PNNL Pumps			Fe	Feed/Recycle/Transfer Pumps				Feed/Re	cycle/Tra	nsfer Pumps	
UTRC Heat Exchanger				-			-	Heat Ex	changer n	nass and volume cut	
	UTRC	GLS	Ga	Gas\Liguid Seperator				Gas\Liqu	uid Sepera	ator	
	UTRC Purific	cation	Ρι	urificatio	n .			Hydroge	n Purifica	tion mass and volume	
	Responsible Organization	Component		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	Tark	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
UTRO	Heat Exchanger		Heat Exchanger mass and volume cut
UTRO	GLS	Gas\Liquid Seperator	Gas\Liquid Seperator
UTRO	Purification	Purification	Hydrogen Purification mass and volume

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

Met

Exceeded

Continuing

Component	Partner	S*M*A*R*T Milestone	Status 10/1/12	Projected Outcome
Materials Development	Ford	Report on ability to develop compacted MOF-5 adsorbent media having a total hydrogen material density of greater than or equal to 0.3 g/t. H2 density of 11 w. % and 33 g/tiler and thermal conductivity of 0.5 W/m-K at P = 60-5 bar and T = 80-160K.	H2 grav. density of the MOF-5 material >11% is possible with .3 g/cc (w/o ENG) at P = 60-5 bar and T = 80-160/k with 60% packing efficiency. H2 vol. density of the MOF-5 material >33 g/l is possible with .5 g/cc (+5% ENG) at P = 60-5 bar and T = 80-160 k with 10% packing efficiency. Thermal conductivity of .5 W/m-K is possible with .3 g/cc to .5 g/cc + 10% ENG with temperatures > 100-120 K.	The capability of achieving specific metric configuration is possible, investigations wi devise a media morphology which will <b>me</b> <b>metrics</b> .
Materials Development	Ford/UM/ BASF	Report on ability to demonstrate a composite MOF-5 adsorbert monoliths having H2 effective kinetics equivalent to 5.6 kg usable H2 over 3 minutes and permeation in packed and powder particle beds with flow rate of 1 m/s superficial velocity and pressure drop of 5 bar.	H2 effective kinetics have been conducted and proven over 240 cycles for MOF-5 powder. The monoilth testing for kinetics is planned. Permeation testing has been conducted for various temperatures and densities. Based on the extrapolation of permiation test data at 0.12 m/s, the 50ar pressure drop milestone is possible (initial assessment of uncompressed darcy) at a media density of 0.3 g/cc but will be a significant challenge beyond this density, <b>meeting the metric</b> .	Met Metric The kinetic response of the MOF-5 materi the desired response while the permeation be a challenge with densities greater than
Materials Development	SRNL/ UQTR	Report on ability to develop a compacted MOF-5 adsorbent media bed having a total hydrogen density of: 11 % g H2/(g MOF) and 33 g H2/(liter MOF) at P = 60 - 5 bar and T = 80 - 160 K	Evaluation of isotherms provided by Ford for initial & final states gives: 1804g/m <sup>1</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=36.7 missing the GC metric	Alternative compaction methods will be pu to identify higher volumetric density morph meeting the metrics.
Structured Bed	GM	Report on ability to develop MOF-5 powder bed having a total hydrogen density of: 15 wt. % g H2/(g MOF) and 20 g H2/(liter MOF) at $P = 60 - 5$ bar and $T = 80 - 160$ K.	Based on the modified Dubinin-Asthakov adsorption model, at 60 - 5 bar and 80 - 160 K the 3 liter test vessel contains 18.6% total deliverable g H2/g MOF) and 30.5% g H2/(liter MOF) surpassing the metric.	Exceeded metric These results will be validated with lab exp
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. <i>Operating this system at 40 K is not feasible</i> . The capability to perform cryogenic cycling has also been implimented.	Safety documentation will be completed a of Type 4 COPVs, pressure testing of Typ be performed at 77K and adding the capal cryogenic cycoic testing capability <b>excee</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 liters. These tanks were designed to operate at 100 bar with a minimum burst ratio of 2.25 (252 bar). The actual burst achieved duing R1 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 2.52 (252 bar). The actual burst achieved during R1 testing was 370 bar. anks have been supplied to JPL for burst testing at 77K to verify low temperature burst pressures. These tanks were appropriately designed having safety factors equivalent to current <b>DOT</b> <b>NHTSA standards</b> for compressed gas fuel containes.	Based on these results single piece 120 li Type 4 tanks will be designed and and ma calculated. It is anticipated that the Type 4 meet hte mass target while the <b>Type 4 ta</b> <b>the mass metric</b> .
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 & different materials it was cocniuded 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 I 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 MLL blanket composed of VDA mylar and dacron separators within a vacuum of at least 16-4 Tor, reduces parasitic heat load to 2 W far exceeding the metric.	25% scale experimental verification has be preliminary results are being analyzed whi 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 <b>exceed the metric</b> for weight and volume, simulation demonstrates that these designs can provide the required discharge performance.	Exceeded metric Laboratory testing is being used to confirm and manufacturing studies have confirmed 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. retueling time and H2 release rate of 0.02 g H2/sec. W/) with a mass less than 6.5 kg and a volume less than 6 liters.	The efficacy of an isolated-loop internal heat exchanger was examined. Computational analyses showed that flowing externally heated hydrogen (fuel cell radiator heated) through isolated heating channels of a fin-and-tube HX within the adsorbert would NOT provide enough heat for the minimum drive cycle requirements. An H2 combustor should be able to raise the H2 temperature high enough, however the fin-and-tube HX has higher mass and volume than a comparable MATI.	This metric was suspended as not viable
Internal flow through HX	SRNL/ UQTR	Report on ability to develop and demonstrate an internal flow through HX system based on compacted media capable of allowing less than 3 min. scaled refueling time and H2 release rate of 0.02 g H2/(sec. kW) with a mass less than 6.5 kg and a volume less than 6 liters.	Models for 6mm 322kg/m3 pellets indicate that, relative to 130kg/m3 powder, flow through cooling requires a significantly larger mass of exhaust hydrogen and a longer time to cool. <b>Compacted MOF will not meet the metric</b> . It appears that <u>180kg/m3 MOF-S powder in an aluminum honeycomb</u> will meet the metric.	Met metric Experiments to validate the models and de concept are in progress at UQTR. Pellets loaded into hex mesh.
Internal flow through HX	GM	Report on ability to develop and demonstrate an internal flow through cooling system based on powder media capable of allowing less than 3 min. scaled refueling time, and an internal heating system for scaled H2 release rate of 0.02 p /µ2(sec. kW with a mass less than 6.5 kg and a volume less than 6 liters.	Model of charging process predicts that for a 60bar system, a 10.3 liter, 27.7 kg heat exchanger is required to successfully discharges 5.6 kg H2 at full-scale. For a 200 bar system, a 5.5 liter 15 kg aluminum helical coil HX is capable of meeting discharge target. The current experimental stainless steel sheathed coils have higher density. Neither HX meets the mass metric.	It is not anticipated that the mass metr achieved. Bypass line and pressure trans added to the test system in order to contra and initial bed temperature at conditions n through cooling experiment. The model pre determined experimentally.
External HX	JPL	Report on ability to develop and demonstrate FC radiator capable of heating 80K hydrogen stream to 233K flowing at 1.6g/sec with no icing at 50%RH with a mass increase of less than 2.5 kg and a volume less than 1.5 liters.	System and detailed segmented models suggest that a small Downstream H2 HX (1.1 kg, 1.0 L) will meet the performance metrics at all but -40°C ambient conditions. An auxiliary heater may be required for such conditions. Results also indicate that a "cold start" heater will be necessary for conditions of T < -10°C. The performance of this HX predicted by modeling meets the metrics.	Met metrics. Changes in funding and scop demonstration, and no experimental valida 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 w validate models and estimate the mass an
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 1 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 = 29 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 terret.	In progress	Will complete by 12/31/12

Suspended

Not Met

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

	Adsorbent System	Partner		S*M*A*R*T Milestone	Status 10/1/12	Projected Outcome
	Materials Development	Ford	Report on ab having a total to 0.3 g/L, H conductivity of	2 develop compacted MOF-5 adsorbent media hydrogen material density of greater than or equal 2 density of 11 wt. % and 33 g/liter and thermal f 0.5 W/m-K at P = 60-5 bar and T = 80-160K.	H2 grav. density of the MOF-5 material >11% is possible with 3 g/cc (w/o ENG) at P = 60-5 bar and T = 80-160K with 60% packing efficiency. H2 vol. density of the MOF-5 material >33 g/l is possible with .5 g/cc (+5% ENG) at 60-5 bar and T = 80-160K with 100% packing efficiency. Thermal conductivity of .5 W/m-K is possible with .3 g/cc 5 g/cc + 10% ENG with temperatures > 100-120 K.	The capability of achieving specific metrics with a given P = configuration is possible, investigations will be continue to to devise a media morphology which will meet all of the metrics.
	Materials Development	Ford/UM/ BASF	Report on ab monoliths ha H2 over 3 min beds with flow of 5 bar.	lity to demonstrate a composite MOF-5 adsorbent wing H2 effective kinetics equivalent to 5.6 kg usable nutes and permeation in packed and powder particle v rate of 1 m/s superficial velocity and pressure drop	H2 effective kinetics have been conducted and proven over 240 cycles for MOF-5 powder. The monolith testing for kinetics is planned. Permeation testing has been conducted for various temperatures and densities. Based on the extrapolation of permiation test data at 0.12 m/s, the 5bar pressure drop milestone is possible (initial assessment uncompressed darcy) at a media density of 0.3 g/cc but will be a significant challenge beyond this density, <b>meeti</b> the metric.	Met Metric The kinetic response of the MOF-5 material will achieve the desired response while the permeation will continue to be a challenge with densities greater than 0.3 g/cc.
	Materials Development	SRNL/ UQTR	Report on ab media bed ha MOF) and 33 K	lity to develop a compacted MOF-5 adsorbent wing 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: 180kg/m <sup>3</sup> (uncompacted) GC=0.15 VC=26.5 missing the VC metric 322kg/m <sup>3</sup> GC=0.10 VC=33.0 missing the GC metric 520g/m <sup>3</sup> GC=0.07 VC=36.7 missing the GC metric	Alternative compaction methods will be pursued with Ford to identify higher volumetric density morphologies meeting the metrics.
	Structured Bed	GM	Report on ab hydrogen der MOF) at P =	lity to develop MOF-5 powder bed having a total isity 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 liter test vessel cont 18.6% total deliverable g H2/(g MOF) and 30.5% g H2/(liter MOF) surpassing the metric.	Exceeded metric These results will be validated with lab experiments.
	Composite Tank	JPL	Report on ab composite ar	lity to develop testing capability to burst test Type 4 id Type 1 (metal) tanks at 40K and demonstrate a minimally 2 5x pominal 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 getterm scovenic, ucline has also been immigrate hear immigrate the interval.	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 concerning exercise testing compliant the
Report on ability to identify Type IV tank liner materials suitable for 40K operation having a mass less than 8 kg and a volume less than 3 liters			i IV IOK an 8 rs	After evaluating 8 di that the liner separa pressure is decreas thickness of 2.55m metric is not feasi	ifferent materials it was concluded ates from the shell when the sed below 35bar with a liner m. With current materials this <b>ble</b> and either a Type 1 or 3 tank	not achievable
(		_	Report on ab	design is necessary	<b>/</b> .	Exceeded metric
	Internal MATI HX	OSU	Adsorption Ta refueling time mass less th	ank Insert capable of allowing less than 3 min. 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 these designs ca provide the required discharge performance.	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 le time and H2 less than 6.5	lity 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 kg and a volume less than 6 liters.	The efficacy of an isolated-loop internal heat exchanger was examined. Computational analyses showed that flow externally heated hydrogen (luce cell relation theated) through isolated heating channels of a fin-and-tube HX within 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 thing her mass and volume than a comparable MATI.	ng he This <b>metric was suspended</b> as not viable.
	Internal flow through HX	SRNL/ UQTR	Report on ab through HX s allowing less rate of 0.02 g volume less f	lity to develop and demonstrate an internal flow ystem based on compacted media capable of than 3 min. scaled refueling time and H2 release 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 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 demonstrate the concept are in progress at UQTR. Pellets have been loaded into hex mesh.
	Internal flow through HX	GM	Report on ab through cooli allowing less heating syste with a mass	lity to develop and demonstrate an internal flow ng system based on powder media capable of than 3 min. scaled refueling time, and an internal m for scaled H2 releaser rate of 0.02 g H2(sec. kW) 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/Lat full-scale. For a 200 bar system, a 5.5 liter 15 kg aluminum helical coll HX i capable of meeting discharge target. The current experimental stainless steel sheathed coils have higher density. Neither HX meets the mass metric.	It is not anticipated that the mass metric can be achieved. Bypass line and pressue transducer will be added to the test system in order to control the intel H2 and initial bed temperature at conditions needed for flow- through cooling experiment. The model predictions will be determined experimentally.
	External HX	JPL	Report on ability to develop and demonstrate FC radiator capable of heating 80K hydrogen stream to 233K flowing at 1.6g/sec with no icing at 50%RH with a mass increase of less than 2.5 kg and a volume less than 1.5 liters.		System and detailed segmented models suggest that a small Downstream H2 HX (1.1 kg, 1.0 L) will meet the performance metrics at all but -40°C ambient conditions. An auxiliary heater may be required for such conditions. Results also indicate that a "coid start" heater will be necessary for conditions of T < -10°C. The performance of th HX predicted by modeling <b>meets the metrics</b> .	Met metrics. Changes in funding and scope have exluded demonstration, and no experimental validation will be conducted.
	Catalytic Combustor	OSU	Report on ab combustor to FC radiator w and volume le	lify to develop and demonstrate a 1 kW catalytic augment partial H2 preconditioning by an existing ith >85% efficiency having a mass less than 0.6 kg ass than 0.5 liters.	Validated simulation results demonstrate that the microchannel combustor has an efficency >95% meeting the metric.	Metric exceeded A small prototype with 7 to 10 unit cells will be tested to validate models and estimate the mass and volume.
	BoP	PNNL	Report on ab external HX adsorbent sy less than 18.	lity to identify BoP materials (excluding internal HX, and combustor) suitable for 60 bar cryogenic stem having mass less than 17 kg and a volume 5 liters.	The BOP mass is significantly reduced with the lower pressure from 200bar to 69bar. The mass of the 69 bar sole 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 loop, and the tank is 6.7kg and 8.5L <b>far exceeding the metric</b> .	Metric exceeded
			System Design         SRNL           SRNL         than 137 kg and a volume less than 279 lifers meeting the all of the HSECoE drive cycles		Several system designs exceeding metricss: - 200 bar, 80 K, Pow	er
	System Design	SRNL	Report on ab than 137 kg a the HSECoE	lity 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 L) - 100 bar, 70 K, Powder MOF-5, FT Cooling + HexCell HX, Type 1 Al Tank (System mass = 127 kg, System volu = 258 L) - 80 bar, 80 K, 80% MPD 0.322 g/cc Compacted MOF-5, MATI, Type 3 Tan (System mass = 120 kg, System volume = 259 L)	ne Metric exceeded

Continuing

Exceeded

Met

Suspended

Not Met

**HSECoE** 

H

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

Exceeded

Met

In progress

Continuing

# Phase 2 Adsorbent System Milestones

	Adsorbent System	Partner		S*M*A*R*T Milestone	Status 10/1/12		Projected Outcome
	Materials Development	Ford	Report on ab having a tota to 0.3 g/L, H conductivity	bility to develop compacted MOF-5 adsorbent media al hydrogen material density of greater than or equal 12 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 be with 60%, packing efficiency. H2 vol. density of the MOF-5 material >33 g/l is possible with .5 g 60-5 bar and T = 80-160K with 100%, packing efficiency. Thermal conductivity of .5 W/m-K is po .5 g/cc + 10% ENG with temperatures > 100-120 K.	r and T = 80-160K /cc (+5% ENG) at P = ssible with .3 g/cc to	The capability of achieving specific metrics with a given configuration is possible, investigations will be continue to devise a media morphology which will meet all of the metrics.
	Materials Development	Ford/UM/ BASF	Report on ab monoliths ha H2 over 3 mi beds with flo of 5 bar.	pility to demonstrate a composite MOF-5 adsorbent aving H2 effective kinetics equivalent to 5.6 kg usable inutes and permeation in packed and powder particle w rate of 1 m/s superficial velocity and pressure drop	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 densit 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 th the metric.	onolith testing for ies. Based on the nitial assessment of is density, <b>meeting</b>	Met Metric The kinetic response of the MOF-5 material will achieve the desired response while the permeation will continue to be a challenge with densities greater than 0.3 g/cc.
	Materials Development	SRNL/ UQTR	Report on ab media bed ha MOF) and 33 K	sility to develop a compacted MOF-5 adsorbent awing a total hydrogen density of. 11 % g H2/(g 3 g H2/(liter MOF) at P = 60 - 5 bar and T = 80 - 160	Evaluation of isotherms provided by Ford for initial & final states gives: 180kg/m <sup>3</sup> (uncompacted) GC=0.15 VC=26.5 m issing the VC metric 322kg/m <sup>3</sup> GC=0.10 VC=33.0 missing the GC metric 232g/m <sup>3</sup> GC=0.07 VC=36.7 missing the GC metric		Alternative compaction methods will be pursued with Ford to identify higher volumetric density morphologies meeting the metrics.
	Structured Bed	GM	Report on ab hydrogen der MOF) at P =	bility to develop MOF-5 powder bed having a total insity 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	Report on ab composite a	bility 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 capability to perform coverse curcling has also been implimented.	been completed. s not feasible. The	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 surgeoid excells testing capability exceeding the
tank liner mate operation havin kg and a volum (2.55 mm thick	in a mass les g a mass les le less than 3 (ness).	for 4 s that 3 lite	IV IOK an 8 rs	that the liner separa pressure is decreas thickness of 2.55mi <b>metric is not feasi</b>	ates from the shell when the sed below 35bar with a liner m. With current materials this <b>ble</b> and either a Type 1 or 3 tank	Metric r	not achievable
			Report on at Adsorption 1	OUCSIGN IS NECESSALY	Current MATI designs exceed the metric for weight and volume. similation demonstrates that	these designs can	Exceeded metric Laboratory testing is being used to confirm simulations
	Internal non-MATI HX	UTRC- SRNL	refueling time mass less the Report on all exchanging I time and H2 less than 6 f	e and H2 release rate of 0.02 g H2/(sec. kW) with a nan 9.4 kg and a volume less than 4.2 liters. Dillity to develop and demonstrate an isolated heat- loop capable of allowing less than 3 min. refueling release rate of 0.02 g H2/(sec. kW) with a mass 5 kg and a withma less than 6 liter.	provide the required discharge performance. The efficacy of an isolated-loop internal heat exchanger was examined. Computational analyses externally heated hydrogen (tuel cell radiator heated) through isolated heating channels of a fin- adsorbent would NOT provide enough heat for the minimum drive cycle requirements. An H2 cor able to raise the H2 temperature high enough, however the fin-and-tube HX has higher mass and	s showed that flowing ind-tube HX within the nbustor should be volume than a	and manufacturing studies have confirmed that aluminum can be used for this component. This <b>metric was suspended</b> as not viable.
	Internal flow through HX	SRNL/ UQTR	Report on ab through HX s allowing less rate of 0.02 ( volume less	big the steam of team of team of the of the second of the	comparable MATL Models for 6mm 322kg/m3 pellets indicate that, relative to 130kg/m3 powder, flow through cooli significantly larger mass of exhaust hydrogen and a longer time to cool. Compacted MOF will metric. It appears that <u>180kg/m3 MOF-5 powder in an aluminum honeycomb</u> will meet the m	ng requires a not meet the etric.	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 less than 11 kg 35 liters.	ty to develop gn having less at 40K having g and volume	a the s tha g a n less	ermal in a iass than	Detailed modeling a experiments have b thermal isolation sy blanket composed o within a vacuum of a heat load to 2 W <b>fa</b>	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>	25% sca been sta being ar <b>exceed</b>	ale experimental verification h arted, and preliminary results halyzed which should prove <b>ing of metric</b> .
	System Design	SRNL	Report on at than 137 kg the HSECoE	bility to identify a system design having a mass less and a volume less than 279 liters meeting the all of E drive cycles	Several system designs exceeding metrics: 22 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 - 826 L) 80 bar, 80 K, 80% MPD 0.22 g/cc Compacted MOF-5,	00 bar, 80 K, Powder L) 7 kg, System volume MATI, Type 3 Tank	Metric exceeded
	Efficiency Analysis	NREL	Calculate an two adsorbe	id model the well-to-powerplant (WTPP) efficiency for nt storage system designs and compare results	(System mass = 120 kg, System volume = 259 L) 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

2.

3.

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 develop a flow through reactor 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 scrubber</b> with a minimum replacment interval of 1800 miles of driving resulting in a minimum outlet borazine concentration of 0.1 ppm (inlet concentration = 4,000 ppm) having a maximum mass of 3.95 kg and maximum volume less of 3.6 liters.	Mass metric achieved but volume metric missed. Compaction of adsorbent media could be conducted to meet the volume metric but emphasis will be placed on reactor testing.	
Report on ability to <b>develop an ammonia scrubber</b> with a minimum replacment interval of 1800 miles of driving resulting in a minimum ammonia outlet concentration of 0.1 ppm (inlet concentration = 500 ppm )having a maximum mass of 1.2 kg and a maximum volume of 1.6 liters.	Met Metric	
Ammonia & Borazine Filters	$\begin{array}{c} 1 \\ 0.8 \\ 0.8 \\ 0.6 \\ 0.4 \\ 0.2 \\ 0.2 \\ \end{array}$	MnCl <sub>2</sub> /IRH-33
0.00001 0.0001 0.001 0.01 0.1 1 PNH3/bar 010% 0% 0% 0% 0% 0% 0% 0% 0% 0% 0% 0% 0% 0	0 0 50 100 150 Time(min) ↓ ↓ ↓ ↓ ↓ ↓ ↓ ↓ ↓ ↓ ↓ ↓ ↓ ↓ ↓ ↓ ↓ ↓ ↓	ACN-210-15
1) HSECOE		Ammonia Borazine

**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)



2.

3.

### 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.
Report on ability to <b>demonstrate a composite MOF-5 adsorbent</b> <b>monoliths</b> 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.	<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	Metric Outcome
Report on ability to develop a thermal insulation design having less than a 5 W heat leak at 40K having a mass less than 11 kg and volume less than 35 liters.	25% scale experimental verification has been started, and preliminary results are being analyzed which should prove <b>exceeding of metric</b> .
<image/>	Image: state stat
	2.7 O Experiment: 30 Layers Prediction: 30 Layers, 43/0

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

0	App ver ½ Billik Internal heat Tank types L-to-D ratios LNs Inner vo Hemispheric Pressure ve Medra pack Full tank pre Full tank ter Empty tank ter pa	roacn on Possibl exchangers (x5) all chiller (x2) all chiller (x2) sel (vith volume sel only vs. se (vith volume secure (x12) perature (x12) peratu	- Fron e System (all options) endcaps () full design ne-% chang ct0) (x4) (x4)	1 OV Com (x45) (x2) (x2) es) ()	ver ½ E	Illion combinations down to 4 Systems system options and combinations of options 52 Million Reasonable Systems Combinations 52 Million Reasonable Systems (18) 52 Million Reasonable Systems (18) 53 Million Reasonable Systems (18) 54 Million Reasonable Systems (18) 54 Million Reasonable Systems (18) 55 Million Reasonable Systems (18) 55 Million Reasonable Systems (18) 55 Million Reasonable Systems (18) 56 Million Reasonable Systems (18) 57 Million Reasonable Systems (18) 58 Million Reasonable Systems (18) 59 Million Reasonable Systems (18) 50				
	Option #1	Option #2	Option #3		Option N	Full tank temperature (x6)     Empty tank temperature (x8)				
	1	1	1		1					
	-	1	1	-	1	Filter the Results				
	N:	1	1		1	Final & Durationary				
	1	2	1		1	These flow through applies with esciptores LIV estimates				
	2	2	1		1	<ul> <li>Intel now-mough cooling with resistance HX options.</li> <li>HavCall with resider MOE 5.</li> </ul>				
						<ol> <li>HexCell with 0.32 plop compacted MOE-5 pellets</li> </ol>				
	N;	N <sub>2</sub>	Ng	••••	NN	3 Helical coil with powder MOE-5				
H	HSECo	E				<ul> <li>One isolated-LN<sub>2</sub> cooling with isolated-H<sub>2</sub> heating option:</li> <li>4. MATI with 0.32 g/cc compacted MOF-5 pucks</li> </ul>				

**HSECoE** 

5

Internal HX and Media	Helical Coll + powder MOF-5	HexCell + powder MOF-5	0.32 g/cc MOF-5 pellets	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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0111	Addar-Libing	12.00	73.00	18.0	1.00		10.00		100	110	1.00	8.18	Employed with a family benefitien to
eu.	Restor	10.00	15.00		10		<b>8</b> .00		10	1.02	580	9110	instant of all with the parts of your Wester May Select 1 - By and Select resulted states PD explorements of 2 May 2.1 L (rescalar-to be assisted)
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### **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 •



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	Met metric for one adsorbent system in process of completion.
results relative to the 60% technical target.	

#### **Drive Cycles**



#### **Energy Efficiency**

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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**

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- 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 *heavya, <u>j</u>, <u>j</u>, <u>heav</u><u>j</u>Acture J.*
- 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 model; (2) the output from heat removal system scoping tool can be used as inputs for the energy balance equation or, alternatively data wailable about the output from heat removal system scoping tool can be used as inputs for the energy balance equation or, alternatively data wailable about the output from heat removal system scoping tool can be used as inputs for the energy balance equation or, alternatively data wailable about the output from heat removal system scoping tool can be used as inputs for the energy balance equation or, alternatively data wailable about the output form heat removal system scoping tool can be used as inputs for the energy balance equation or, alternatively data wailable about the output form heat removal system scoping tool can be used as inputs for the energy balance equation or, alternatively data wailable about the output form heat the scope about the output form heat removal system scope and the scope about 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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	Julia Interpolation 7 (Bh)		22.674	Initial M2 Concentration (mol/m02)	
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Interpolation 15 (%)     Interpolation	Interpolation 14 (Ek)	0.314	8.3140	Gas Constant (Jymoi-K)	
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Vi Isterpidion 20 (27) Sterpidion 20 (27)	Interpolation 19 (Dv)	n) 14	14.000	Velocity of Injected H2 in Feed Tube (m/s)	
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## **Metal Hydride FEM Model**



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# **Metal Hydride FEM Model**





**HSECoE** 

# **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
3	MH Framework Model	UTRC	Model complete <i>(TBR)</i> 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 li	nked to HSECoE webs	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**

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Phase 3 goal for this system:	specific targ	gets: IVIOF-5 c	ryoadsorber	it system																		
System/material form: powder/	compacted? Fl Target	ow-through/MA 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 respons (10%-90% & 90%- 0%)	e Fuel purity (SAE J2719 & ISO/PDTS 14687-2)	Permeation & leakage	Toxicity	Safety	Loss of usable H <sub>2</sub>
	Unit	wt%	g-H <sub>2</sub> /L	\$/kWh net	\$/gge at pump	°c	"с	cycles	bar (abs)	bar (abs)	%	%	kg-H2/min	(g/s)/kW	5	5	5	%H2	Scch/h			(g/h)/kg-H2 stored
	2017 Ultimate	5.5	40 70		2-6 2-3	-40 - 60 (sun) -40 - 60 (sun)	-40/85 -40/85	1500	5	12	90	60	1.5	0.02	5	15	0.75	99.97 99.97	See note See note	See note See note	See note See note	0.05
Will this target be tested?		Yes-Partial	Yes-Partial	Maybe	No	Indirect via modeling	Indirect via modeling	Yes-Partial	Yes	Yes	Yes	Indirect via modeling	Yes	Indirect via modeling	Yes	Indirect via modeling	Yes	Yes	No	Yes-Partial	Yes	Yes
What is the test or model approach?		Actual weights instrumented BOP list; Instrumentation and hardware add to system;What w could build today;	Separate lists of volumes (as for s weights) e	Cost of lab system will be known. Production system costs at 500K units/year will be estimated by HSECoE and DTI	Cost to refuel will be estimated by Paster and Thornton	Test will be at room temperature	Will measure H2 delivery temperature Separate component test	Stress models ASME. Limited material cycling test (possibly 500 cycles?) + extrapolation	Test both 3 and 5 bar.	Verify pressure regulation to 12 ba functions over specified operatin conditions	Determine work/heat input to r release H2 and warm system to g specified final temperature. Modeing:	Modeling: Thornton, Hardy	Detailed model car estimate what flow rates / sorbent/ minimum temperature and what pressure?	Modeling: Tamburello & Hardy, Pasini	Experiments: Chahine	Modeling: Tamburello & Hardy	Modeling: Hardy; Experiments: Chahine	Direct measurement of H2 purity from storage tank via mass spec or RGA. Done at beginning of tests and	Consider for Phase 2 at JPL with composite tank. Reiter and Simmons	Dust cloud ignition	Design should be robust and testing procedures should be vetted in advance for possible risks	Clarify whether I Phase 3 will require a MLVI and jacket
What exactly should be measured in this test to verify the target or model?		Usable capacity. Include 5 bar & 3 bar operating pressure as test matrix and see effect on gravimetric	Usable capacity	Estaimated costs o lab scale system to actual cost of lab scale system	f 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/afte	H2 outlet pressure at a function of charge state and discharge rate r	<ul> <li>H2 outlet pressure at a function of charge state and discharge rate</li> </ul>	Energy input to tank to induce H2 release	Cost and energy inputs during refill	Time to complete fill as a function of tank starting temperature and state of charge	H2 outlet flow as a function of state of charge and "drive cycle"	Time to achieve full flow	Time to achieve full flow. Consider extrapolating 20 C data to -20 C.	Time to achieve desired response in flow rate	Composition of desorbed gas using Mass spectrometer or RGA.	Transport of H2 through liner. Other?	N/A. BASF and/or UTRC will conduct dust cloud tests?	Meets appicable safety standards	Temperature of tank vs time. Vacuum level in insulated jacket.
What is the reference test or model ner	E' refers to experiments; 'M' refers to models	4.3 - System Fill Test 4.4 - System Delivery Test E: Chahine M: Tamburello	4.3 - System Fill Test 4.4 - System Delivery Test E: Chahine M: Tamburello	Sytem Cost Projections M: Weimar & Veenstr	WTW Efficiency Projections M: a Thornton	<insert model<br="">name&gt; M: Tamburello</insert>	<insert model<br="">name&gt; M: Tamburello</insert>	Cycle Tests; E: Chahine and Simmons	4.4 System Deliver Test; E: Chahine	ry 4.4 System Deliver Test; E: Chahine	y 4.4 System Deliver Test; E: Chahine	/ 4.3 System Fill test M: Thornton, Hard	4.3 System Fill Test t; E: Chahine, M: y Hardy & Tamburrello	4.4 System Deliver Test and 4.6 System Dynamic Test; M: Pasini, Tamburello Hardy; E: Chabine	4.5 - System start- up test; E: Chahine	4.5 - System start- up test; M: Tamburello and Hardy	4.6 System Dynamic Test; E: Chahine	H2 Purity Test: E: Veenstra, Siegel, and Chahine	Permeation Test: E Reither and Simmons	Dust cloud test; E: Khalil and/or BASF	Safety Protocols; E Chahine	: Insulation Test; E: Reiter
Does the test involve possible scaling? (Will the system size be varied in Phase 3 to examine finite-size effects?)		No. Only one size will be tested	No. Only one size will be tested	Yes. Scaling for higher volume volume manufacturing wil be included in the analysis	Yes. Models should scale to account for economies of scale (large number of vehicles and fueling stations)	d r No. Only one size will be tested	No. Only one size will be tested	No. Only one size will be tested	No. Only one size will be tested	No. Only one size will be tested	No. Only one size will be tested	No. Only one size will be tested	Possibly. Should detemine how fill time varies with state of charge and initital temperature	No. Only one size will be tested	No. Only one size will be tested	No. Only one size will be tested	No. Only one size will be tested	N/A	Consider for Phase 2 at JPL	N/A	N/A	Yes, examine different amounts of insulation
Is modeling required to justify scaling? (Should modeling be used to determine the size of the system or magnitude of effect to be tested?)		Yes. Need to quantify tradeoff between finite- size effects and th size of system which can realistically be tested.	Yes. Need to quantify tradeoff between finite- size of system which can realistically be tested.	<sup>te</sup> Yes	Yes	No	No	No	No	No	Yes	No	Yes. Need to quantify tradeoff between finite- size effects and the size of system which can realistically be tested.	Yes	No	No	Yes	No	No	No	No	Yes
Is there any contraints to the test set- up (i.e. test facility limits, materials availability, etc.) ?		See UQTR limits below	See UQTR limits below	N/A	N/A	Unlikely that heating or cooling system to these temperatures will be possible.	Chahine	Cycle test is limite by time to complete a cycle and consumables (H2, N2)	d No	No	No	N/A	Note limitations or UQTR cooling rate of compressed H2	N/A	No? Chahine	N/A	Chahine	Test rig should be designed to enable sampling of H2 purity	Reiter	N/A	Chahine	Availability of MLV is a concern. JPL to address

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## **System Test Matrixes**

	Т	arge	et		Gravi cap	metri acity	с	V	olume capaci	etric ty		Syste	em cos	st		Fuel c	cost		Ar tem	nbien peratu	t ıre
		Unit	t		w	't%			g-H <sub>2</sub> /	'L		\$/kV	Vh ne	t	\$/{	gge at	pump			°C	
Phase 3 ideas for testing specific ta Phase 3 goal for this system: System/material form: powder/compacted		2017	_		5	5.5			40							2-6	5		-40 -	60 (si	un)
Target	L	litima	te <sub>System cost</sub>	Poercost	/	<u>′.5</u>	IIIC (1/4 LATIX LO		/0	afficiants.	alaat affinia aa i	system ini rate	Million now rate	Raue (20***)	8 ( 20°C)	2-5	32/15 & 150/1015	Inchase	-40 -	60 (SL	JN)
Unit	wt%	g-H <sub>2</sub> /L	\$/kWh net	\$/gge at pump	*C	°C	full) cycles	bar (abs)	bar (abs)	%	%	kg-H2/min	(g/s)/kW	s	s	0%) s	14687-2) %H <sub>2</sub>	Scch/h			(g/h)/kg-H2 stored
2017 Ultimate	5.5 7.5	40 70	_	2-6 2-3	-40 - 60 (sun) -40 - 60 (sun)	-40/85 -40/85	1500 1500	5 3	12 12	90	60	1.5 2	0.02 0.02	5	15 15	0.75	99.97 99.97	See note See note	See note See note	See note See note	0.05
Will this target be tested?	Yes-Partial	Yes-Partial	Maybe	No	Indirect via modeling	Indirect via modeling	Yes-Partial	Yes	Yes	Yes	Indirect via modeling	Yes	Indirect via modeling	Yes	Indirect via modeling	Yes	Yes	No	Yes-Partial	Yes	Yes
What is the test or model approach?	Actual weights instrumented BOP list; Instrumentation and hardware adds to system;What we could build today;	Separate lists of volumes (as for weights)	Cost of lab system will be known. Production system costs at 500K units/year will be estimated by HSECoE and DTI	Cost to refuel will be estimated by Paster and Thornton	Test will be at room temperature	Will measure H2 delivery temperature Separate component test	Stress models ASME. Limited material cycling test (possibly 500 cycles?) + extrapolation	Test both 3 and 5 bar.	Verify pressure regulation to 12 bar functions over specified operating conditions	Determine work/heat input to release H2 and warm system to specified final temperature. Modeing:	Modeling: Thornton, Hardy	Detailed model can estimate what flow rates / sorbent/ minimum temperature and what pressure?	Modeling: Tamburello & Hardy, Pasini	Experiments: Chahine	Modeling: Tamburello & Hardy	Modeling: Hardy; Experiments: Chahine	Direct measurement of H2 purity from storage tank via mass spec or RGA. Done at beginning of tests and	Consider for Phase 2 at JPL with composite tank. Reiter and Simmons	Dust cloud ignition	Design should be robust and testing procedures should be vetted in advance for possible risks	Clarify whether Phase 3 will require a MLVI and jacket
What exactly should be measured in this test to verify the target or model?	Usable capacity. Include 5 bar & 3 bar operating pressure as test matrix and see effect on gravimetric	Usable capacity	Estaimated costs o lab scale system to actual cost of lab scale system	f 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	H2 outlet pressure at a function of charge state and discharge rate	H2 outlet pressure at a function of charge state and discharge rate	Energy input to tank to induce H2 release	Cost and energy inputs during refill	Time to complete fill as a function of tank starting temperature and state of charge	H2 outlet flow as a function of state of charge and "drive cycle"	Time to achieve full flow	Time to achieve full flow. Consider extrapolating 20 C data to -20 C.	Time to achieve desired response in flow rate	Composition of desorbed gas using Mass spectrometer or RGA.	Transport of H2 through liner. Other?	N/A. BASF and/or UTRC will conduct dust cloud tests?	Meets appicable safety standards	Temperature of tank vs time. Vacuum level in insulated jacket.
E'refers to What is the reference test or model nae seperiments; M refers to models	4.3 - System Fill Test 4.4 - System Delivery Test E: Chahine M: Tamburello	4.3 - System Fill Test 4.4 - System Delivery Test E: Chahine M: Tamburello	Sytem Cost Projections M: Weimar & Veenstr	WTW Efficiency Projections M: a Thomton	<insert model<br="">name&gt; M: Tamburello</insert>	<insert model<br="">name&gt; M: Tamburello</insert>	Cycle Tests; E: Chahine and Simmons	4.4 System Deliver Test; E: Chahine	y 4.4 System Delivery Test; E: Chahine	r 4.4 System Delivery Test; E: Chahine	/ 4.3 System Fill test M: Thornton, Hardy	4.3 System Fill Test; E: Chahine, M: Hardy & Tamburrello	4.4 System Delivery Test and 4.6 System Dynamic Test; M: Pasini, Tamburello, Hardy; E: Chahine	4.5 - System start- up test; E: Chahine	4.5 - System start- up test; M: Tamburello and Hardy	4.6 System Dynamic Test; E: Chahine	H2 Purity Test: E: Veenstra, Siegel, and Chahine	Permeation Test: E: Reither and Simmons	Dust cloud test; E: Khalil and/or BASF	Safety Protocols; E Chahine	: Insulation Test; E: Reiter
Does the test involve possible scaling? (Will the system size be varied in Phase 3 to examine finite-size effects?)	No. Only one size will be tested	No. Only one size will be tested	Yes. Scaling for higher volume volume manufacturing will be included in the analysis	Yes. Models should scale to account for economies of scale (large number of vehicles and fueling stations)	No. Only one size will be tested	No. Only one size will be tested	No. Only one size will be tested	No. Only one size will be tested	No. Only one size will be tested	No. Only one size will be tested	No. Only one size will be tested	Possibly. Should detemine how fill time varies with state of charge and initital temperature	No. Only one size will be tested	No. Only one size will be tested	No. Only one size will be tested	No. Only one size will be tested	N/A	Consider for Phase 2 at JPL	N/A	N/A	Yes, examine different amounts of insulation
Is modeling required to justify scaling? (Should modeling be used to determine the size of the system or magnitude of effect to be tested?)	Yes. Need to quantify tradeoff between finite- size effects and the size of system which can realistically be tested.	Yes. Need to quantify tradeoff between finite- e size effects and the 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
is there any contraints to the test set- up (i.e. test facility limits, materials availability, etc.) ?	See UQTR limits below	See UQTR limits below	N/A	N/A	Unlikely that heating or cooling system to these temperatures will be possible.	Chahine	Cycle test is limited by time to complete a cycle and consumables (H2, N2)	No	No	No	N/A	Note limitations on UQTR cooling rate of compressed H2	N/A	No? Chahine	N/A	Chahine	Test rig should be designed to enable sampling of H2 purity	Reiter	N/A	Chahine	Availability of MLVI is a concern. JPL to address

### **System Test Matrixes**

	Target		Gravi cap	metri acity	с	V	olume capaci	etric ty		Syste	em cos	st		Fuel c	ost		Ar tem	nbien peratu	t ure
	Unit		wt%			g-H <sub>2</sub> /	'L		\$/k\	Wh ne	t	\$/{	ge at	pump			°C		
Phase 3 ideas for testing specific ta Phase 3 goal for this system:	2017		5.5			40							2-6	5		-40 -	60 (sı	un)	
System/material form: powder/compacted:	Ultimate		7	7.5			70							2-3	3		-40 -	60 (si	un)
Will this target be	tested?	ge at pump 2-6 2-3	*C -40 - 60 (sun) -40 - 60 (sun)	C -40/85 -40/85 Indirect via	full) cycles 1500 1500	pressure to FC bar (abs) 5 3	pressure to FC bar (abs) 12 12	efficiency % 90	plant efficiency % 60 Indirect via	kg-H <sub>2</sub> /min 1.5 2	(g/s)/kW 0.02 0.02 Indirect via	flow (20°C) s 5 5	flow (-20°C) s 15 15 Indirect via	0%) 5 0.75 0.75	12719 4150/P013 14687-2) %H <sub>2</sub> 99.97 99.97	leakage Scch/h See note See note	See note See note	See note See note	(g/h)/kg-H2 stored 0.05 0.05
		o refuel will imated by and ton	modeling Test will be at room temperature	modeling Will measure H2 delivery temperature Separate component test	Yes-Partial Stress models ASME. Limited material cycling test (possibly 500 cycles?) + extrapolation	Yes Test both 3 and 5 bar.	Yes Verify pressure regulation to 12 ban functions over specified operating conditions	Yes Determine work/heat input to release H2 and warm system to specified final temperature. Modeing:	modeling Modeling: Thornton, Hardy	Yes Detailed model car estimate what flow rates / sorbent/ minimum temperature and what pressure?	modeling Modeling: Tamburello & Hardy, Pasini	Yes Experiments: Chahine	modeling Modeling: Tamburello & Hardy	Yes Modeling: Hardy; Experiments: Chahine	Yes Direct M2 purity from storage tank via mass spec or RGA. Done at beginning of tests and	No Consider for Phase 2 at JPL with composite tank. Reiter and Simmons	Yes-Partial	Yes Design should be robust and testing procedures should be vetted in advance for possible risks	Yes Clarify whether Phase 3 will require a MLVI and jacket
			d External temperature	H2 outlet temperature	Fatigue behavior. Structure of tank internals before/after cycling (tomography?). H2 purity before/after	H2 outlet pressure at a function of charge state and discharge rate	H2 outlet pressure at a function of charge state and discharge rate	Energy input to tank to induce H2 release	Cost and energy inputs during refill	Time to complete fill as a function of tank starting temperature and state of charge	H2 outlet flow as a function of state of charge and "drive cycle"	Time to achieve full flow	Time to achieve full flow. Consider extrapolating 20 C data to -20 C.	Time to achieve desired response in flow rate	Composition of desorbed gas using Mass spectrometer or RGA.	Transport of H2 through liner. Other?	N/A. BASF and/or UTRC will conduct dust cloud tests?	Meets appicable safety standards	Temperature of tank vs time. Vacuum level in insulated jacket.
What is the test or model approach?		Efficiency tions M: ton	<insert model<br="">name&gt; M: Tamburello</insert>	<insert model<br="">name&gt; M: Tamburello</insert>	Cycle Tests; E: Chahine and Simmons	4.4 System Delivery Test; E: Chahine	4.4 System Delivery Test; E: Chahine	/ 4.4 System Delivery Test; E: Chahine	r 4.3 System Fill test M: Thornton, Hard	4.3 System Fill Test ; E: Chahine, M: y Hardy & Tamburrello	4.4 System Delivery Test and 4.6 System Dynamic Test; M: Pasini, Tamburello, Hardy; E: Chahine	4.5 - System start- up test; E: Chahine	4.5 - System start- up test; M: Tamburello and Hardy	4.6 System Dynamic Test; E: Chahine	H2 Purity Test: E: Veenstra, Siegel, and Chahine	Permeation Test: E: Reither and Simmons	Dust cloud test; E: Khalil and/or BASF	Safety Protocols; E Chahine	: Insulation Test; E: Reiter
		odels shoul o account fo mies of scale number of es and g stations)	d rr e 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 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 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	N/A	No? Chahine	N/A	Chahine	Test rig should be designed to enable sampling of H2 purity	Reiter	N/A	Chahine	Availability of MLVI is a concern. JPL to address

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
ase 3 ideas for testing specific ta se 3 goal for this system: tem/material form: powder/compacted	2017	5.5	40		2-6	-40 - 60 (sun)
	Ultimate	7.5	70		2-3	-40 - 60 (sun)
this target be t	tested?	Yes-Partial	Ves-Partial	Maybe	No	Indirect via modeling
Will this target be tested? What is the test or model approach?		Actual weights instrumented BOP list; Instrumentation and hardware adds to system;What we could build today; Alternate list of what it could be.; actual capacity of system	Separate lists of volumes (as for weights)	Cost of lab system will be known. Production system costs at 500K units/year will be estimated by HSECOE and DTI	Cost to refuel will be estimated by Paster and Thornton	Test will be at room temperature
What exactly should be measured in 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 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
	se 3 Ideas for testing specific to a goal for his system: em/material form: powde/compacted this target be t is the test or t exactly shou est to verify t	Target   Unit   solution   indentation   and indentation   and indentation   tist the test or model approach? texactly should be measured in est to verify the target or model?	TargetGravimetric capacityUnitwt%20175.5Ultimate7.5Ultimate7.5this target be tested?Yes-PartialActual weights instrumented BOP list; Instrumentation and hardware adds to system;What we could build today; Alternate list of what it could be.; actual capacity. Include 5 bar & 3 bar operating pressure as test matrix and see effect on gravimetric capacity.	TargetGravimetric capacityVolumetric capacityUnitwt%g-H_J/L***********************************	TargetGravimetric capacityVolumetric capacitySystem costUnitwt%g-H <sub>2</sub> /L\$/kWh net20175.540Ultimate7.570this target be tested?Yes-PartialYes-PartialActual weights instrumented BOP list; Instrumented BOP sistem cold build today; Alternate list of what it could be.; actual capacity.Cost of lab system will be known. Production system costs at 500K units/year will be estimated by HSECoE and DTIet exactly should be measured in est to verify the target or model.Usable capacity. Include 5 bar & 3 bar operating pressure as test marix and see effect on gravimetric capacity.Usable capacity. lisable capacity.	TargetGravimetric capacityVolumetric capacitySystem costFuel costUnitwt%g-H_2/L\$/kWh net\$/gge at pump20175.5402-6Uttimate7.5702-3this target bet bet of uttimateYes-PartialMaybeNoActual weights instrumented BOP list; tist the test or model approach?Actual weights instrumented BOP units/ware adds system; What we volumes (as for volumes (as for system)Cost of lab system will be known. Production system costs at 500K units/year will be estimated by HSECOE and DTI actual capacity of 

**HSECoE** 

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Component	Assumed Validation in Phase II	Responsible Design Organization	What can be validated with modeling rather than experimental work?	Rationale for including/excluding from Phase III	Areas of Concern Requiring Testing	Limitations on Scaling	Include in Phase
Internal Heat Exchanger: HexCell Resistance Heater with Flow- Through Cooling	Modeling and partial experimental validation of individual components/capabilities	SRNL / UQTR	1 <sup>st</sup> -order thermal behavior (already completed).	Simple, low-cost design; Verify capability for rapid cooling: dynamic behavior (such as channeling) can only be evaluated experimentally	Cool-down time; non- uniform temperature distribution; robustness of HX with respect to temperature/pressure cycling; efficiency (energy consumed during fill)	N/A	Yes
Cryo-Adsorbent Material: <b>Powder MOF-5</b>	Modeling and experimental validation	SRNL / UQTR / Ford (BASF)	Theoretical H2 uptake; heat transfer (partial)	Integral part of system; validate capacity projections; Quantify effects due to bed inhomogeneities (non- uniform packing)	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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	^	ccumo/	d Validation	Respo	onsible	What can be validated with modeling rather than experimental wor			
Compone	nt <sup>P</sup>	lssumer D		De	sign				
			nase n	Organ	ization				
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: <b>Powder MOF-5</b>	Modeling and experimental validation	SRNL / UQTR / Ford (BASF)	Theoretical H2 uptake; heat transfer (partial)	Integral part of system; validate capacity projections; Quantify effects due to bed inhomogeneities (non- uniform packing)	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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Co	Assume Component				d Validation in Phase II			onsible sign ization	What can be validated with modeling rather than experimental wor			
Internal H Exchange HexCell R Heater w Through (	leat r: Resistance ith Flow- Cooling	Modeling experimer of in componen	g and par ntal valida dividual its/capabi	tial ation llities	SRNL /	UQTR	1 <sup>st</sup> -orde (alre	er thermal beh eady completed	avior I).	Simple, Verify c cooling: (such a only ex	low-cost design; apability for rapid dynamic behavior s channeling) can be evaluated perimentally	
"Th	ermos Bottle"	models to show the need/benefit	Composites	can	be modeled	within the ch evaluated e	annel must be xperimentally	phase change	re	main intact		
Inte Excl with Hea LN2	ernal Heat hanger: MATI h Isolated-H2 ating and Isolated- 2 Cooling	ATI experimental validation H2 of individual of individual components/capabilities OSU 1 <sup>st</sup> -order thermal behavior has already been verified. at Modeling and partial experimental validation (BASF) Theoretical H2 uptake; heat transfer (partial)		1 <sup>st</sup> -order thermal behavior has already been verified.		hermal behavior ly been verified. Quantify a cooling rate volume; V cooling ca cooling ca		advantages in     Welds, cycling, and       ate and system     verification of       cycrify rapid     adsorption/desorption       capability and     behavior, design       n performance     complexity/robustness		N/A	Yes – partially	
Cryo Mat Con "pu	o-Adsorbent terial: mpacted MOF-5 ucks" (0.32 g/cc)			Integral pa validate c kinetic proje robustnes transfer	rt of system; apacity and ctions; Assess and heat limitations	Cracking/crumbling, heat transfer, and adsorbent behavior		N/A	Yes – partially			
Тур pre:	Type 1 Aluminum Design and pa pressure vessel experimental val		LC	Mass, v	olume, and cost	Integral pa validate proie	rt of system; capacity ections	Cryo-burst testing		N/A	Yes	
Mul insu	lti-layer vacuum ulation	Modeling of heating rate/dormancy performance	JPL	Parti pe	ial dormancy rformance	Validate dor vacuum le robustnes	mancy model; vel stability; ss of design	No supplier (JPL work scope reduction)		N/A	No	

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Componen	t A	Assumed P	umed Validation in Phase II				onsible sign ization	Wh wi than	at can b th mode experim	at can be validated h modeling rather experimental work?		
Internal Heat Exchanger: HexCell Resistance Heater with Flow- Through Cooling	rnal Heat hanger: Cell Resistance ter with Flow- bugh Cooling Modeling and experimental w of individ components/ca				UQTR	1 <sup>st</sup> -orde (alre	er thermal bel ady complete	havior ed).	Simple, Verify ca cooling: c (such as only exp	low-cost design; pability for rapid lynamic behavior channeling) can be evaluated erimentally		
Cryo-Adsorbent Material: <b>Powder MOF-5</b>	Modeling and experimental valid			SRNL / L Ford (E	JQTR / BASF)	Theo heat	retical H2 upt transfer (par	ake; tial)	Integra valio projec effec inhomo unif	l part of system; date capacity tions; Quantify ts due to bed ogeneities (non- orm packing)		
Type 1 Aluminum pressure vessel Multi-layer vacuum insulation	Design and partial experimental validation LC Mass Modeling of heating rate/dormancy JPL P		Mass, v Part pe	al dormancy		rt of system; capacity ections mancy model; vel stability;	Cryo-burst testing No supplier (JPL work scope reduction)		N/A N/A	Yes		
	Ferrormanoe				robustnes	is of design						

# **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

(FI) HSECOE

## **Phase 3 Gantt Chart**

WBS	Task Name	Resource Names	Duration	Start	Finish				2014				2015	
						Qtr 2	Qtr 3	Qtr 4	Qtr 1	Qtr 2	Qtr 3	Qtr 4	Gtr 1	Qtr 2
3.1	Design subscale prototype systems		66 days	Mon 7/1/13	Mon 9/30/13			•						
3.1.1	Adsorbent	SRNL/OSU	66 days	Mon 7/1/13	Mon 9/30/13			1						
3.1.2	Chemical	LANL/PNNL	66 days	Mon 7/1/13	Mon 9/30/13			-						
3.2	Synthesize/Modify Materials		326 days	Mon 7/1/13	Mon 9/29/14		•							
3.2.1	Adsorbent	FMC	111 days	Mon 7/1/13	Mon 9/29/14									
3.2.2	Chemical	PNNL	111 days	Mon 7/1/13	Mon 9/22/14									
3.3	Complete test facilities		196 days	Mon 7/1/13	Mon 3/31/14		•		· ·	•				
3.3.1	Adsorbent	UQTR/OSU	196 days	Mon 7/1/13	Mon 3/31/14					հ				
3.3.2	Chemical	lani	196 days	Mon 7/1/13	Mon 3/31/14				:	Н				
3.4	Acquire BoP/System Components		60 days	Wed 10/9/13	Tue 12/31/13			<u> </u>	Ý.					
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				H					
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				Ľ	H				
3.5.2	Chemical	LANL/UTRC	64 days	Wed 1/1/14	Mon 3/31/14				<u> </u>	Н				
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					Ľ			4	
3.6.2	Chemical	lani	197 days	Tue 4/1/14	Wed 12/31/14					Ľ				
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					Ľ			ġ.	
3.7.2	Chemical	PNNL	197 days	Wed 4/2/14	Thu 1/1/15					Ĭ			<b>.</b>	
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					Ľ			ih ا	
3.8.2	Chemical	lani	197 days	Tue 4/1/14	Wed 12/31/14					Ľ			۹L – L	
3.9	Post updated models on WEB	SRNL/UTRC/PNNL/NREL	20 days	Thu 1/1/15	Wed 1/28/15							1	Ť.	
3.10	Decommission prototypes as necessary		40 days	Thu 1/1/15	Wed 2/25/15							I	÷	
3.10.1	Adsorbent	UQTR/OSU	40 days	Thu 1/1/15	Wed 2/25/15								L .	
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								4	
3.12.2	Chemical	LANL/PNNL	198 days?	Mon 3/31/14	Wed 12/31/14								4	
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								<u> </u>	
3.13.2	Adsorbent	UM	457 days	Mon 7/1/13	Tue 3/31/15				:				<u>.</u>	
3.13.3	Chemical	lani	457 days	Mon 7/1/13	Tue 3/31/15				:				ų.	
3.14	Write Final Report	All	66 days	Thu 1/1/15	Thu 4/2/15							I	<del>۴ – – •</del>	<b>.</b>

(F1) HSECOE

### **Phase 3 Gantt Chart**

WBS	Task Name	Resource Names Duration Start Finish							2015					
						Qtr 2	Qtr 3	Qtr 4		Qtr 2	Qtr 3	Qtr 4	Qtr 1	Qtr 2
3.1	Design subscale prototype systems		66 days	Mon 7/1/13	Mon 9/30/13	l	·	•						
3.1.1	Adsorbent													
3.1.2	Chemical			lesto	nes e	einc	l De	veio	pea i	OLES	acn			
3.2	Synthesize/Modify Materials			<b>~</b> ·			<b>`</b>		•			1		
3.2.1	Adsorbent	Contribution in Resources												
3.2.2	Chemical													
3.3	Complete test facilities		196 d	Mon 7/1/13	Mon 3/31/14	I	÷			•				
3.3.1	Adsorbent	UQTR/OSU	196 c	Mon 7/1/13	Mon 3/31/14					∎ŋ				
3.3.2	Chemical	lani	196	Mon 7/1/13	Mon 3/31/14					■-				
3.4	Acquire BoP/System Components		ys	Wed 10/9/13	Tue 12/31/13			<u> </u>	<b>-</b>					
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			1						
3.5	Fabricate/assemble prototype system		64 days	Wed 1/1/14	Mon 3/31/14				<u> </u>	•				
3.5.1	Adsorbent	UQTR/OSU	64 days	Wed 1/1/14	Mon 3/31/14				Ľ.					
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					Ľ			<b>I</b>	
3.7	Compare to and refine models		197 days	Wed 4/2/14	Thu 1/1/15								<b>•</b>	
3.7.1	Adsorbent	SRNL/OSU	197 days	Wed 4/2/14	Thu 1/1/15					1			<b>İ</b>	
3.7.2	Chemical	PNNL	197 days	Wed 4/2/14	Thu 1/1/15					1			<b>İ</b>	
3.8	Modify test apparatus/prototype		197 days	Tue 4/1/14	Wed 12/31/14					<u>.</u>			Ý.	
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					Ľ			£	
3.9	Post updated models on WEB	SRNL/UTRC/PNNL/NREL	20 days	Thu 1/1/15	VVed 1/28/15								ý – v	
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	VVed 2/25/15								Ľ.	
3.10.2	Chemical	lani	40 days	Thu 1/1/15	VVed 2/25/15								ř.	
3.11	Performance/Cost Model Updates		164 days?	Fri 5/16/14	Wed 12/31/14					-			Ý	
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					· · · · ·			Ý	
3.12.1	Adsorbent	FMC/SRNL	198 days?	Mon 3/31/14	Wed 12/31/14								<b>i</b>	
3.12.2	Chemical	LANL/PNNL	198 days?	Mon 3/31/14	Wed 12/31/14						-			
3.13	Project Management		457 days	Mon 7/1/13	Tue 3/31/15	''	-							•
3.13.1	Center	SRNL	457 days	Mon 7/1/13	Tue 3/31/15					-				1
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					-			Ų	1
3.14	Write Final Report	All	66 days	Thu 1/1/15	Thu 4/2/15								¥	•

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



### 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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Fuel cell system

**HSECoE** 




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