IV.B.2 Systems Engineering of Chemical Hydrogen Storage, Pressure Vessel, and Balance of Plant for Onboard Hydrogen Storage

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Contract Number: DE-AC05-76RL01830

Project Start Date: February 1, 2009
Project End Date: January 31, 2014

Overall Objectives

- Develop engineering and design models to further the understanding of onboard storage energy management requirements.
- Develop innovative onboard system concepts for chemical hydrogen storage and cryogenic adsorption materials-based storage technologies.
- Develop and validate models for a chemical hydrogen storage system.
- Work with our partners to integrate our validated models into system framework that will lend insight into overall fuel cycle efficiency.
- Develop materials characteristic performance envelope for chemical hydrogen storage systems.
- Demonstrate key components for chemical hydrogen and cryo-sorbent-based materials.
- Reduce system volume and mass while optimizing system storage capability and performance through value engineering of heat exchangers and balance-of-plant (BOP) components.
- Mitigate materials incompatibility issues associated with hydrogen embrittlement, corrosion, and permeability through suitable materials selection for vessel materials, heat exchangers, plumbing and BOP components.
- Project the cost of chemical and cryo-sorbent materials-based hydrogen storage systems.

Fiscal Year (FY) 2013 Objectives

- Chemical Hydrogen Storage Design
  - Validate models and concepts via experiments
  - Scale up slurry production
  - Assess feasibility of liquid-slurry chemical hydrogen storage
  - Assess feasibility of volume-exchange tank
  - Assess feasibility of slurry use with heat exchanger, pump, valves
  - Project system efficiency, mass, and volume
- Pressure Vessel for Cryo-Adsorbent Hydrogen Storage
  - Exercise “tankinator” model to assess materials and design options for Type I, III, and IV vessels
  - Optimize vessel design in terms of cost
  - Assess vessel cost as function of pressure and temperature
  - Project system mass and volume
- BOP
  - Maintain BOP library
  - Size components (heat exchangers, valves, pumps, etc.)
  - Determine material compatibility
  - Identify where improvements can be made
- Cost Modeling to project the systems cost at various production levels

Technical Barriers

This project addresses the following technical barriers for Hydrogen Storage from the Fuel Cell Technologies Office Multi-Year Research, Development, and Demonstration Plan:

General to all storage approaches:

(A) System Weight and Volume

(B) System Cost

(C) Efficiency

(D) Durability/Operability

(E) Charging/Discharging Rates

(G) Materials of Construction

(H) Balance of Plant (BOP) Components:

(I) Dispensing Technology

(J) Thermal Management

(K) System Life-Cycle Assessments

(N) Hydrogen Venting

Off-Board regenerable specific

(R) By-Product/Spent Material Removal

Technical Targets

The technical targets for this project are presented in Table 1.

FY 2013 Accomplishments

- Completed testing of eight materials for use in Type IV pressure vessels determining tensile strength, storage modulus, elongation, and glass transition temperatures under cryogenic conditions.
- Identified BOP components for a cryo-sorbent hydrogen storage system with a total mass less than 9.4 kg and volume less than 11.6 L exceeding our targets of 17 kg and 18.5 L.
- Developed manufacturing approaches for Type I and III cryo-sorbent pressures.
- Completed a tradeoff study on joining techniques and identified friction stir welding as the most likely candidate to be able to join the tanks during the manufacturing process without damaging the sorbent materials.
- Developed the thermos bottle concept to enable fast tank cooling with liquid nitrogen rather than cryogenic hydrogen. This concept would potentially reduce the excess hydrogen required for a 5.6-kg fill from over 11 kg to ~1.1 kg depending on initial tank pressure.

TABLE 1. Progress towards Meeting Technical Targets for Hydrogen Storage

Hydrogen Storage Enginering Center of Excellence

Phase 2 System Status

6/30/2013

			Adsorbent System			Chemical Systyem		
			Phase 2 *Actual (automotive scale)*			Projected System HSECoE Go/No-Go*What could be built in the future (full scale)*		
Target	Units	2017 DOE Goal (System)	Phase 2 HSECoE Targets (Material)	Phase 2 HSECoE Targets (BOP only)	Phase 2 HSECoE Targets (System)	Phase 2 HSECoE Targets (Material)	Phase 2 HSECoE Targets (BOP only)	Phase 2 HSECoE Targets (System)
Gravametric Capacity	kg H2/kg system	0.055	0.187	0.10	0.0352	0.0872	0.15	0.055
mass	*kg*	*102*		*16.1*	159			*102*
Volumetric Capacity	kg H2/L system	0.04	0.03	0.053	0.0175	0.078	0.132	0.049
Volumetric	*liters*	*140*		*16.9*	320			*114*
System Cost	$/kWh net	6	3.5	5.62	12.74			
	$	*1,119*		*1048*	2376			
Fuel Cost	$/gge at pump	2-6			4.89			
Min Operating Temp	°C	-40			-40			-20
Max Operating Temp	°C	60			60			60
Min Delivery Temp	°C	-40			-40			-20
Max Delivery Temp	°C	85			85			85
Cycle Life	Cycles	1500			1500			1000
Min Delivery Pressure	bar	5			5			5
Max Delivery Pressure	bar	12			12			12
Onboard Efficiency	%	90			92			95
Well to Power Plant Efficiency	%	60			39.2			37
System Fill Time	min	3.3			3.3			2.9
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			5			1
Start Time to Full Flow (-20°C)	sec	15			15			1
Transient Response	sec	0.75			0.75			0.5
Fuel Purity	%H2	99.97			99.99			99.97
Permeation, Toxicity, Safety	Scc/h	Meets or Exceeds Standards			s			s
Loss of Useable Hydrogen	(g/h)/kg H2 stored	0.05			0.44			0.05

- Completed the development of the "tankanator" model and provided it to Savannah River National Laboratory (SRNL) for insertion into their models.
- Completed costing of 135 cryo-sorbent tank configurations and identified a 100-bar, Type I vessel with MOF-5 as the lowest cost option.
- Reduced projected cost of the cryo-sorbent hydrogen storage system from >$3,000/system in FY 2012 to less than $2,500/system in FY 2013.
- Terminated work on Type IV pressure vessels for 40 K cryogenic operation due to liner separation from the shell at pressures less than 35 bar and limitations on low-cost liner materials.
- Validated reactor model for an exothermic (slurry ammonia borane, AB) and endothermic (slurry alane as simulant) chemical hydrogen systems.
- Developed chemical hydrogen storage system model which included instrumentation, controls, controls logic, and engineering improvements increase the parts in the system from 12 in FY 2012 to 47 in FY 2013. This was used for cost, mass and volume calculations.
- Developed a feasible pathway to achieve DOE gravimetric and volumetric hydrogen storage targets using exothermic chemical hydrogen materials.
- Reduced projected costs from ~$4,700/system to ~$3,000/system by moving from a solid chemical hydrogen system to a slurry chemical hydrogen system.
- Validated the slurry flow-through reactor, heat exchangers, and volume exchange tanks.
- Demonstrated that the slurry could successfully flow at -20°C.
- Identified the need for pump development for size and mass reduction for fresh AB.
- Demonstrated that a pleated membrane could be used in a volume exchange tank for chemical hydrogen slurries.
- Demonstrated fluidization of settled solids and removal of slurry from a volume exchange tank such that a hydrogen storage system based on this concept could be drained and filled within 5 minutes, meeting the DOE targets.
- Demonstrated a 50 wt% AB slurry with a viscosity less than 1,500 cP meeting DOE targets.
- Measured settling and flocculation rates of spent and fresh AB.
- Demonstrated that Triton X-15 significantly reduces foaming at low weight percent loadings (1-3%) in AB slurries.
- Scaled up slurry production process from <150 mL batches to >750 mL batches.

INTRODUCTION

Multiple onboard vehicle-scale hydrogen storage demonstrations have been done, including several studies to examine characteristics that impact systems engineering. However, none of these demonstrations have simultaneously met all of the DOE hydrogen storage sub-program goals. Additionally, engineering of new chemical hydrogen storage approaches is in its infancy, with ample opportunity to develop novel systems capable of reaching the DOE targets for storage capacity. The goal of the Hydrogen Storage Engineering Center of Excellence (HSECoE), led by SRNL, is to develop and demonstrate low-cost, high-performing, onboard hydrogen storage through a fully integrated systems design and engineering approach. Toward this end, PNNL is working with HSECoE partners to design and fabricate a system based on slurry chemical hydrogen storage media.

APPROACH

As part of the HSECoE, PNNL actively contributes to all five technology areas and targets six key objectives to optimize performance characteristics and reduce the size, weight, and cost of a H_2 storage system. This is being accomplished through engineering and integrated design approach, including application of advanced materials (structural and H_2 storage), and assessments of manufacturing and cost impact based on established models/approaches for technology tradeoff or "viability" studies.

PNNL serves multiple leadership roles within the HSECoE technology area structure to help facilitate collaboration across the center partnership and to feed technical results to other HSECoE partners. Achieving the objectives enables PNNL, SRNL, and other HSECoE partners to demonstrate onboard hydrogen storage with the potential to meet DOE technical targets. This technology and design knowledge will be transferred to the participating automotive original equipment manufacturers, thus advancing the hydrogen market sector and production of future hydrogen-powered vehicles. As appropriate, the models, catalogues, and lessons learned will be made available to the fuel cell community to accelerate fuel cell technology commercialization.

RESULTS

Cryo-Sorbent Hydrogen Storage

The cryo-sorbent hydrogen storage system work completed in FY 2013 was focused on: Type IV pressure vessel evaluation, optimal vessel type selection, cost projection, BOP identification to meet mass and volume targets, and hydrogen filling optimization.

Analysis completed in Phase I of the project (FY 2012) indicated that the pressure vessel accounted for the majority of cost, and BOP mass and volume. Therefore we began a systemic study with our partners to identify the optimal conditions and vessel type to minimize cost while increasing the volumetric and gravimetric hydrogen content. Therefore we evaluated Type I, III, and IV pressure vessels in various system configurations. Type IV pressure vessels use a polymer liner with carbon fiber outer layers. They offer a light-weight solution compared to the other pressure vessel types. Through computer modeling, we determined that the polymer liner needed to be limited to 2.55 mm in order to meet the volumetric and gravimetric BOP targets. We tested eight materials for hydrogen permeation, tensile strength, fatigue, coefficient of thermal expansion, elongation, and storage modulus in cryo-genic conditions, and we measured their glass transition temperatures. Hexagon Lincoln tested the materials for weld strength and impact. Halar and high-density polyethylene had the best properties. However, we found that even the best materials, when used as a liner, would separate from the shell when the hydrogen pressure was less than 35 bar. This would mean that the hydrogen pressure would always need to remain >35 bar, severely limiting the usable hydrogen. Therefore, the Type IV pressure vessels were out-selected.

PNNL developed the "tankinator" model which combined the predictive performance and sizing models with costs to be able to predict tank costs at different pressures and temperatures. Specifically, the tankinator code estimated the necessary wall thickness for pressure vessels given a Type (I, II, or III), operating pressure, cost, and two out of the following three: storage volume, diameter, or length. Its ability to estimate reasonable wall thickness and pressure vessel mass was validated against tank geometry designs available in the open literature and some proprietary tank design information. It includes a winding model that evaluated the amount of fiber and resin required. For manufacturing, it included the winding time. We adapted a model that Thiokol used to estimate the costs of Type II and Type IV tanks to evaluate the costs. We added Type III pressure vessels and a manufacturing process flow model that examined the steps in the manufacturing process, identifying equipment and costs, cycle times, and labor required. The cost estimation component of the analysis was validated against a proprietary database of existing tank designs. The cost estimation was also validated through cross comparison of the PNNL cost model to a third-party manufacturing process flow cost model. Figure 1 has a snapshot of the model inputs, Type I pressure vessel. The model predicts the total system cost, amount of fiber used, materials costs, manufacturing costs, and BOP costs. This model was used to predict the costs of 135 different cases and identified 100-bar Type I system with MOF-5 as the lowest cost option. The Center developed a detailed system schematic which included BOP instrumentation, controls, control logic, etc. The BOP was optimized using the 100-bar Type I system. PNNL optimized the system BOP to minimize mass and volume and identified a system with BOP having a mass of 9.4 kg and volume of 11.6 L which was under our targets of 17 kg and 18.5 L. This was a bottom-up design.

Finally, the Center examined the challenge of cooling the pressure vessel during filling. An "empty" tank may have a temperature of 180 K and needs to be cooled to 80 K for a complete fill. The conventional approach for filling the cryo-sorbent tanks is to cool the tank by flowing cryo-compressed hydrogen. The hydrogen would cool the sorbent media, tank walls, etc., to the desired operating temperature. This process is highly inefficient and is particularly poor at cooling the tank walls. SRNL determined that it is nearly impossible meet the DOE fill time target using only flow-through hydrogen to cool and fill a cryo-sorbent tank at 100 bar, assuming temperatures above 180 K. Lowering tank pressure would make it even less likely to meet the fill time target. Furthermore, we determined that flow-through hydrogen to

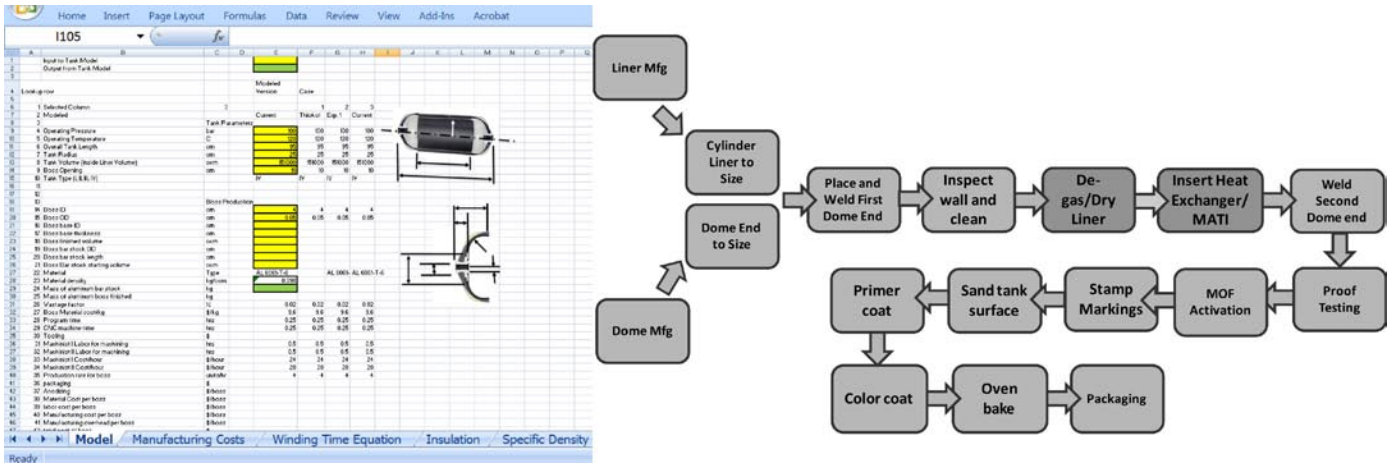

FIGURE 1. Tankinator Model Inputs and Example Manufacturing Flow Chart

cool the tank requires a loss of up to 11 kg of H_2 for a 5-6 kg H_2 fill. While the excess hydrogen can be recompressed and cooled, this additional processing would increase costs. SRNL's analysis indicated that the sorbent media is relatively quickly cooled by the hydrogen, but the pressure vessel and insulation required the majority of the excess hydrogen to reach the desired temperatures. PNNL developed a thermos concept (Figure 2) which would utilize liquid nitrogen to cool the pressure vessel outer surface. SRNL projected that using liquid nitrogen as a pre-fueling coolant can reduce the waste of hydrogen fuel from 11 kg/fill to 1.1-2.4 kg depending on tank pressure. Coupling the Modular Adsorption Tank Insert design being developed by Oregon State University with the thermos concept would virtually eliminate excess hydrogen. With or without the Modular Adsorption Tank Insert, the thermos concept would enable an empty tank to fill within the 5 minute DOE Target.

Chemical Hydrogen Storage

PNNL's chemical hydrogen storage work in the Center was focused on: model validation, BOP identification, key part validation, and AB slurry production and characterization. Developing and validating system models is a key objective of this project. Los Alamos National Laboratory (LANL) provided PNNL data from their flow reactor for both an exothermic chemical hydrogen material (AB slurry) and an endothermic chemical hydrogen material (alane slurry). The model fit the AB slurry experimental data without any need for modification. However, the alane experimental results did not fit the model. This was because the model used reaction kinetics for an "active" alane developed by Graetz [1]. The alane used in LANL's experiments was not activated. Therefore we used data from one of the experimental runs to fit the data for the less active alane. The new kinetic equation was put into the model. Other experimental runs at different flow rates were compared to the model and found to have a good fit. Figure 3 contains the results of the AB slurry experimental and model data and the fixed alane experimental and model data.

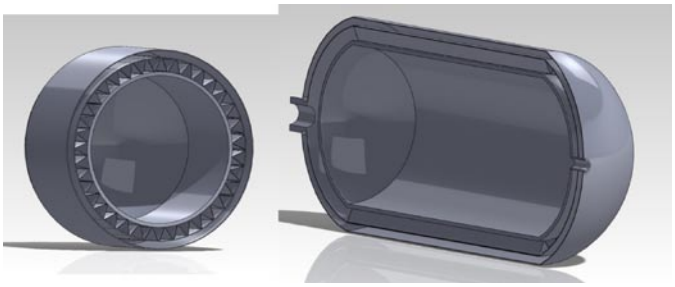

FIGURE 2. Conceptual Design for the Thermos Bottle Concept to Reduce Cooling Time and Excess Hydrogen Requirements during Filling

Previously, PNNL worked with United Technologies Research Center, and LANL to develop a chemical hydrogen storage system schematic. In FY 2013, we added instrumentation, controls, and control logic to the schematic. This increased the part count from 12 to over 47 and was used to predict the mass, volume and cost of the system. PNNL identified off-the-shelf parts that could be used to build the design. We believe that the part count can be reduced to ~34. The system mass was 137 kg with the BOP accounting for approximately 54 kg. We then identified a pathway to reduce the BOP mass to 38 kg meeting our 41 kg target. We proposed that the pump, radiator, and valves mass could be reduced by 25%; the mass of the mixers for the tank could be reduced by 50%; and the clean-up system mass could be reduced by 75% by using a material that did not produce as much impurities. In order to achieve the 5.5 wt% gravimetric target, these BOP improvements would be required, plus the hydrogen content would need to be increased to ~8 wt%. However, if a liquid chemical hydrogen material that did not require mixing and had minimal

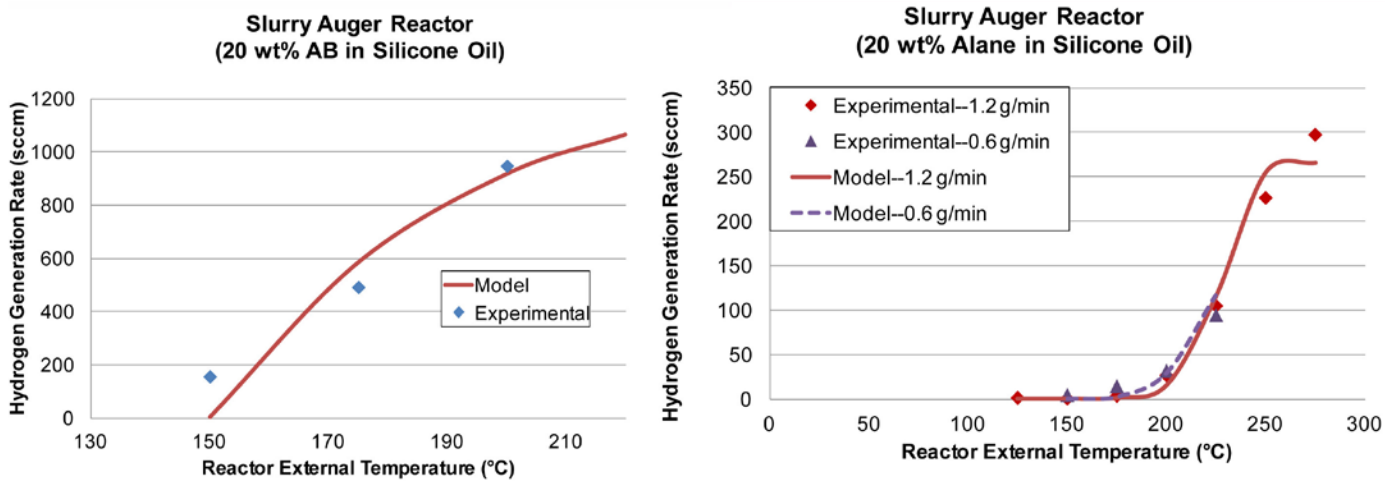

FIGURE 3. Model Validation for Slurry AB and Slurry Alane

hydrogen clean-up was used, the required gravimetric capacity to meet the DOE targets could be reduced to 7.8 wt%.

The proposed schematic's key components were the reactor, gas-liquid phase separator, pumps, valves, heat exchangers, volume displacement tank, and hydrogen cleanup system. PNNL validated the heat exchangers (FY 2012), volume displacement tanks (FY 2013), and pumps (FY 2013). The gear pump identified in FY 2012 worked well with the simulant and spent AB. However, with fresh AB slurry the pump seized. Syringe and peristaltic pumps could successfully pump the fresh AB slurry. Unfortunately, syringe and peristalitic pumps are not suitable options for a vehicle, so future work would be needed to develop a suitable pump for slurry AB should the DOE or others move forward with it. In FY 2013 we assembled a simple system composed of a prototypical heat exchanger, pump, Swagelok® fittings, and valves to study the impact of slurry setting and to validate the heat exchanger model. We used simulant for the majority of the tests, although spent AB slurry was also used. We operated the system with the simulant for several hours and then turned off the pump. The slurry was allowed to settle overnight. The system successfully re-started the next day. We did this cycle several times and then pulled apart the system looking for deposits of material. We found a slight deposit in the 90 degree elbows. By removing the 90 degree elbow this problem can be resolved. In addition, we decreased the system temperature to -20°C and tested the system in the same way. The system with the settled slurry was able to start and operate at the low temperatures.

For a liquid chemical hydrogen system, both the fresh and spent fuel must be stored onboard. Rather than use separate tanks for fresh and spent fuel, we proposed a volume exchange tank. We ran chemical compatibility tests on various materials, ethylene propylene diene monomer, Viton®, and Buna-N, to ensure that the materials can work well with AB and spent AB. None of the materials showed significant changes in tensile strength or elongation. Viton® had the lowest mass and length change. To minimize the stress on the membrane we developed a pleated membrane which rather than stretch, unfolds to the desired shape (Figure 4a). We also examined ways to homogenize a settled slurry and flocculated slurry by using an ultrasound, impeller mixer, French press, jet mixing, and vibration. French press was identified as the best candidate. Using 11 kg of simulant slurry, we demonstrated that a volume exchange tank with a French press can homogenize a fully settled slurry and remove 98% of it within 1.7 minutes (Figure 4b). This rate would meet the DOE targets in a full-scale device.

In FY 2013 we completed our AB slurry work. We measured the flocculation and settling rate of a 45 wt% AB slurry (Table 2) and scaled up slurry manufacturing from 100-ml to 750-ml batches. In addition, we completed our investigation into additives for the slurry by examining DOW's Triton™ X-15, X-35, and X-45. When added to a 35-wt% AB slurry at 1-wt% mass, the X-15 reduced foaming during reaction and increased slurry stability (decreased the slurry's tendency to solidify). The additive X-35 reduced the foaming but not as much as X-15, and X-45 had no visible effect. Therefore, we added the X-15 to all future slurries developed and tested. We demonstrated this slurry in a flow-through reactor equipped with a mixer. At a set point of 200°C, 300 rpm mixing, and 1.75 min residence time (same order of magnitude as a full-scale system), no plugging of

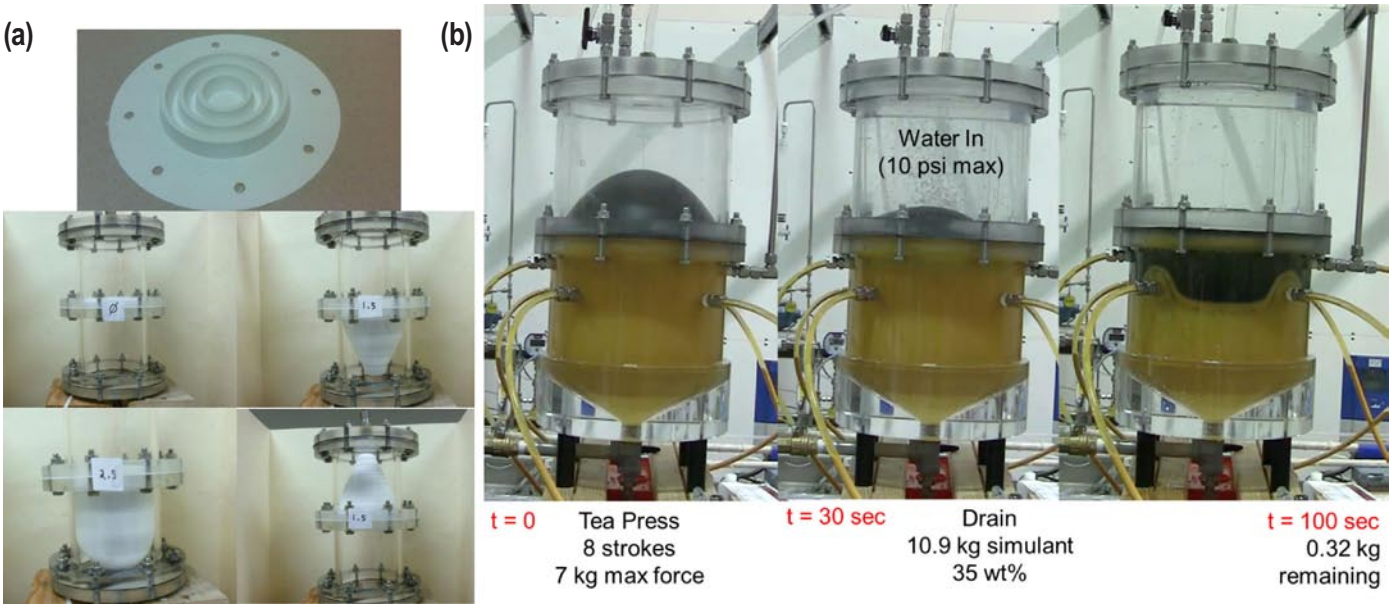

FIGURE 4. Volume Exchange Tank (a) Pleated Membrane (b) Mixing and Removal of Spent AB Slurry

TABLE 2. Flocculation Rate and Settling Rate of 45 wt% AB Slurry

Time	Fresh AB Flocculation	Spent AB Settling
0 min	-	-
5 min	10.4%	21.1%
10 min	21.1.%	26.3%
1h	21.1%	26.3%
2 h	26.3%	36.8%
3 h	26.3%	36.8%
24 h	26.3%	36.8%

the reactor was observed. The product was a foam which reformed a slurry with slight mixing. Nuclear magnetic resonance testing revealed that over 2 equivalents of hydrogen had been released from the AB. LANL continued the flow reactor testing and quantifying the hydrogen production rate and impurities. LANL's data was used to validate the model.

Finally, a 50 wt% AB slurry has been developed. The fresh slurry had a viscosity of 966 cP, significantly higher than that of a 45 wt% slurry (270 cP). This indicates that the liquid carrier (silicon oil) was almost fully loaded and that higher solid loadings would be difficult.

Cost Analysis

In FY 2013 we completed the cost analysis for the more detailed schematics described previously. Vender quotes were used for the off-the-shelf components such as valves, fittings, insulations, and heat exchangers. For specialty components, cost quotes were done following procedures described in previous annual reports. In addition, we included estimates for manufacturing and system assembly as well as applied standard learning curves. System costs were calculated for yearly productions ranging from 10,000 to 500,000 units per year. We worked with our partners to identify lower cost parts and improved manufacturing compared to previous years. This resulted in cost reduction for the cryo-sorbent-based storage system from $3,000/unit to ~$2,500/unit. For the chemical hydrogen system, we previously had priced the solid- rather than a slurry-based system. Changes to a liquid-based system significantly reduced cost from ~$4,600/unit to ~$3,000/unit. Much of the cost reduction is in lower BOP cost due to the reduction in the number of valves. Comparing these costs to those reported by TIAX for 350-bar, 700-bar and cryo-compressed hydrogen all with carbon fiber tanks revealed that both the slurry AB and the sorbent were the same as or less expensive than the compressed gas storage and that the cryo-sorbent was competitive with cryo-compressed (Figure 5).

CONCLUSIONS AND FUTURE DIRECTIONS

PNNL's cryo-sorbent-based storage system efforts resulted in down-selection to a relatively low-cost storage system. We out-selected the Type IV pressure vessels. We also were able to identify BOP components that meet the Center's BOP targets for mass and volume. We developed manufacturing schemes for systems using Types I, III, and

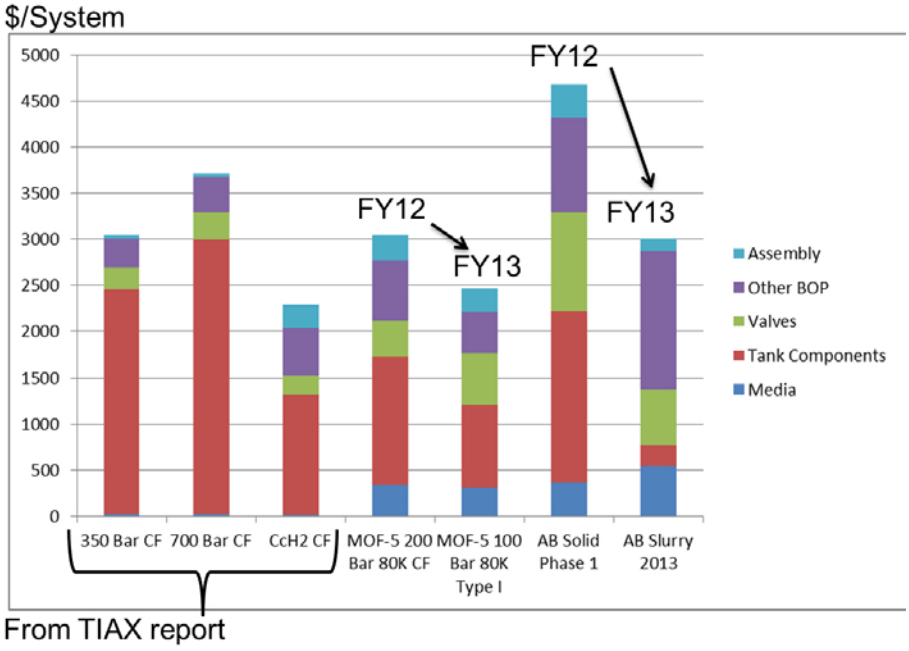

FIGURE 5. Projected Hydrogen Storage System Costs

IV pressure vessels. We completed our tankinator model and provided it to SRNL for inclusion in their models. We invented the thermos bottle concept to decrease the fill time and drastically reduced the excess hydrogen required for tank cooling. Finally, we showed a projected cost reduction for the sorbent based systems.

PNNL's chemical hydrogen efforts in FY 2013 were on validating the model and key components. We developed a pathway to achieve the DOE's gravimetric targets. Our analysis showed that if the gravimetric targets were achieved the volumetric targets would also be realized. We validated the heat exchangers and volume exchange tank. We developed the pleated membrane for the volume exchange tank and French press for mixing. We demonstrated that off-boarding/onboarding could be done at rates sufficient for a 5-minute fill. We showed that the settled slurry would not necessarily clog the system and that the slurry was flowable at temperatures as low as -20°C, meeting the DOE targets. Finally, we projected a 35% cost reduction by changing from the solid-based AB system to the liquid-based system.

FUTURE WORK

- Design sub-scale cryo-adsorbent system prototype (joint with partners)
- Complete chemical hydrogen model verification:
  - Compare model to additional reactor data provided by LANL
  - Refine model if necessary
  - Materials requirements
- Demonstrate advanced pressure vessel system for dormancy, etc. (with Hexagon Lincoln)
- Elevated design concepts
  - Sorbent: reduce part count by up to 30%
- Refine cost model
  - Update BOP
  - Improve manufacturing estimates

FY 2013 PUBLICATIONS/PRESENTATIONS

Publications

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2. Holladay JD, KP Brooks, E Ronnebro, and AJ Karkamkar. 2012. "Chemical Hydrogen for On-Board Vehicle Hydrogen Storage." Presented by Jamie Holladay at Fuel Cell Seminar and Energy Exposition, Uncasville, CT on November 9, 2012. PNNL-SA-91871.

3. Ronnebro E, MP Westman, J Chun, AJ Karkamkar, and KP Brooks. 2013. "HSECoE TTR Materials Operating Requirements - Chemical Hydrogen Storage." Presented by Ewa Ronnebro (Invited Speaker) at US Drive - Hydrogen Storage Tech Team Meeting, Detroit, MI on March 21, 2013. PNNL-SA-94267.

4. Simmons KL, KP Brooks, E Ronnebro, and JD Holladay. 2013. "System Modeling and Balance of Plant for the Chemical Hydrogen Storage Systems." Presented by Kriston Brooks (Invited Speaker) at Hydrogen Storage Technical Team Meeting, Southfield, MI on March 21, 2013. PNNL-SA-94281.

5. Simmons KL, MR Weimar, KP Brooks, BA Van Hassel, and M Veenstra. 2013. "HSECoE 2013 Tech Team Meeting Chemical Hydrogen BOP/Cost." Presented by Kevin L Simmons, Mark Weimar at Hydrogen Storage Engineering Center of Excellence Tech Team Review, Southfield, MI on March 21, 2013. PNNL-SA-94408.

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