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8 June 2017

Project ID# ST100

Overview

Timeline

- Project Start Date: 9/30/16
- Project End Date: 9/29/21
- % complete: 10% of five-year project (in Year 1 of 5)

Budget

- Total Funding Spent
 - \$145k (though March 2017, including subs)
- Total DOE Project Value
 - \$1.5M (over 5 years, including Lab funding)
- Cost Share Percentage: 0% (not required for analysis projects)

Barriers

- A: System Weight and Volume
- B: System Cost
- K: System Life-Cycle Assessment

Partners

- Pacific Northwest National Laboratory (PNNL)
- Argonne National Laboratory (ANL)



Relevance & Impact

Objective

 Conduct rigorous, independent, and transparent, bottoms-up techno-economic analysis of H₂ storage systems

Relevance and Impact

- DFMA[®] analysis can be used to predict costs based on both mature and nascent components and manufacturing processes depending on what manufacturing processes and materials are hypothesized
- Identify the cost impact of material and manufacturing advances and to identify areas of R&D interest
- Provide insight into which components are critical to reducing the costs of onboard H₂ storage and to meeting DOE cost targets

DFMA[®] Methodology

- Process-based, bottoms-up cost analysis methodology which projects material and manufacturing cost of the complete system by modeling specific manufacturing steps
- Predicts the actual cost of components or systems based on a hypothesized design and set of manufacturing & assembly steps
- Determines the lowest cost design and manufacturing processes through repeated application of the DFMA[®] methodology on multiple design/manufacturing potential pathways

Approach/Activities In Past year

- 500 bar Cryo-Compressed H₂ (CcH₂) for bus applications

- Super-Critical H₂ (90 123 K at 500 bar)
- Based on performance analysis by ANL and system design from Lawrence Livermore National Laboratory (LLNL)
- Completed preliminary cost analysis of CcH₂ for bus applications (40 kg usable H₂)

Cold-compressed H₂ for light-duty vehicles

- Cold gaseous hydrogen storage (150 250 K; 400-600 bar)
- Based on PNNL system design
- Investigated potential carbon fiber composite and insulation cost trade-offs for lightduty applications (5.6 kg usable H₂)

MOF-74 Material Cost Analysis

- Adsorbed H₂
- Based on materials development at Lawrence Berkeley National Laboratory (LBNL)
- Analyzed cost of MOF-74 made from two linker isomers: m-dobdc and p-dobdc

- Type 4 Compressed Natural Gas (CNG) Analysis

- 3,600 psi natural gas storage in Type 4 pressure vessels for light-duty and heavy-duty on-board storage
- Provided baseline cost analysis in support of the Institute for Advanced Composites Manufacturing Innovation (IACMI) and the Advanced Manufacturing Office (AMO)

500 bar Cryo-Compressed H₂ storage system cost

Worked with partners ANL and PNNL to leverage past work and define system in sufficient detail to inform cost analysis



500 bar Cryo-Compressed H₂ storage system cost

Emphasis placed on transparent and rational cost/design assumptions & internal consistency

Design Parameter	Base Case Value	Basis/Comment
Rated Storage Pressure	500 bar	ANL modeling assumption
Burst Pressure	1,125 bar	2.25 safety factor per SAE J2579
Minimum (Empty) Pressure	5 bar	Minimum delivery pressure to fuel cell system
Storage Temperature Range	93-123 K	Determined by LH ₂ refueling schedule, insulation parameters, LH ₂ pump efficiency
Tank Volume (Water Capacity)	169.1 L	ANL modeling assumption
Usable H ₂	10 kg	ANL modeling assumption
Aspect Ratio (L/D)	5	ANL modeling assumption. Based on I.D.
Pressure Vessel Dimension	176 cm x 35.2 cm	Calculated from volume, aspect ratio and assumed spheroid dome shape of r_minor/r_major = 0.2
Liner Thickness	2 mm	ANL modeling assumption
Carbon Fiber Type	T700S	ANL modeling assumption
Resin	Ероху	ANL modeling assumption
Total Allowable Heat Leak	10 W	ANL assumption
Insulation Thickness	7 mm	$K_{eff} = 5E-5 W/m-K; \Delta Q_{insulation} \le 3W$
Vacuum Pressure (design)	10 ⁻³ Torr	LLNL feedback (ANL assumes 10 ⁻⁵ Torr)
Liner Material	316L	ANL modeling assumption
Minimum Fatigue Life	15,000 cycles	SAE code for bus applications
Vacuum Gap	8.4 mm	1.2 x insulation thickness to facilitate assembly and avoid crushing insulation

CcH₂ Manufacturing Process Flow



Capital equipment reported in 2007\$

Preliminary CcH₂ Cost Breakdowns

Need to investigate BOS component reductions, through system simplification, multi-functionality, or improved design to reduce cost



- Balance of system (BOS) dominates cost
 - Valves (four per system) account for nearly half the BOS cost
 - Current component cost estimates are a mix of low volume quotes and 700 bar ambient temperature storage components
- As prod. volume increases, composite cost is a larger fraction of total system cost due to improved equipment utilization
- Cost of applying insulation modeled using orbital wrapping leads to relatively low cost compared to hand lay-up
- Insulation vacuum process (degassing) may be a major cost item
 Up to 1 week in lab to achieve stable pressure adds ~\$3/kWh



500 bar Cryo-Compressed H₂ storage system cost

Insulation materials and wrapping are not major cost items



Method for Applying Multi-Layer Insulation (MLI)

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- Applying MLI by hand is labor intensive and leads to non-uniformity in insulation
- Feedback from industry is that MLI orbital wrapping techniques are considered proprietary and closely guarded
- Patent suggests range of possible wrapping times from 7-70 min depending on vessel size
- ~ 0.6 RPM (polar)
- ~ 6 RPM (orbital)
- Current modeling assumptions:
 - polar wrapping only
 - 7 cm (2.75 in) roll width
 - 10 m/min wrapping speed (~2.5 RPM)
 - 44 m² total MLI area
 - 60 min wrapping time



STRATEGIC ANALYSIS

Orbital

US3708131A (1966) https://patents.google.com/patent/US3708131A/en.

Accomplishments & Progress: 500 bar Cryo-Compressed H₂ storage system cost

Comparison of CcH₂ with baseline 700 bar compressed

	Cryo-Compressed H ₂	700 Bar Type 4 H ₂ *
Application	Bus	LDV (light duty vehicle)
Available H ₂ per Tank	10 kg	5.6 kg
Internal Volume per Tank	169.1 L	147 L
Composite Mass per Tank	64.2 kg	107 kg

- As a fraction of stored hydrogen, cryo-compressed leads to significant reductions in composite (~2/3 the composite mass to store 2x H₂).
- Balance of system components are more complex for cryo-compressed H₂ and more expensive (as currently modeled), and therefore make up a larger fraction of total system cost at all volumes analyzed.
- Balance of system is amortized over a larger mass of stored hydrogen for cryocompressed H₂.

* Comparison is made to 60% volume fraction carbon fiber composite with epoxy resin to be consistent with assumptions for cryocompressed system. Lighter 700 bar tanks are possible using vinyl ester resin as demonstrated by PNNL.

500 bar Cold-Compressed H₂ storage system cost analysis

Leveraged cryo-cH₂ and ambient temperature 700 bar Type 4 models to explore design space and potential cost savings for 5.6 kg cold compressed Type 4 for LDV



- Composite cost savings are possible for lower temperature and pressure assuming a constant performance factor for a constant or lower volume
- Assuming Type 4 tank with containment and insulation same design as cryo-CH₂
 - Composite reduction would save ~-\$3/kWh
 - MLI would add ~+\$0.30/kWh
 - Containment vessel would add ~+\$0.20/kWh
 - Estimated savings ~\$2.5/kWh

Anticipated Refueling station considerations in order of least to most expensive:

- Gaseous 700 bar, 298 K
- Gaseous 500 bar, 200 K
- Liquid 500 bar, 100 K

Accomplishments & Progress: Tool Development

Tools and methods are being developed to better understand and explore cost trade-offs in design space



Cost savings are with respect to Type 4 (5.6 kg usable H_2) at 700 bar, 300 K

Liner

Туре 3

- 2 mm 316 L stainless steel
- Impact extrusion formed
- Type 4
 - 0.5 mm HDPE
 - Blow mold
- Boss/Throat
 - Туре 3
 - Hot spin-formed from extruded liner
 - Туре 4
 - Cast and machined Aluminum
- Composite
 - T700-S carbon fiber
 - Epoxy resin
- Next steps
 - Add BOS and insulation to analysis
 - Extend to other storage systems (e.g. sorbents and metal hydrides)
 - Trade-off between Type 1 and Type 3

<u>Preliminary</u> results showing potential cost savings as a function of temperature and pressure for cold-gas Type 3 and Type 4 tanks

Metal Organic Frameworks

Recently published SA analysis showed that alternative MOF synthesis routes have potential to reduce cost*



LAG: Liquid-assisted grinding

*DeSantis et al "Techno-Economic Analysis of Metal-Organic Frameworks for Hydro-Gen and Natural Gas Storage." *Energy & Fuels* (2017)

**Kapelewski, et al. " M_2 (m-dobdc) (M = Mg, Mn, Fe, Co, Ni) Metal–Organic Frameworks Exhibiting Increased Charge Density and Enhanced H_2 Binding at the Open Metal Sites." JACS (2014).

- Previous analysis of Hexcell and MATI cryo-sorbent storage systems suggest
- -50 kg MOF required for LDV system
- -<u>\$10/kg MOF</u> is a reasonable cost target
- LBNL investigated MOF-74**
 - Shows similar/improved H₂ binding properties of Mg₂(m-dobdc) vs. traditional Mg₂(p-dobdc)
 - m-dobdc made from <u>low-cost</u> starting material: resorcinol
- Linker costs were not well understood
 - Not produced at high volume, thus quotes costs are difficult to obtain
 - <u>Linker costs were modeled</u> to understand cost impacts of alternative isomers being investigated for MOF

Focused on alternate (potentially low-cost) linker: meta-dobdc

m-dobdc is lower cost than p-dobdc due to lower cost starting materials



- Analyzed linker costs using methods described in 1, 2
- Linker costs dominated by materials cost
- m-dobdc is ~50% of p-dobdc

¹·Guang et al. "Improved One-Pot Synthesis of 4_6-Dihydroxylsophthalic Acid and 2,3-Dihydroxyterephthalic Acid." Chinese Chemical Letters 16, no. 8 (2005): 1039–42. ² Sikkema et al. "Process for dicarboxylating dihydric phenols." US6040478, issued March 2000.

0%

Metal Organic Frameworks

m-dobdc prepared by liquid assisted grinding (LAG) may achieve <\$10/kgMOF goal



- Solvent (primarily DMF) is the main cost driver of MOF from solvo-thermal synthesis
- Liquid assisted grinding (LAG) and aqueous synthesis both show promise for reducing the cost of MOF synthesis
- m-dodbc (made from lower cost starting materials) is projected to cost \$9.87/kgMOF at 500k systems/year
- p-dobdc is projected to cost \$14.57/kgMOF when produced using LAG

Accomplishments & Progress: 3,600 psi Type 4 CNG system Analysis

Established baseline costs for CNG systems by leveraging past 700 bar Type 4 H₂ system models



- Leveraged existing 700 bar H₂ storage system design to analyze cost for two CNG storage systems for LDV (64.4 L) and HDV (537.5 L)
- Integrated valve, fittings and tubing are modeled and validated against commercially available CNG components
- Pressure regulator prices are based on quotes from a CNG supplier

Accomplishments & Progress: 3,600 psi Type 4 CNG system Analysis

Modeled system masses are in good agreement with commercial comparison system masses

		LDV	HDV
Modeled Masses			
Boss	kg	1.75	1.75
Liner	kg	5.07	23.65
Composite	kg	16.30	135.95
Shoulder Foam	kg	0.17	0.57
Total	kg	23.29	161.92
Reported Mass (TUFFSHELL)	kg	27.21	176.42
Boss, Liner, Composite w/o Fiberglass, and Foam only TUFFSHELL Mass	kg	23.76	154.14
Relative Difference	%	-2%	+5%

- Fiberglass is not included in the model, but is used in Hexagon Lincoln vessels
- Assumed 12.5% of total composite mass is fiberglass
 - Adjusted composite masses in good agreement for LDV, but model overestimates composite for HDV
- Model assumes 0.5 cm thick liner
 - Hexagon Lincoln liner is thinner for LDV and thicker for HDV

Accomplishments & Progress: 3,600 psi Type 4 CNG system Analysis

CNG cost results show expected trends when compared to H₂ systems



- Composite cost for H₂ pressure vessel is based on vinyl ester resin and lower cost PAN-MA carbon fiber as described in the 2015 FCTO Program Record*
- Composite cost for the CNG systems is based on epoxy resin and Toray T700S
- Cost comparisons show expected trends:
 - Cost decrease with increased production volume
 - Large CNG systems (537L) less expensive than small CNG systems (64L) on a per kWh and per Liter basis primarily due to improved amortization of (mostly) fixed valve costs.
 - High pressure vessels (10kpsi) are more expensive than lower pressure vessels (3.6kpsi).
 - Cost differences are exaggerated

*https://www.hydrogen.energy.gov/pdfs/15013_onboard_storage_performance_cost.pdf

Accomplishments and Progress: Responses to Previous Year's Reviewers' Comments

Reviewer's Comments	Response to Reviewer's Comment
Nearly all effort during the past year has been on the Type 4 700 bar compressed gas system, which is the only current contender for hydrogen FCEVs.	This year, we have completed preliminary analysis of cryo-compressed systems for buses, analysis of alternative MOFs, and have plans to analyze other materials-based storage approaches.
It would be beneficial to the community to analyze newly emerging materials and storage approaches, such as alane, especially when attempting to drive the cost of this material to below \$10/kg.	We plan to investigate both chemical and metal hydrides later in the year.
Analyses conducted on 700 bar Type 4 systems may not be entirely applicable to other up-and coming storage concepts (e.g., cryo-compressed employing composite overwrapped pressure vessels). In these cases, other factors will need to be addressed.	We are currently investigating differences in manufacturing approaches for cryogenic storage and plan to validate our approach against existing industries, e.g. LNG.

Collaborations

Partner	Project Role
Pacific Northwest National Laboratory (PNNL) (sub on project)	Contributed information on developments within cryo-compressed H ₂ , and manufacturing variations
Argonne National Laboratory (ANL) (sub on project)	Conduct system analysis to determine the carbon fiber requirement for compressed gas Type 4 tanks; support SA in cost analysis activities.
Lawrence Livermore National Laboratory (LNNL)	Review and feedback on cryo-compressed analysis
Lawrence Berkeley National Laboratory (LBNL)	Review and feedback on MOF-74 analysis
Institute for Advanced Composite Manufacturing Innovation (IACMI)	CNG baseline analysis
Hexagon Lincoln	Provided feedback on CNG baseline analysis

Remaining Barriers and Challenges

Cryo-Compressed H₂ System

- Balance of System
 - Uncertainty in component costs at relevant volumes leads to uncertainty in system cost
- Vacuum space evacuation
 - Constricted flow due to many layers of insulation and out-gassing from epoxy lead to very long times to achieve stable vacuum pressure in the lab (up to 1 week)
 - Currently assumed short vacuum times lead to low costs, but there is uncertainty in this assumption

Cold-Compressed H₂ System

• Preliminary analysis suggests cost savings, but a validation system is needed to fully understand system cost trade-offs

Metal Organic Frameworks

• Need reliable hydrogen uptake data to estimate required MOF mass for system analysis

Storage System/Refueling Station Cost Trade-offs

• A holistic approach should be taken to best understand trade-offs between the storage system and refueling station costs

Proposed Future Work

Refine CcH₂ analysis

- Discuss industry best practices with LNG system manufacturer to understand manufacturing issues around insulation
- Collaborate with cryogenic component suppliers to better understand balance of system costs and to identify potential cost savings
- Extend analysis to Light-Duty Vehicles
- Analyze 2010 system assumptions to compare against current

Cold-Compressed H₂

- Leverage CcH₂ learnings to model full system cost
- Reverse engineering
 - Use cost models to identify system component and materials cost reduction requirements to meet DOE targets

Any proposed future work is subject to change based on funding levels.

Technology Transfer Activities

Not Applicable to SA's Cost Analysis

Summary

Completed preliminary CcH₂ storage system cost

- Balance of system is nearly half the total cost
 - Plan to work with LNG and cryogenic suppliers to refine BOS costs and to identify potential savings
- Automated insulation wrapping is predicted to lead to insulation costs of ~\$1.20/kWh at high volume
- Vacuum-degassing time uncertainty could lead to significant costs
 - Plan to work with LNG or other cryogenic manufacturers to better understand vacuum processing times
 - Alternative, low vapor pressure resins may be a better solution for Type 3 storage vessels

Identified preliminary savings for light-duty storage using cold compressed H₂

Preliminary analysis suggests ~\$2.50/kWh system savings are possible at 500 bar and 200 K

Completed analysis of MOF-74 suggesting <\$10/kg is achievable using LAG</p>

- System level cost with new MOF costs will be estimated in future work

• Completed 3,600 psi Type 4 CNG analysis for IACMI

 Additional analyses may be done on liner-less tanks (Type 5) and based on projects resulting in lower cost composites and manufacturing processes

Technical Backup Slides

Approach:

SA's DFMA[®] - Style Costing Methodology

- DFMA[®] (Design for Manufacture & Assembly) is a registered trademark of Boothroyd-Dewhurst, Inc.
 - Used by hundreds of companies world-wide
 - Basis of Ford Motor Co. design/costing method for the past 20+ years
- SA practices are a blend of:
 - "Textbook" DFMA[®], industry standards and practices, DFMA[®] software, innovation, and practicality

Estimated Cost = (Material Cost + Processing Cost + Assembly Cost) x Markup Factor



STRATEGIC ANALYSIS

10,000 to 500,000 H₂ storage systems per year

Machine Rate, \$/min

Solvo-Thermal Synthesis



- Process is based on scaled-up lab scale synthesis assuming 90% solvent and reagent recycle
- Manufacturing scale chosen to provide enough MOF for 500k FCEVs per year
- Cost is dominated by precipitation reactor size and solvent material cost (DMF)

DeSantis et al "Techno-Economic Analysis of Metal-Organic Frameworks for Hydro-Gen and Natural Gas Storage." Energy & Fuels (2017)

Comparison of Linker Production

p-dobdc Process Flow



Comparison of Linker Production

m-dobdc Process Flow



3,600 psi, Type 4 CNG Storage Systems @500k tanks/year



• Processing steps are identical to those of H₂ vessels

Painting

Comparison of CNG Tank Dimensions

	units	TUFFSHELL	CNG Model	TUFFSHELL	CNG Model	Hydrogen
		LDV	LDV	HDV	HDV	(2013)
Fill Pressure	MPa	24.8	24.8	24.8	24.8	70.0
Water Volume	L	64.4	64.4	537.5	537.5	146.6
Performance Factor	In		1.04E+06		1.04E+06	1.04E+06
Carbon Fiber Volume Fraction	%		60.0		60.0	60.0
Composite Mass	kg		16.3		135.9	102.0
External Diameter	cm	33	31.8	53.3	52.8	
External Length	cm	109.2	100.4	304.8	286.9	
Boss Stem Length	cm		2.5		2.5	
Internal Diameter	cm		29.6		49.6	39.1
Internal Length	cm		106.7		302.3	129.3
Total Mass of Fuel (@ Fill Pressure)	kg		10.3		86.1	5.76
Mass of Usable Fuel (@ Empty Pressure)	kġ		9.5		79.0	5.6

- Composite mass is a function of the performance factor, which depends on volume & pressure
 - Modeled CNG tank lengths and diameters were selected to provide reasonable matches to Hexagon TUFFSHELL CNG pressure vessels
 - The critical physical dimension is internal tank volume
 - Dome shape and boss stem length were estimated to give tank reasonable external dimensions
 - Calculated external dimensions assume equal composite thickness in both dome and cylinder
- Regulator assumed to require a minimum of 2 MPa inlet pressure per discussions with supplier
 - This affects the kg of gas within vessel upon the "empty" condition, and thus affects the mass of usable fuel stored

Key Differences in System Design and Manufacturing Between H₂ and CNG Models

	H ₂	CNG
Physical Dimensions and Pressure	700 bar, 147 L	250 bar, 64 L & 538 L
Composite	PAN-MA based CF/vinyl ester	T700S/epoxy
Valve	Integrated in-tank valve pricing based on DFMA [®] modeling	Integrated external valve pricing based on supplier quotes
Regulator	Integrated regulator pricing based on DFMA [®] modeling	Regulator, low pressure transducer, and manual defuel valve pricing based on supplier quotes
He Fill and Leak Test	Modeled after a fast fill fueling station with cascade compression	Modified for lower CNG pressures at 10k-500k tanks/year Simplified system design with single stage pump at 1k tanks/year

Hydrogen Storage System Placement on Fuel Cell Electric Bus (FCEB)



Images courtesy of ANL