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2017 DOE Hydrogen and Fuel Cells Program Review

Hydrogen Storage Cost Analysis

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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)

Barriers

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

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)

Partners

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

Relevance & Impact

- **Objective**
  - Conduct rigorous, independent, and transparent, bottoms-up techno-economic analysis of H_2 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 H_2 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 H_2 (CcH_2) for bus applications**
  - Super-Critical H_2 (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 CcH_2 for bus applications (40 kg usable H_2)
- **Cold-compressed H_2 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 light-duty applications (5.6 kg usable H_2)
- **MOF-74 Material Cost Analysis**
  - Adsorbed H_2
  - 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)

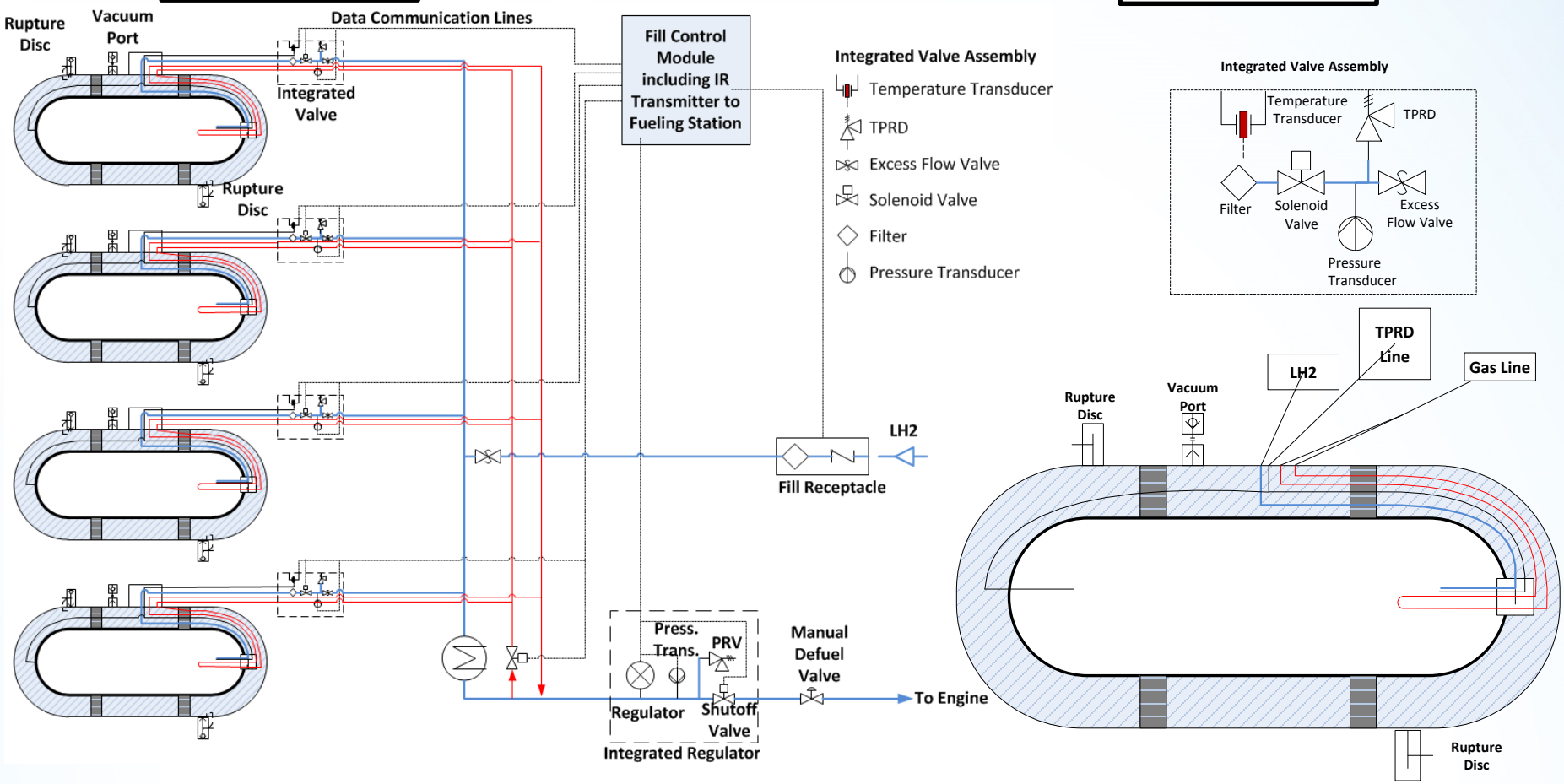
Accomplishments & Progress:

500 bar Cryo-Compressed H_2 storage system cost

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

Full system

Single Tank



Accomplishments & Progress:

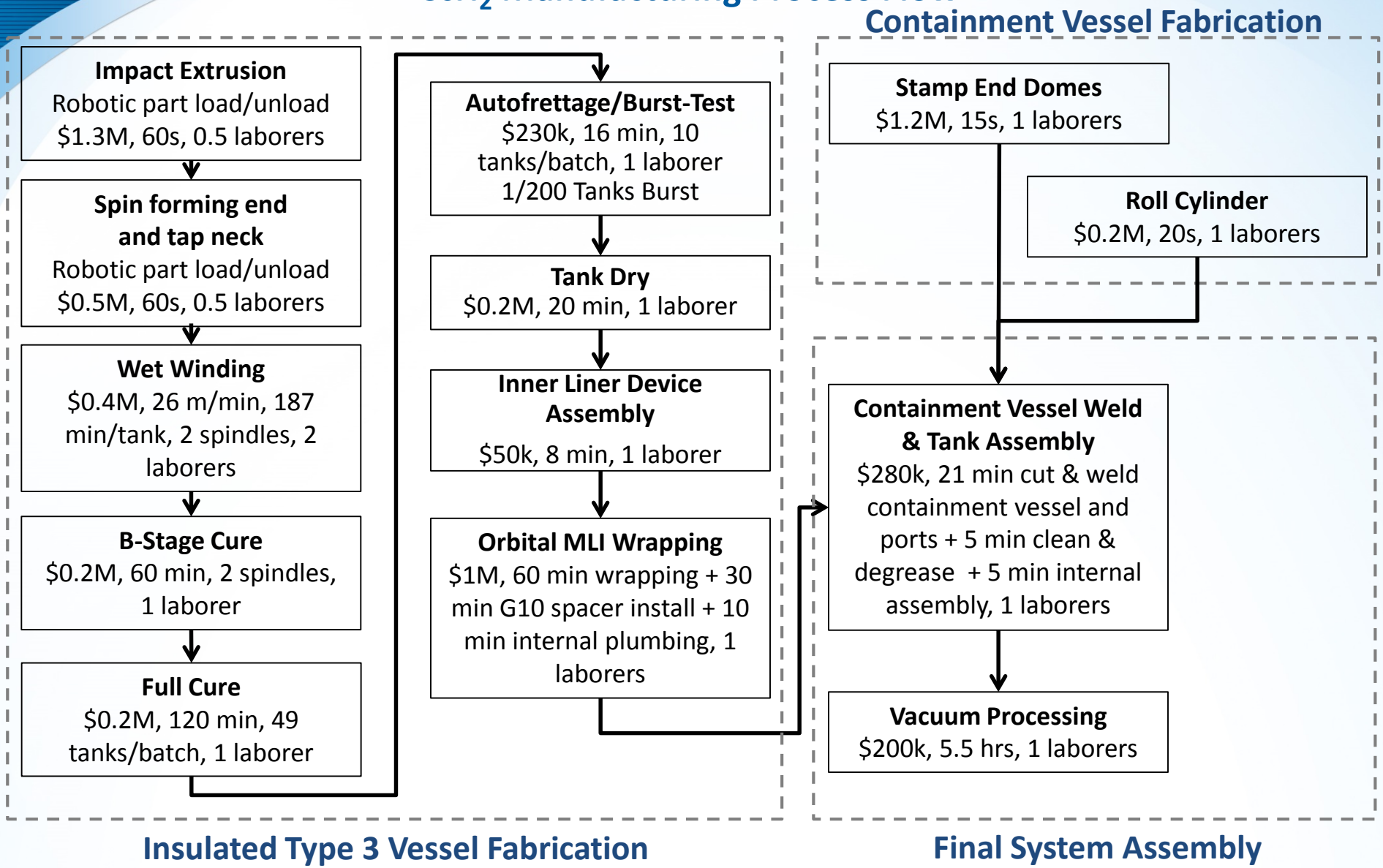
500 bar Cryo-Compressed H_2 storage system cost

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	Epoxy	ANL modeling assumption
Total Allowable Heat Leak	10 W	ANL assumption
Insulation Thickness	7 mm	K_{eff} = 5E-5 W/m-K; $\Delta Q_{insulation} \leq 3W$
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

Accomplishments & Progress

CcH_2 Manufacturing Process Flow

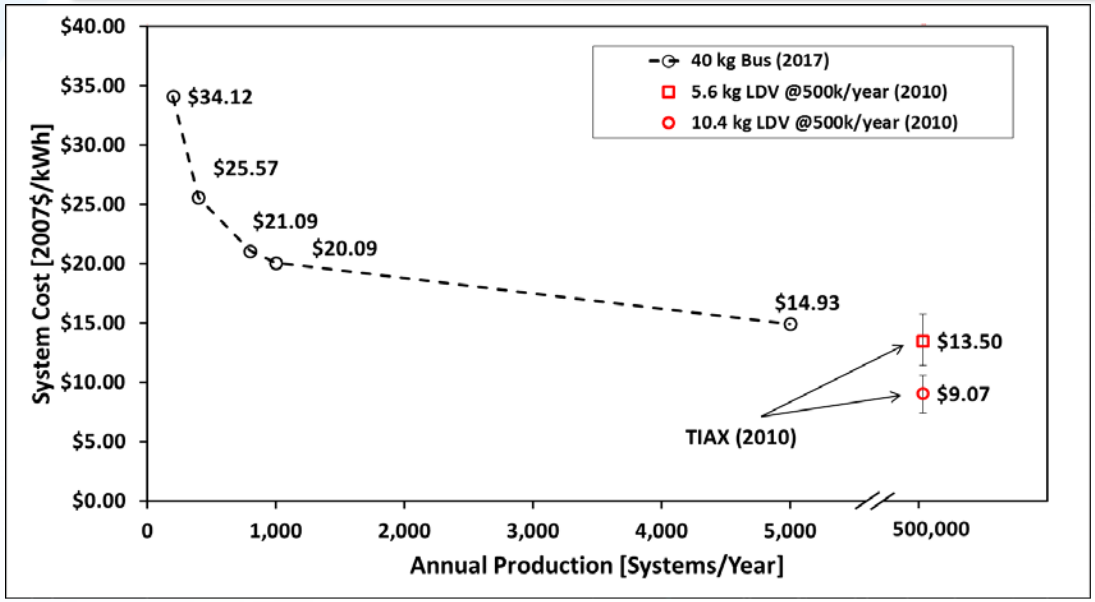


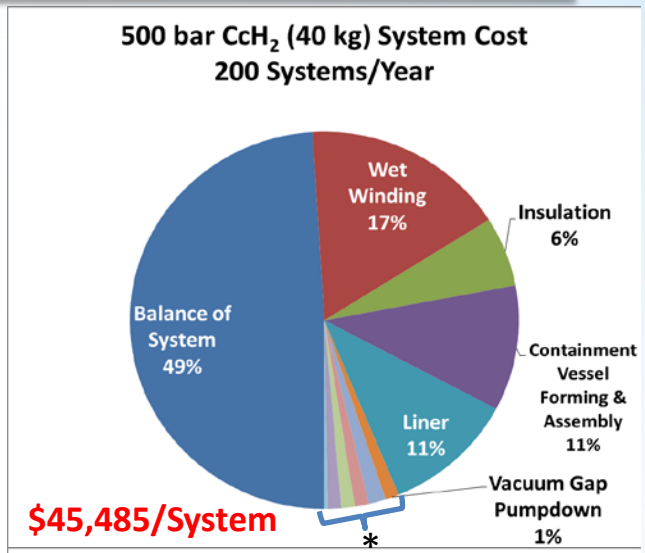
Capital equipment reported in 2007$

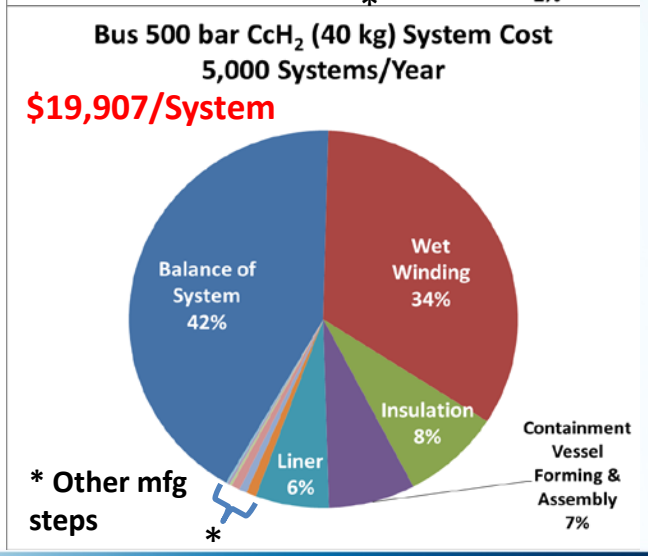
Accomplishments & Progress

Preliminary CcH_2 Cost Breakdowns

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







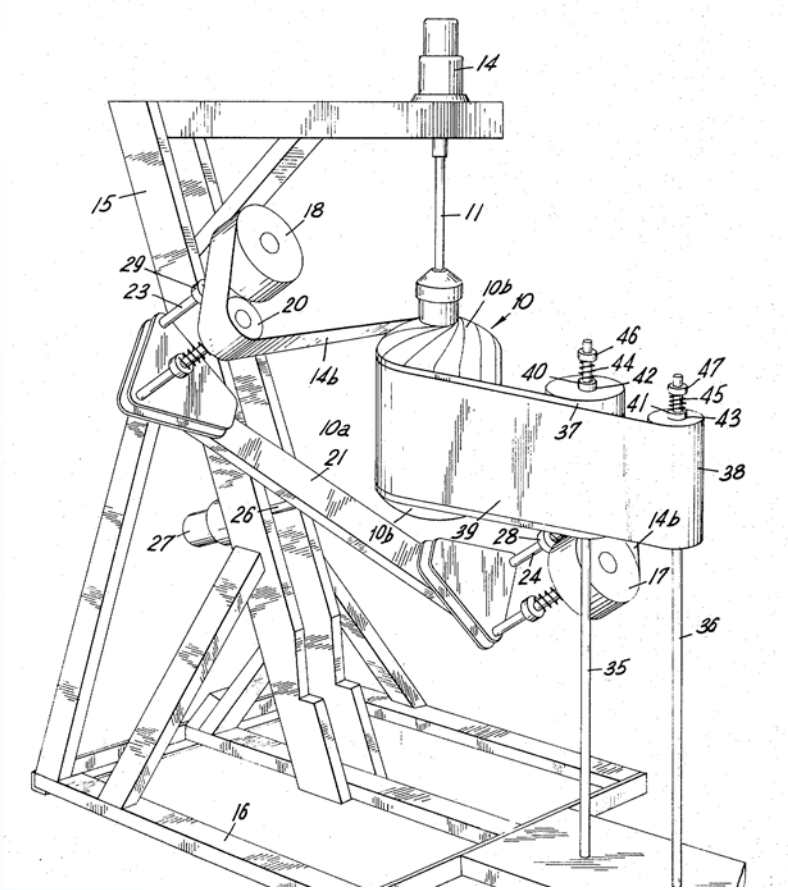
- Balance of system (BOS) dominates cost
  - Valves (four per system) account for nearly half the BOS cost
  - Current component cost estimates are a mix of low volume quotes and 700 bar ambient temperature storage components
- As prod. volume increases, composite cost is a larger fraction of total system 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

Accomplishments & Progress:

500 bar Cryo-Compressed H_2 storage system cost

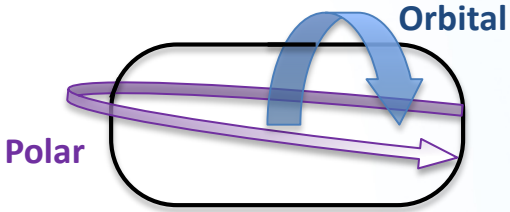
Insulation materials and wrapping are not major cost items

Method for Applying Multi-Layer Insulation (MLI)



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

- 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 m^2 total MLI area
  - 60 min wrapping time



Accomplishments & Progress:

500 bar Cryo-Compressed H_2 storage system cost

Comparison of CcH_2 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

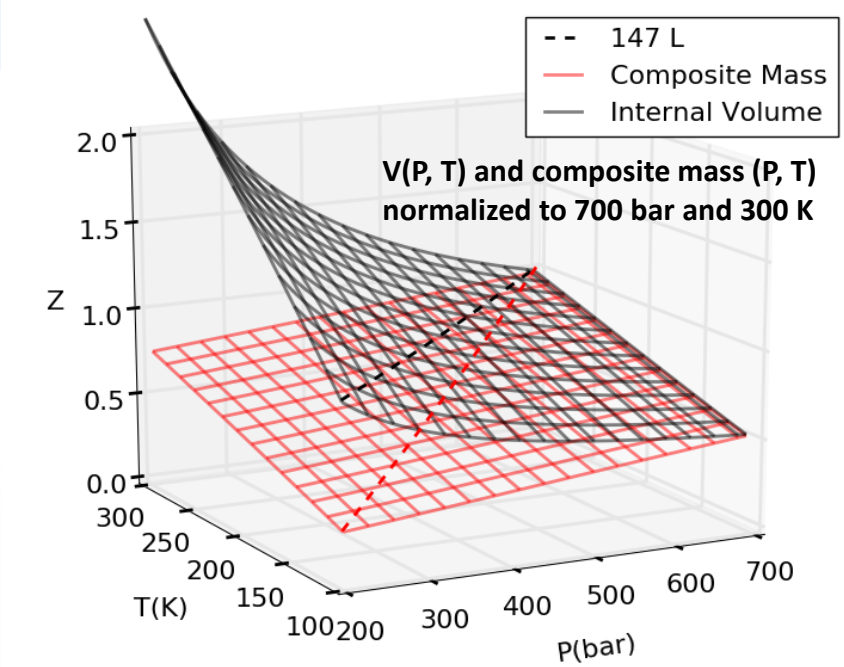
- As a fraction of stored hydrogen, cryo-compressed leads to significant reductions in composite (~2/3 the composite mass to store 2x H_2).
- Balance of system components are more complex for cryo-compressed H_2 and more expensive (as currently modeled), and therefore make up a larger fraction of total system cost at all volumes analyzed.
- Balance of system is amortized over a larger mass of stored hydrogen for cryo-compressed H_2.

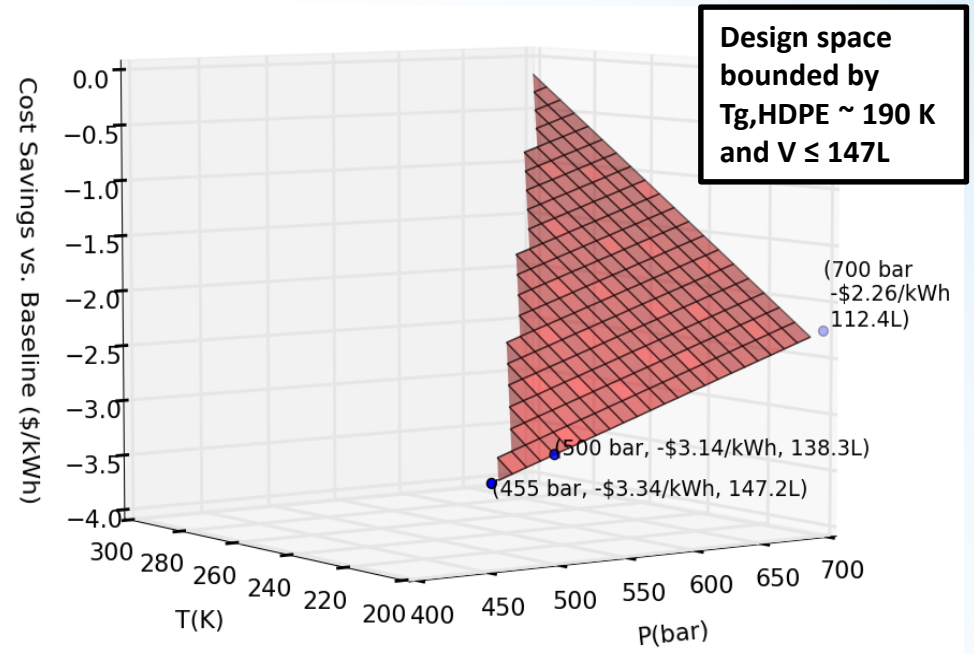
* Comparison is made to 60% volume fraction carbon fiber composite with epoxy resin to be consistent with assumptions for cryo-compressed system. Lighter 700 bar tanks are possible using vinyl ester resin as demonstrated by PNNL.

Accomplishments & Progress:

500 bar Cold-Compressed H_2 storage system cost analysis

Leveraged cryo-cH_2 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





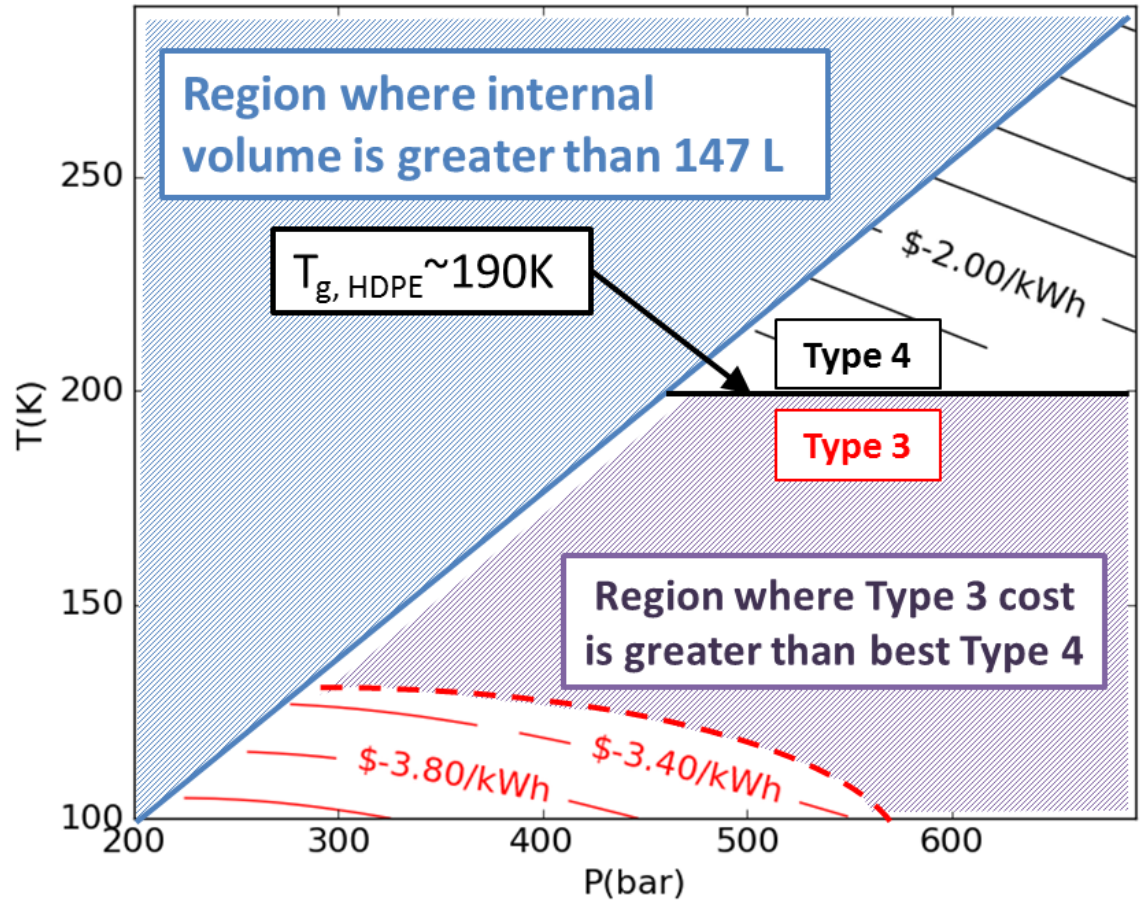
- Composite cost savings are possible for lower temperature and pressure assuming a constant performance factor for a constant or lower volume
- Assuming Type 4 tank with containment and insulation same design as cryo-CH_2
  - Composite reduction would save **~-$3/kWh**
  - MLI would add **~+$0.30/kWh**
  - Containment vessel would add **~+$0.20/kWh**
  - **<u>Estimated savings ~$2.5/kWh</u>**

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

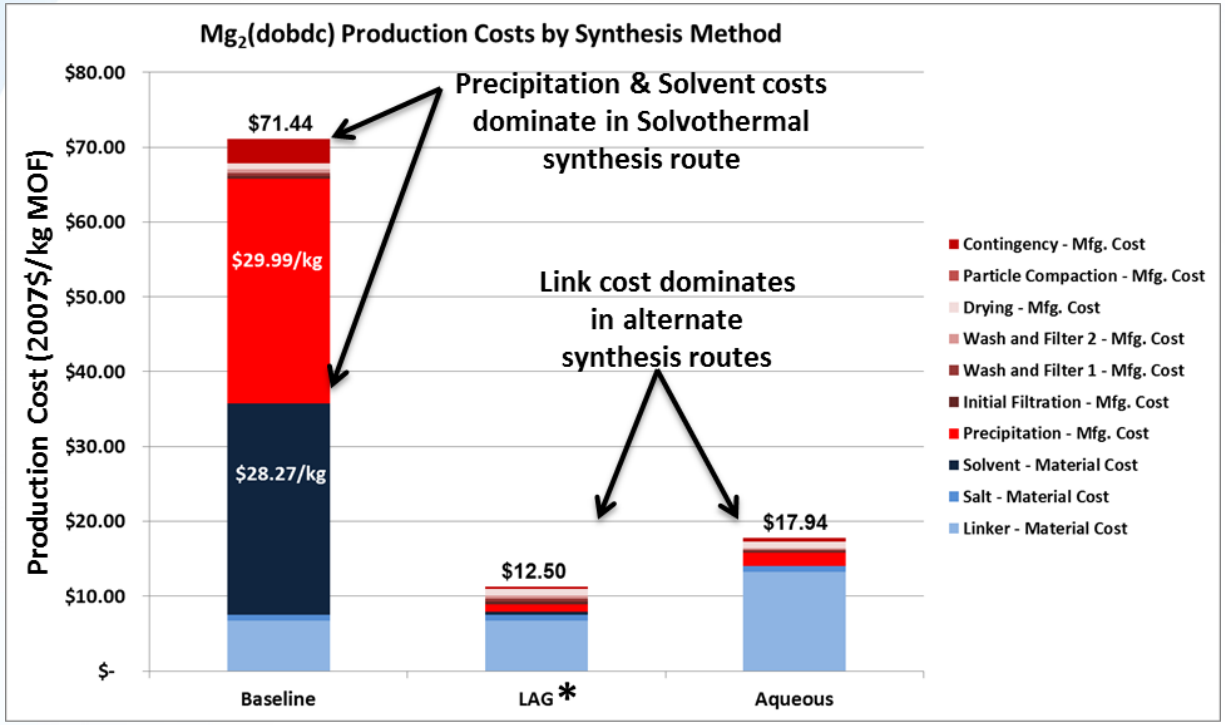


- Cost savings are with respect to Type 4 (5.6 kg usable H_2) at 700 bar, 300 K
- Liner
  - Type 3
    - 2 mm 316 L stainless steel
    - Impact extrusion formed
  - Type 4
    - 0.5 mm HDPE
    - Blow mold
- Boss/Throat
  - Type 3
    - Hot spin-formed from extruded liner
  - Type 4
    - Cast and machined 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

Accomplishments & Progress:
Metal Organic Frameworks

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



- Previous analysis of Hexcell and MATI cryo-sorbent storage systems suggest
  - 50 kg MOF required for LDV system
  - $10/kg MOF is a reasonable cost target
- LBNL investigated MOF-74**
  - Shows similar/improved H_2 binding properties of Mg_2(m-dobdc) vs. traditional Mg_2(p-dobdc)
  - m-dobdc made from low-cost starting material: resorcinol
- Linker costs were not well understood
  - Not produced at high volume, thus quotes costs are difficult to obtain
  - Linker costs were modeled to understand cost impacts of alternative isomers being investigated for MOF

LAG: Liquid-assisted grinding

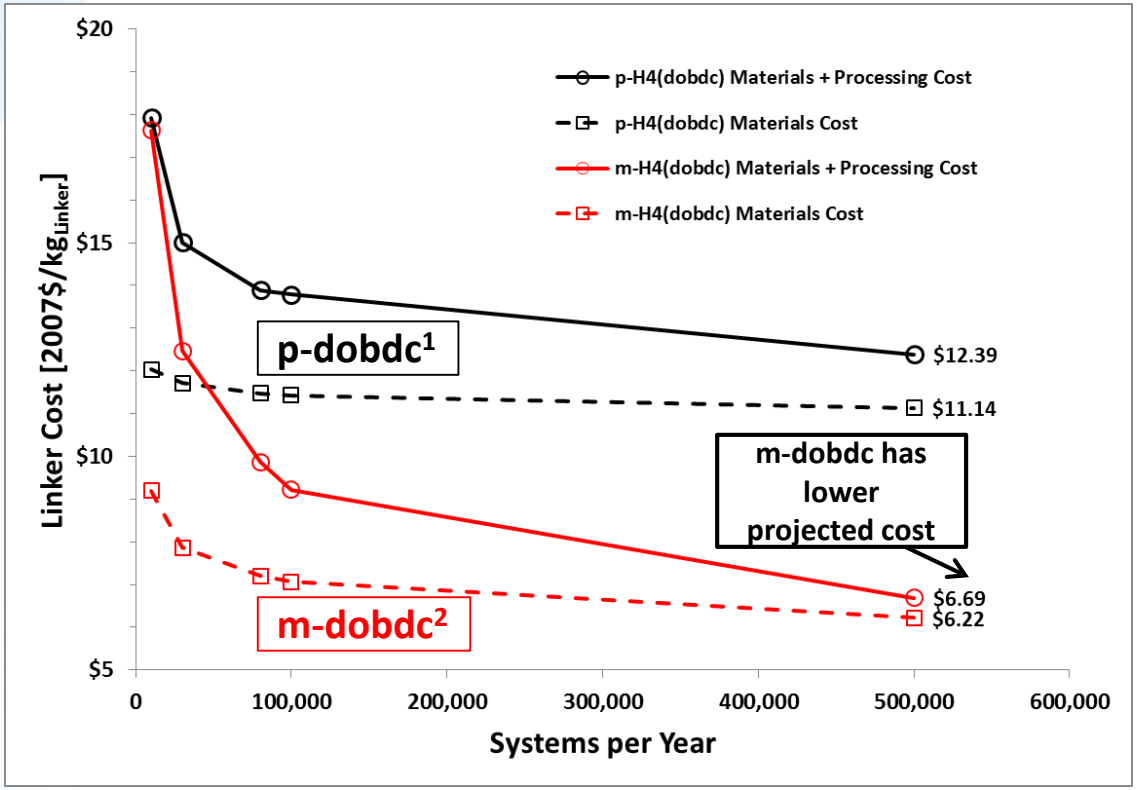
*DeSantis et al "Techno-Economic Analysis of Metal-Organic Frameworks for Hydro-Gen and Natural Gas Storage." *Energy & Fuels* (2017)

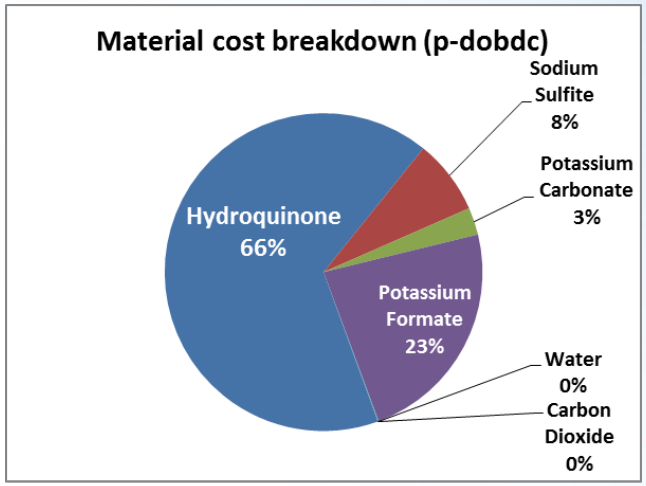
**Kapelewski, et al. "M_2(m-dobdc) (M = Mg, Mn, Fe, Co, Ni) Metal–Organic Frameworks Exhibiting Increased Charge Density and Enhanced H_2 Binding at the Open Metal Sites." JACS (2014).

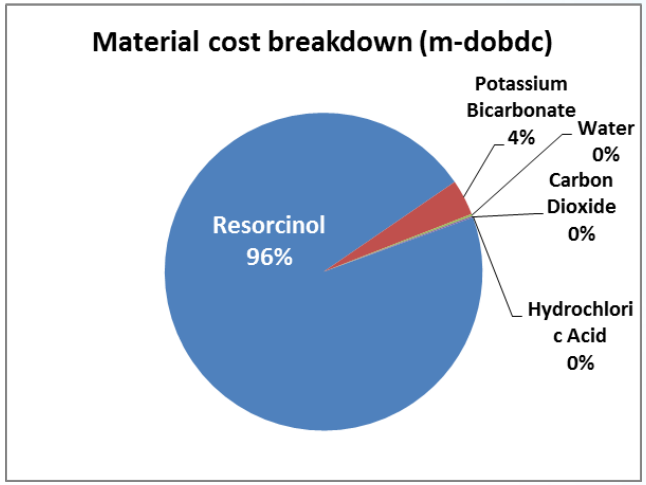
Accomplishments & Progress:

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

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







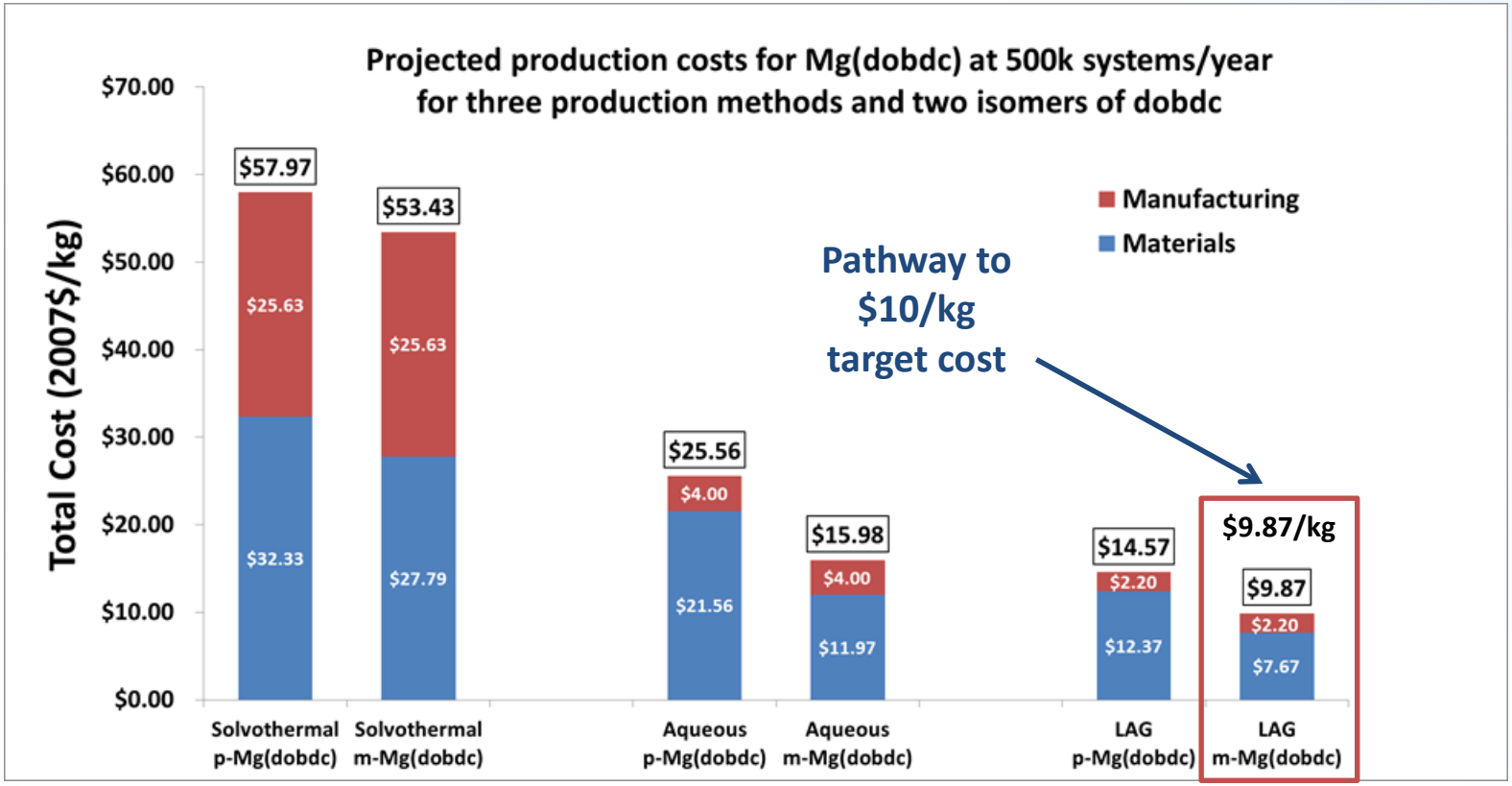
- **Analyzed linker costs using methods described in 1, 2**
- **Linker costs dominated by materials cost**
- **m-dobdc is ~50% of p-dobdc**

[1] Guang et al. "Improved One-Pot Synthesis of 4_6-Dihydroxyisophthalic 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.

Accomplishments & Progress:

Metal Organic Frameworks

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

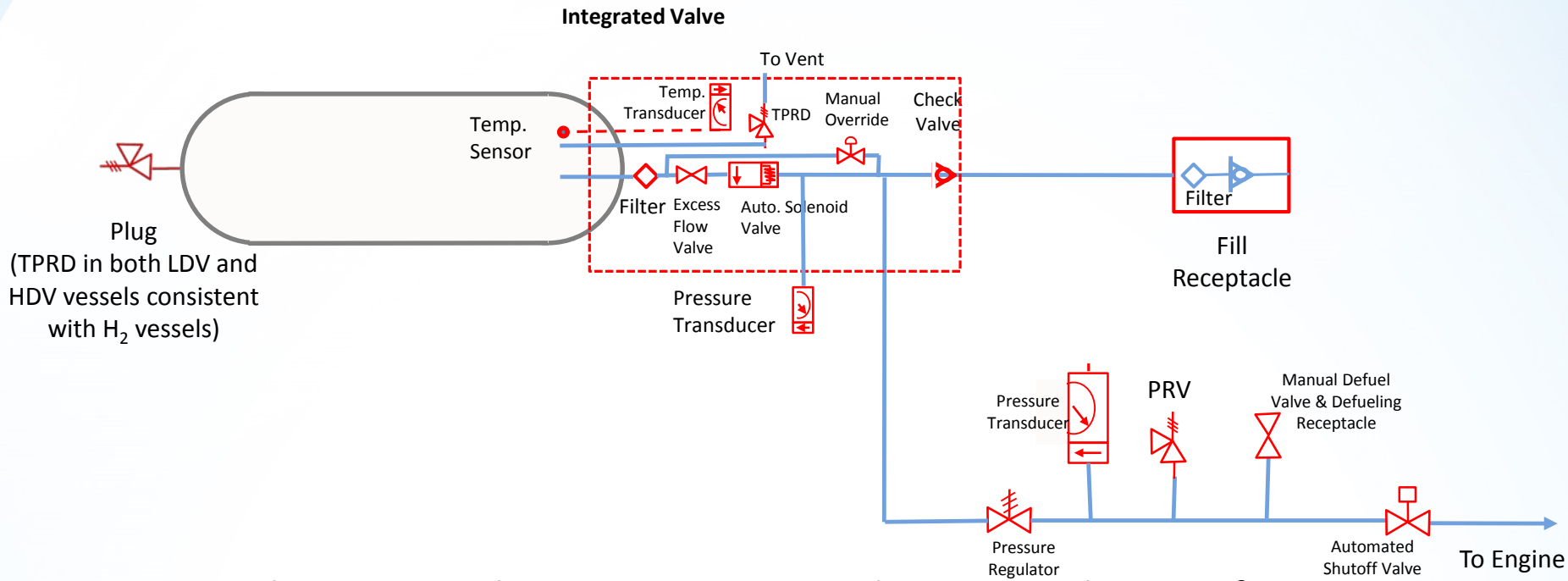


- Solvent (primarily DMF) is the main cost driver of MOF from solvo-thermal synthesis
- Liquid assisted grinding (LAG) and aqueous synthesis both show promise for reducing the cost of MOF synthesis
- m-dodbc (made from lower cost starting materials) is projected to cost $9.87/kgMOF at 500k systems/year
- 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 H_2 system models



- Leveraged existing 700 bar H_2 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

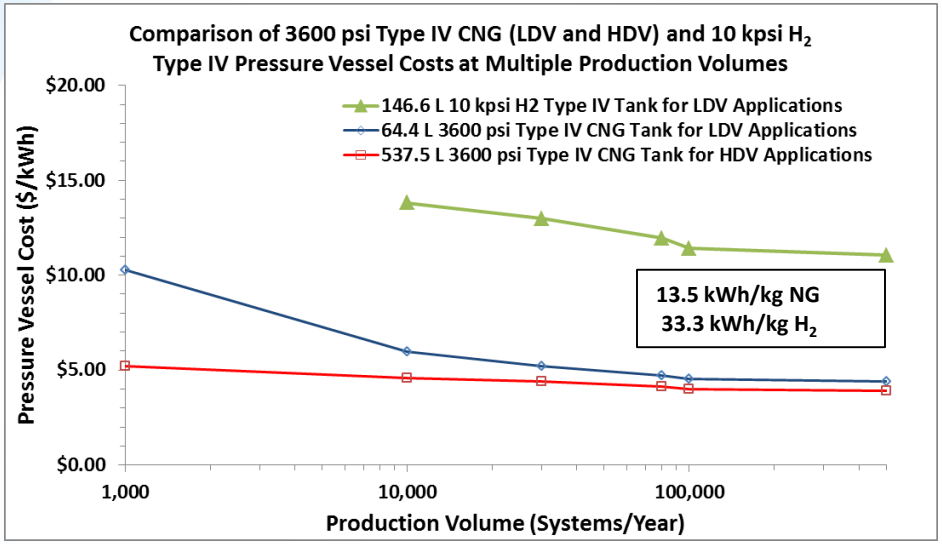
Modeled system masses are in good agreement with commercial comparison system masses

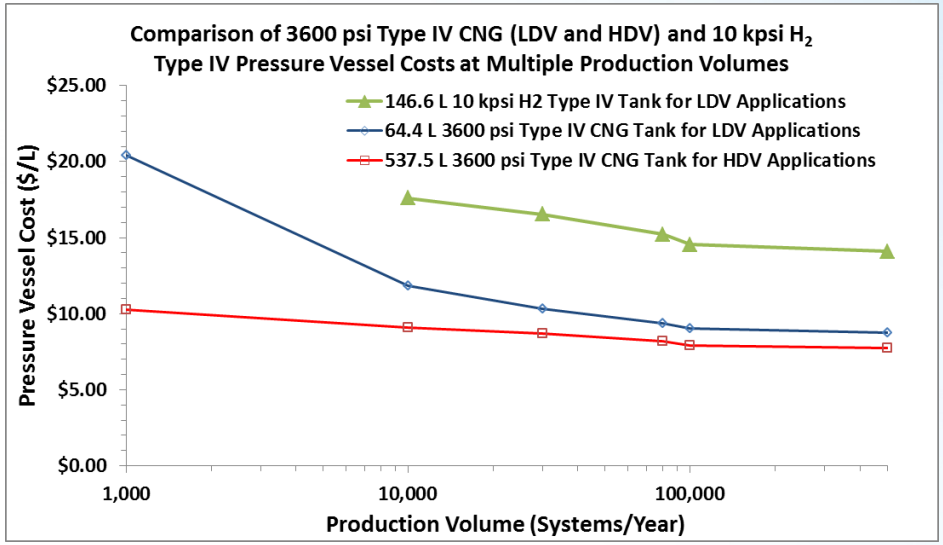
		LDV	HDV
Modeled Masses			
Boss	kg	1.75	1.75
Liner	kg	5.07	23.65
Composite	kg	16.30	135.95
Shoulder Foam	kg	0.17	0.57
Total	**kg**	**23.29**	**161.92**
Reported Mass (TUFFSHELL)	kg	27.21	176.42
Boss, Liner, Composite w/o Fiberglass, and Foam only TUFFSHELL Mass	kg	23.76	154.14
Relative Difference	%	-2%	+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 over-estimates 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 H_2 systems





- **Composite cost for H_2 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 H_2 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 H_2 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 CcH_2 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 H_2**
  - Leverage CcH_2 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 CcH_2 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 H_2**
  - 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**
  - 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

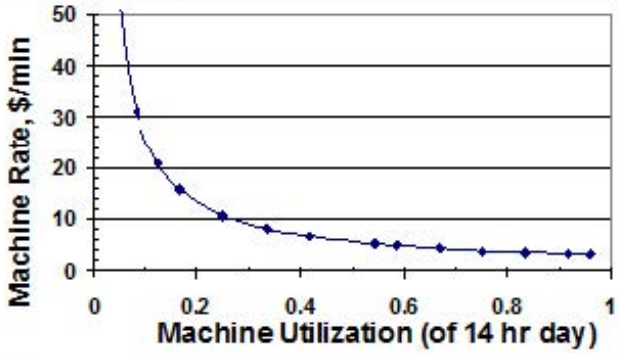
- DFMA® (Design for Manufacture & Assembly) is a registered trademark of Boothroyd-Dewhurst, Inc.
  - Used by hundreds of companies world-wide
  - Basis of Ford Motor Co. design/costing method for the past 20+ years
- SA practices are a blend of:
  - "Textbook" DFMA®, industry standards and practices,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

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

Manufacturing Cost Factors:

1. Material Costs
2. Manufacturing Method
3. Machine Rate
4. Tooling Amortization

Methodology reflects cost of under-utilization:



Methodology Reflects Cost of Under-utilization:

Capital Cost
Installation
} **Initial Expenses** → **Used to calculate annual capital recovery factor based on:**
- Equipment Life
- Interest Rate
- Corporate Tax Rate

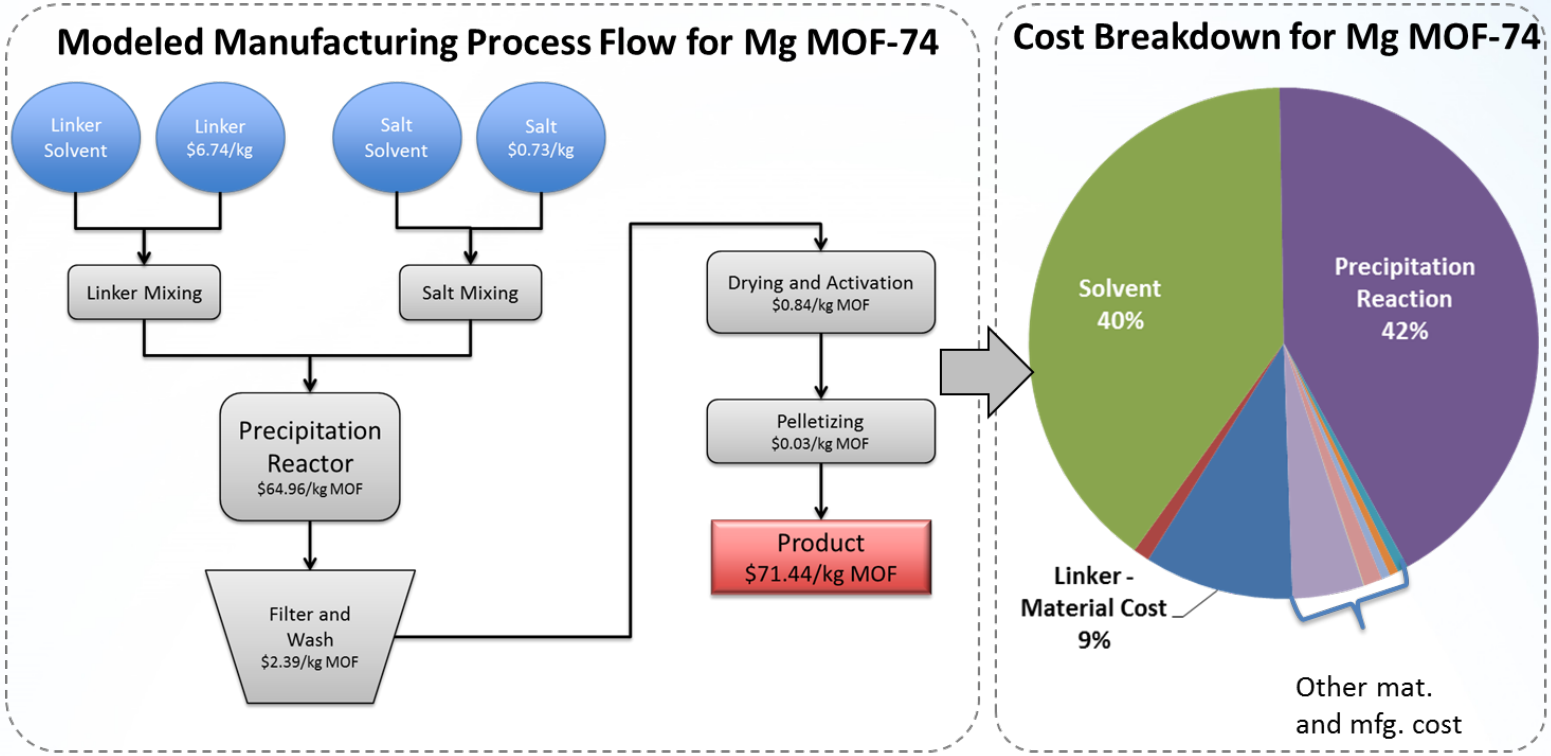
Maintenance/Spare Parts Utilities Miscellaneous
} **Operating Expenses**

$$\frac{\left(\text{Annual Capital Repayment} + \text{Annual Operating Payments}\right)}{\left(\text{Annual Minutes of Equipment Operation}\right)} = \text{Machine Rate } (\$/\text{min})$$

Production Volume Range of Analysis:

10,000 to 500,000 H_2 storage systems per year

Solvo-Thermal Synthesis

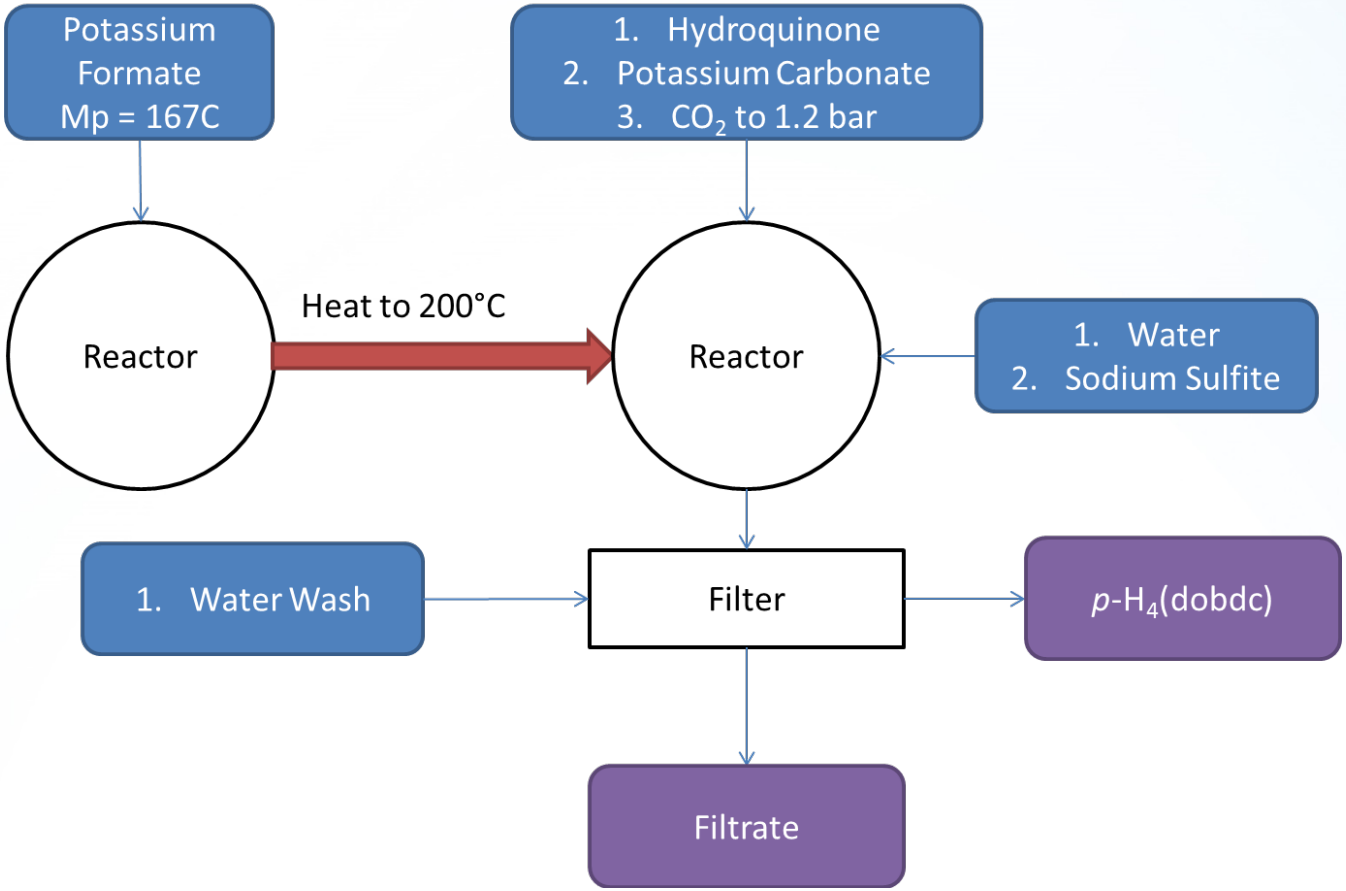


- Process is based on scaled-up lab scale synthesis assuming 90% solvent and reagent recycle
- Manufacturing scale chosen to provide enough MOF for 500k FCEVs per year
- Cost is dominated by precipitation reactor size and solvent material cost (DMF)

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

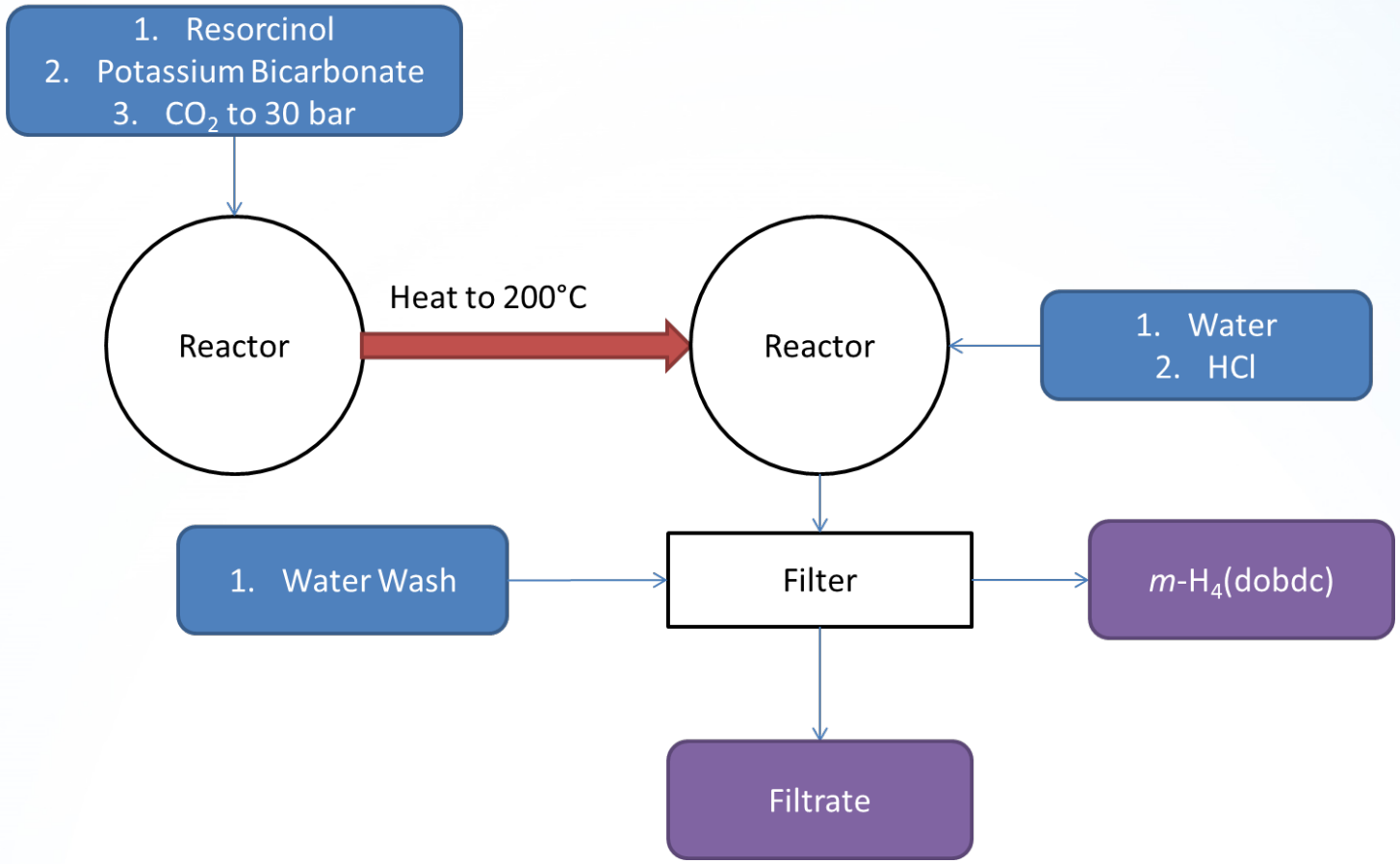


p-dobdc
(from Guang Dong et al)

95% Yield

Comparison of Linker Production

m-dobdc Process Flow

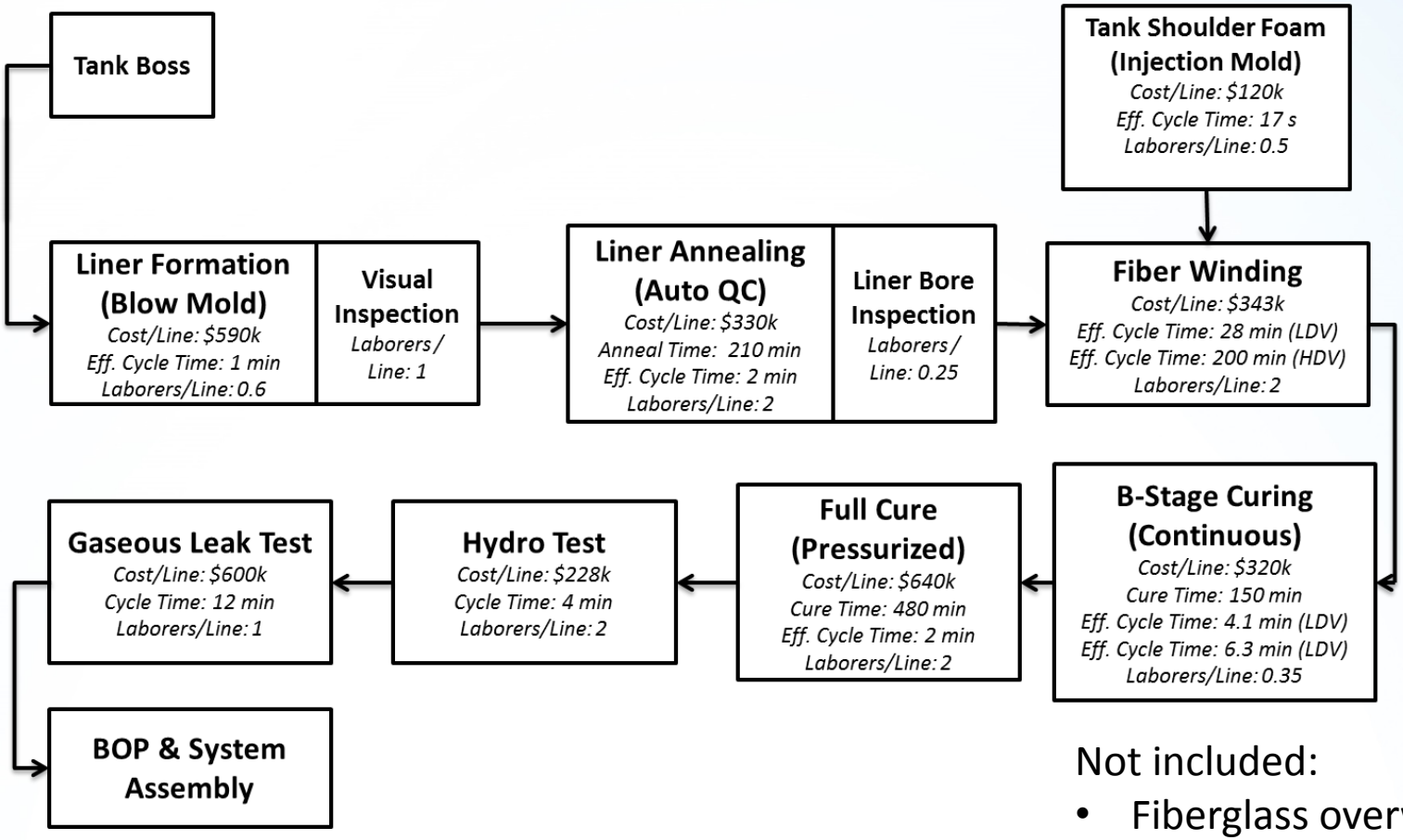


m-dobdc
(from Sikkema et al)

93% Yield

Accomplishments & Progress:

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



Not included:

- Fiberglass overwrap
- Gel coating
- Painting

- Processing steps are identical to those of H_2 vessels

Comparison of CNG Tank Dimensions

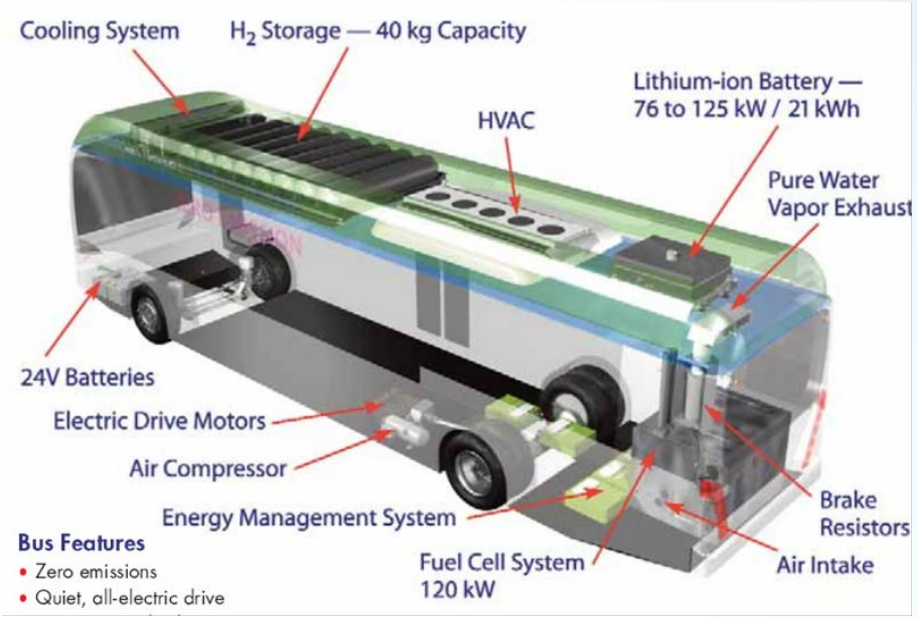
	units	TUFFSHELL LDV	CNG Model LDV	TUFFSHELL HDV	CNG Model HDV	Hydrogen (2013)
Fill Pressure	MPa	24.8	24.8	24.8	24.8	70.0
Water Volume	L	**64.4**	**64.4**	**537.5**	**537.5**	146.6
Performance Factor	In	--	**1.04E+06**	--	**1.04E+06**	**1.04E+06**
Carbon Fiber Volume Fraction	%	--	60.0	--	60.0	60.0
Composite 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)	kg	--	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 H_2 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