System Level Analysis of Hydrogen Storage Options

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2015 DOE Hydrogen and Fuel Cells Program Review

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Project ID: ST001

Overview

Timeline

- Project start date: Oct 2009
- Project end date: N/A
- Project continuation and direction determined annually by DOE

Barriers

- H_2 Storage Barriers Addressed:
  - A: System Weight and Volume
  - B: System Cost
  - C: Efficiency
  - E: Charging/Discharging Rates
  - J: Thermal Management
  - K: Life-Cycle Assessments

Budget

- FY14 DOE Funding: $480 K
- FY15 DOE Funding: $480 K

Partners/Interactions

- Storage Systems Analysis Working Group (SSAWG)
- PNNL, Tank OEMs
- Delivery Team
- Hydrogen Storage Engineering Center of Excellence (HSECoE): SRNL, LANL
- SA

Objectives and Relevance

Develop and use models to analyze the on-board and off-board performance of physical and material-based automotive hydrogen storage systems

- Conduct independent systems analysis for DOE to gauge the performance of H_2 storage systems
- Provide results to material developers for assessment against system performance targets and goals and help them focus on areas requiring improvements
- Provide inputs for independent analysis of costs of on-board systems.
- Identify interface issues and opportunities, and data needs for technology development
- Perform reverse engineering to define material properties needed to meet the system level targets

Impact of FY2015 work

- Evaluated relationship between HDPE liner properties and liner failure at cryogenic temperatures to support cryo/cold H_2 storage work
- Proposed lower and upper limits to free energy of decomposition (ΔG^0) for energetic off-board regeneration of chemical hydrogen materials
- Established desired range of ΔH and decomposition temperature to satisfy on-board storage system targets with chemical hydrogen materials

Approach

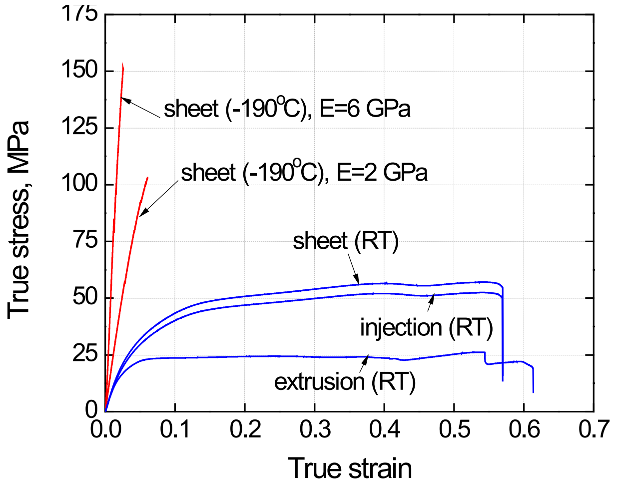
- Develop thermodynamic and kinetic models of processes in physical, complex metal hydride, sorbent, and chemical H_2 storage systems
  - Address all aspects of on-board and off-board storage targets, including capacity, charge/discharge rates, emissions, and efficiencies
  - Perform finite-element analysis of compressed hydrogen storage tanks
  - Assess improvements needed in materials properties and system configurations to achieve storage targets
- Select model fidelity to resolve system-level issues
  - On-board system, off-board spent fuel regeneration, reverse engineering
  - Conduct trade-off analyses, and provide fundamental understanding of system/material behavior
  - Calibrate, validate, and evaluate models
- Work closely with DOE technology developers, HSECoE and others in obtaining data, and provide feedback
- Participate in SSAWG meetings and communicate approach and results to foster consistency among DOE-sponsored analysis activities

Summary: FY2015 Tasks and Accomplishments

1. Physical storage
   - ABAQUS simulations of HDPE liners at 150-200 K (in progress)
   - On-board cold gas H_2 storage system and off-board WTT efficiency
   - Validate ABAQUS models for tanks with advanced materials and winding techniques (pending)
2. H_2 storage in metal hydrides
   - Published paper in IJHE on reverse engineering to determine material properties needed to meet system targets with low-temperature metal hydrides
3. H_2 storage in sorbents
   - Publishing paper in IJHE on reverse engineering to determine material properties needed to meet system targets including well-to-tank (WTT) efficiency
   - Validate and update sorbent model utilizing HSECoE data (pending)
4. Chemical hydrogen storage
   - Reverse engineering to determine material properties needed to meet system targets including well-to-tank efficiency
   - Validate and update reactor and BOP models utilizing HSECoE data (ongoing)

Technical Accomplishments: Stress and Strain Behavior in HDPE

Collaborating with PNNL to determine the relationship between HDPE liner properties and liner failure at cryogenic temperatures in support of work on cryo/cold hydrogen storage in Type 4 tanks



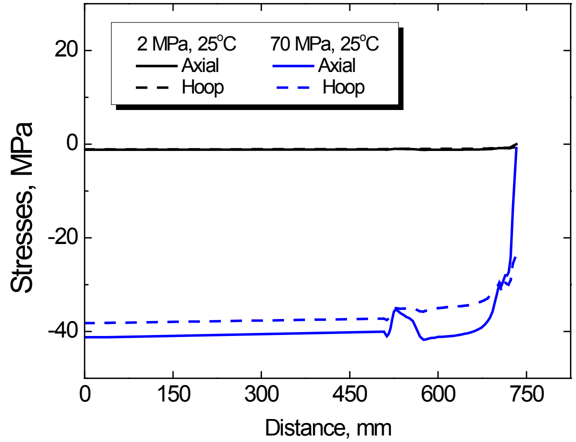
PNNL Data (David Gotthold)

Liner behavior at room temperature

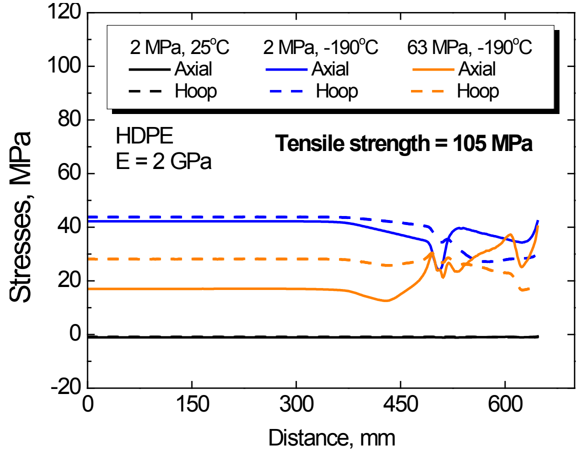
- Small compressive stresses at 2 MPa, increasing to -41 MPa (axial), -38 MPa (hoop) at 70 MPa
- No failure anticipated

At -190°C, liner is in tension

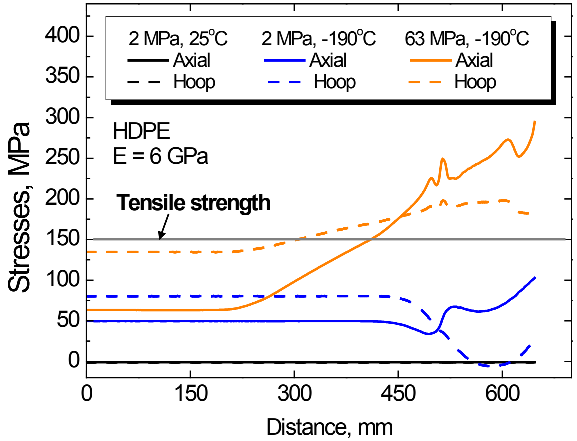
- For HDPE with E = 2 GPa, tensile stress in the liner is below the tensile strength
- For HDPE with E = 6 GPa, tensile stress in the dome is well above the 150-MPa tensile strength, tank failure is predicted



T = 25 °C



T = -190°C, E = 2 GPa

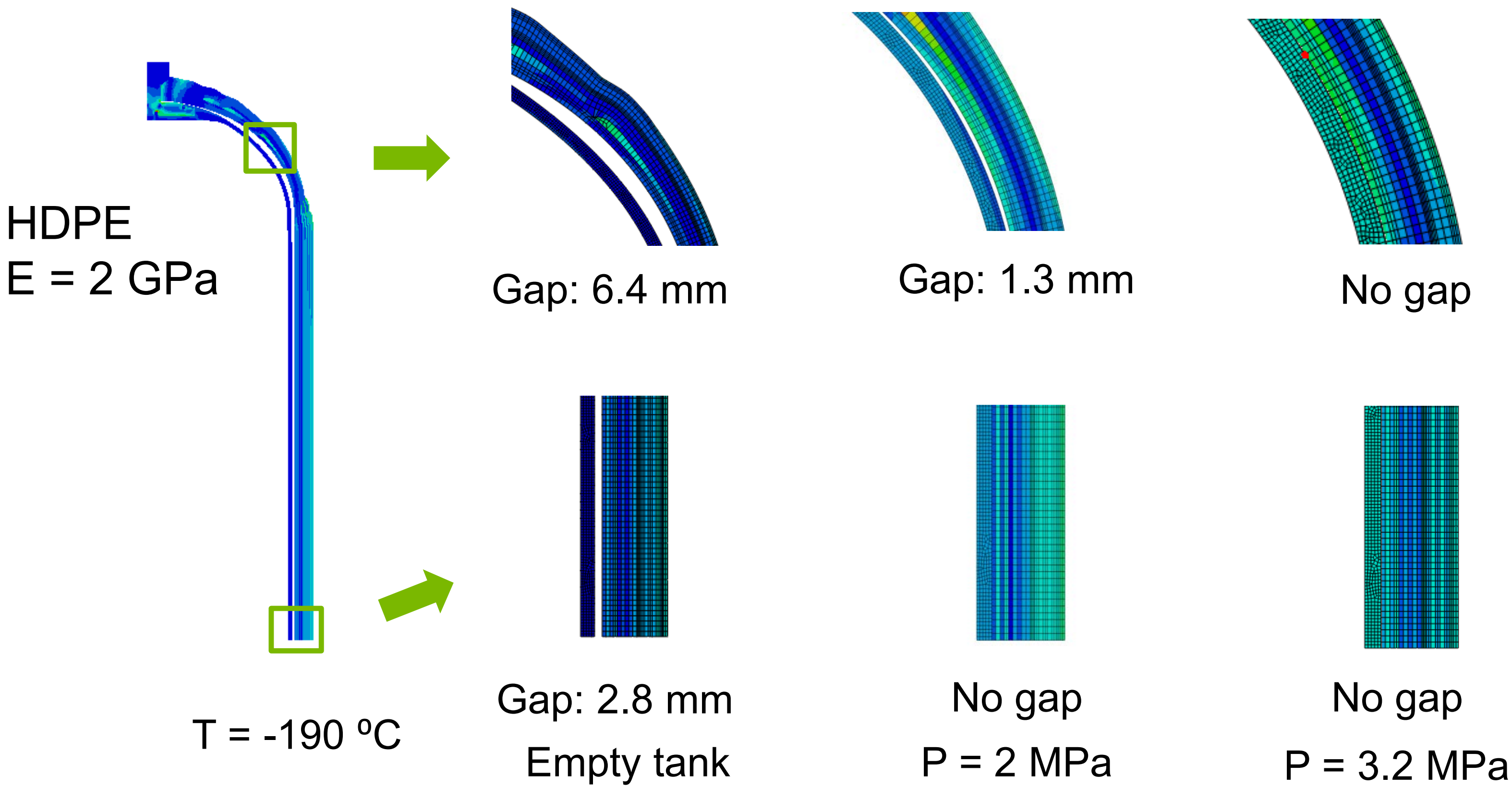


T = -190°C, E = 6 GPa

***ABAQUS simulations for full-sized 5.6 kg H_2 tank pressurized to 70 MPa**

Liner Separation at Low Temperature

- Minimum internal pressure needed to avoid liner separation at near LN_2 temperatures (-190°C)
  - Gaps exist between the liner and CF in the cylinder and dome sections of the tank as a result of differential CTEs if the internal pressure is <2 MPa
  - Gap exists in the dome if the tank internal pressure is <3.2 MPa

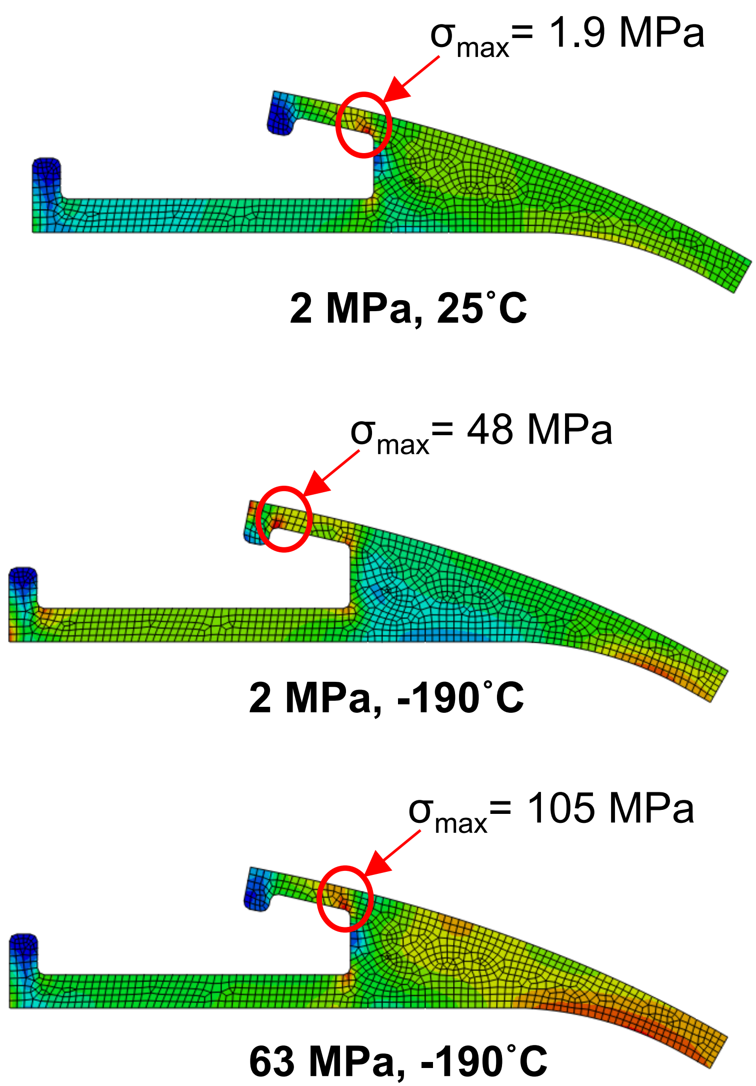


Stress Concentration at Liner/Boss Interface

ABAQUS simulations of a full-sized tank with HDPE liner (E = 2 GPa) reveal high stress concentration region at the interface corners

- Simulation results at P = 2 MPa
  - Compared to peak stress at 25°C, 25-fold increase at -190°C due to CTE mismatch between HDPE liner and Al-6061
  - Peak stress is below 105-MPa tensile strength of liner
- Simulation results at P = 63 MPa
  - Peak stress at -190°C approaches the tensile strength of liner
- For comparison, testing of two Type-4 tanks at LN_2 temperature by Hexagon Lincoln showed that both tanks leaked at <28 MPa and cracks occurred at the liner/boss interface

von Mises Stress Contours

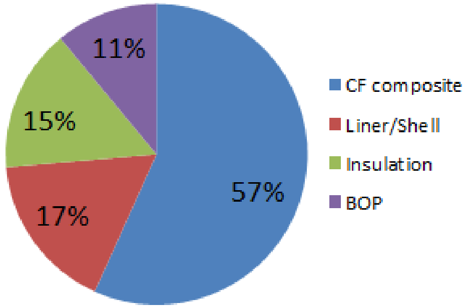


Cold Gas Storage Option: Off-Board Analysis

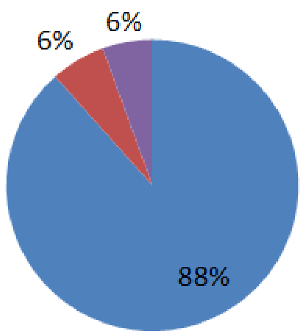
- Netting analysis calibrated with ABAQUS model to determine weight and volume for 2.25 safety factor and 5500 pressure cycles, and constrained by ISO container dimensions and trailer payload
- Onboard conditions: baseline (700 bar, 300K), cold gas (400 bar, 200 K)
- Baseline tubes require significantly more CF than cold gas tubes

	Unit	Trailer Tube		Cascade Storage Tube	
		Base Case	Cold Gas	Base Case	Cold Gas
Type		4	3	3	3
Nominal Storage Pressure	bar	340	340	945	534
Nominal Storage Temperature	K	300	83	300	116
H_2 Stored	kg	116	137	46	45.3
H_2 Volume	m^3	5.1	2.25	0.96	0.77
Carbon Fiber Composite Weight	kg	1148	425	712	278
Total Tube Weight	Kg	1421	1483	958	856

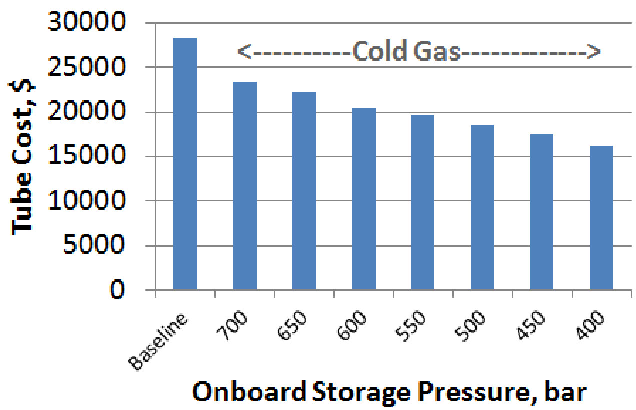
Trailer tube, cold gas
$25,637



Trailer tube, base case
$41,588

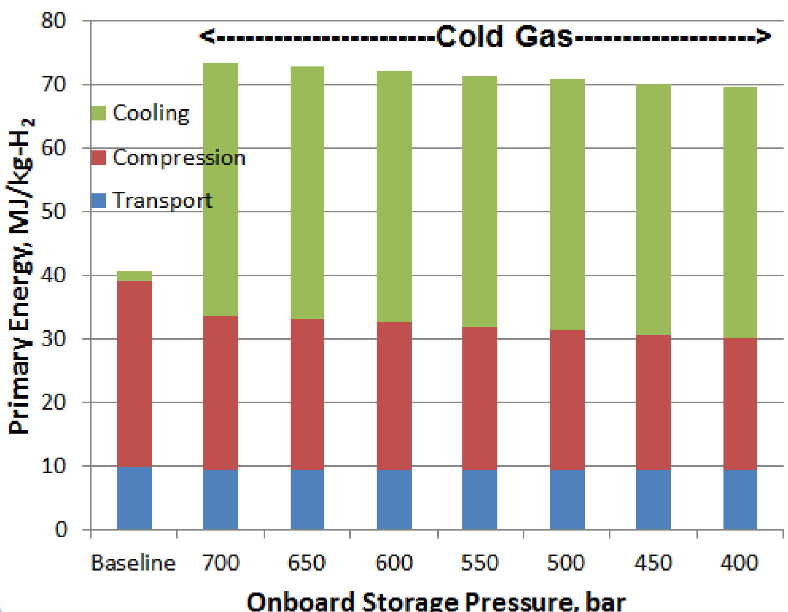


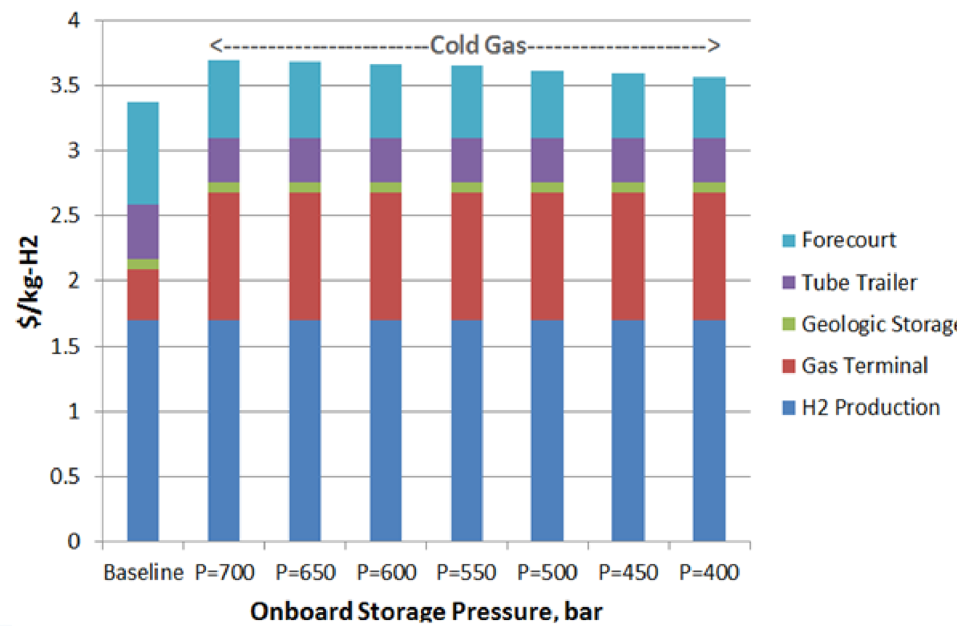
Cascade tubes



Off-Board Analysis: Energy Consumption and Fuel Cost

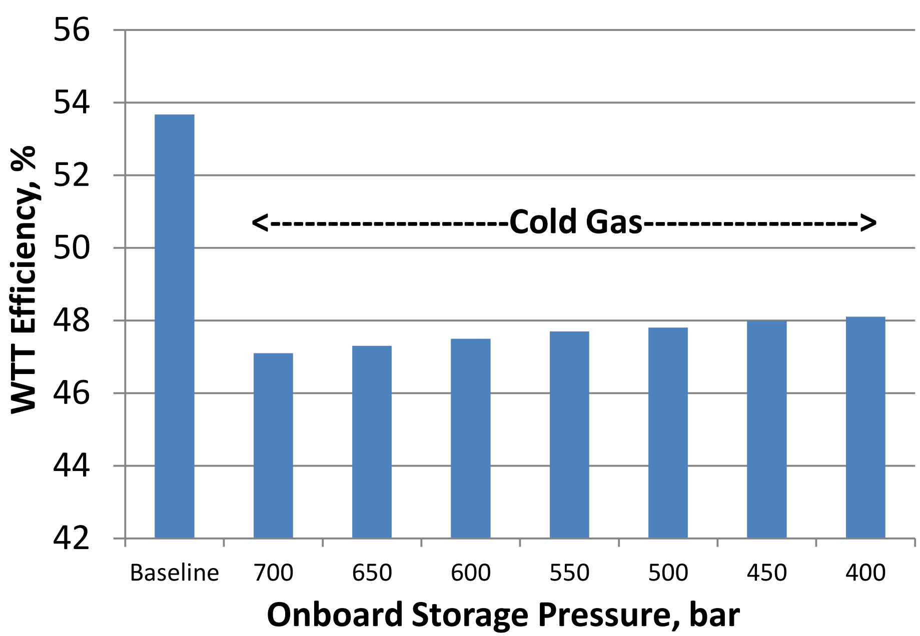
- Off-board primary energy consumption for cold gas option is equivalent to ~60% of H_2 LHV, and is ~73% higher than for baseline
  - ➢Cooling with LN_2, GCtool analysis: 7 kg LN_2 is needed per kg H_2
  - ➢Compression energy is lower because of lower gas temperature
- Off-board cost for cold gas is \$0.18 - \$0.31/kg-H_2 higher than baseline
  - ➢Significantly higher at the gas terminal
  - ➢Lower costs at forecourt and tube trailer
- Storage pressure of cold gas has only small effect on off-board energy consumption and fuel cost (<7% variation between 400 and 700 bar)





WTT Efficiency

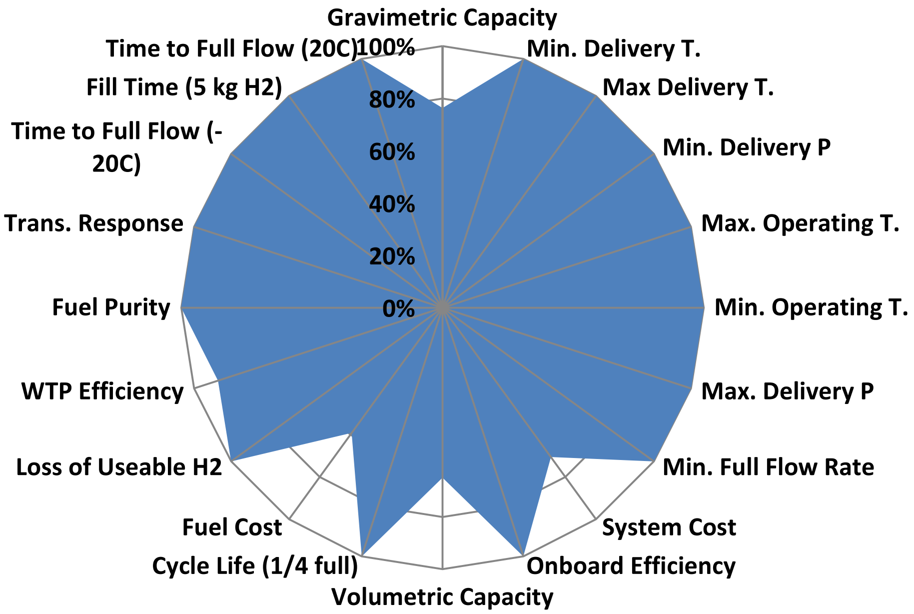
- WTT efficiency for cold gas storage < 50%, ~6 percentage points lower than baseline because of cooling requirement
- WTT efficiency can improve by 1.3 percentage points for baseline and 0.2 – 0.7 percentage points for cold gas if Linde ionic compressor is used at forecourt



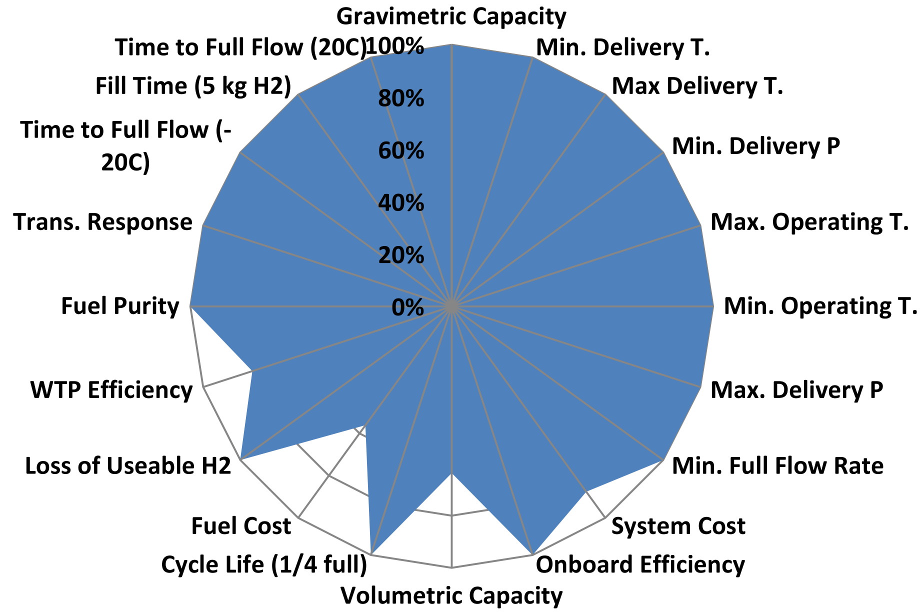
Process/Process Fuels	Nominal Value	Source/Comments
Electricity production	35.1% thermal efficiency	EIA projected U.S. grid 2015, inclusive of 6.5% transmission loss
North American natural gas production	93.5 % efficiency	GREET
H_2 production by SMR	73% efficiency	Advanced industrial SMR plant
Pipeline transmission	50 bar	Pressure drop
H_2 compressor isentropic efficiency	88% central 65% forecourt	HDSAM
H_2 cooling with LN_2		
- LN_2 production	0.55 kWh/kg	Large plants
H_2 delivery by tube trailers	up to 9 tubes/trailer	Weldship
- Tube pressure	340 bar	CF overwrap for reinforcement
- Temperature	83 K	Requires insulation
- Water volume	2.254 m^3	Weldship
- H_2 capacity per tube	135 kg	
- RT distance/fuel economy	100 km/ 6 mpg	HDSAM

Summary of Cold Gas Storage Option

- Cold gas storage option has the potential to meet the gravimetric capacity target but unlikely to meet the volumetric capacity target (little change versus baseline)
- Fuel cost is ~5% higher than baseline, but onboard system cost is ~20% lower (50% savings in CF requirement, offset by added insulation and shell costs)
- WTP efficiency for cold gas storage is ~6 percentage points lower than baseline and is unlikely to meet DOE target



700 bar, 300 K



400 bar, 200 K

Chemical Hydrogen Storage Materials

Class of storage materials that release hydrogen through a non-equilibrium process and, therefore, cannot be regenerated by reacting the dehydrogenated product with H_2 gas.

- Require off-board regeneration using electrochemical or catalytic processes

1. Negative free energy of decomposition

- Thermodynamically unstable at room temperature and are stabilized by extremely slow kinetics (alane, ammonia borane) or by other chemical means (addition of 3% NaOH to aqueous $NaBH_4$)

2. Positive free energy of decomposition

- Stable at room temperature but can be decomposed at elevated temperatures
- Require a catalyst for adequate kinetics at low temperatures
- APCI patent identifies many cyclic hydrocarbons including perhydrogenated n-ethyl carbazole
- On-board storage system efficiencies may be low since $\Delta H > T\Delta S$, i.e., $\Delta H > 38.8$ kJ/mol for $\Delta S = 130.2$ J/mol.K
- High off-board efficiencies may be possible since the regeneration reaction is exothermic

Off-Board Regeneration of Chemical Hydrogen Storage Materials

Well-to-tank efficiency (η_{WTT})*

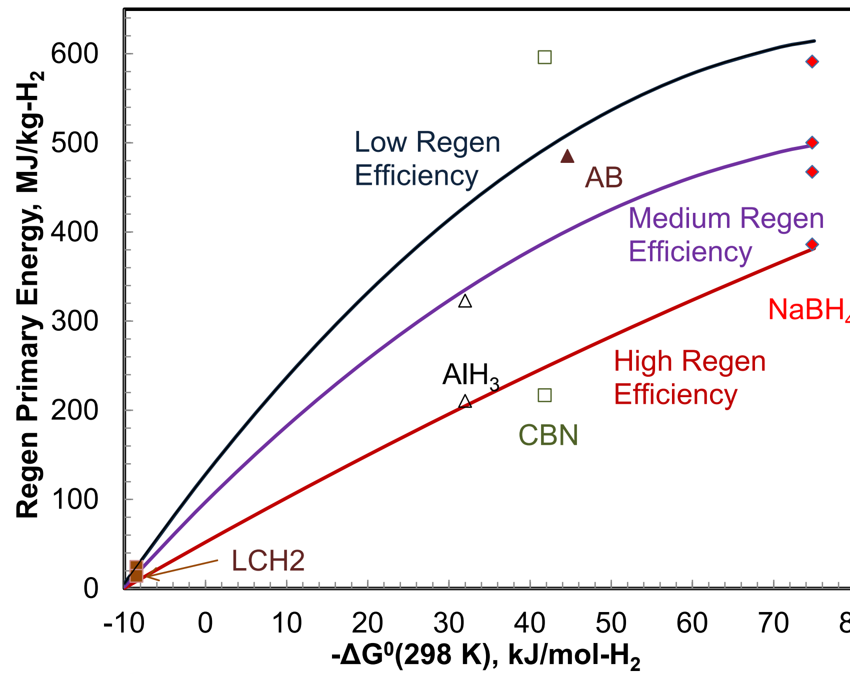
- Ratio of LHV of H_2 produced to the primary energy (Q^f) consumed in producing (subscript *p*), delivering (subscript *d*) and storing (subscript *s*) H_2

$$\eta_{WTT} = \frac{\Delta H_{LHV}}{Q_p^f + Q_d^f + Q_s^f} \qquad Q_r^f = Q_d^f + Q_s^f$$

ΔG determines the off-board regeneration efficiency. Materials with large negative ΔG require elaborate regeneration processes with high demands for primary energy.

- WTT efficiency: 16-21% for $NaBH_4$ (-75 kJ/mol), 8-18% for AB (-45 kJ/mol), 24-31% for AlH_3 (-32 kJ/mol), 60-63.2% for n-ethyl carbazole

	ΔG^0 (298 K) kJ/mol-H_2	ΔH^0 (298 K) kJ/mol-H_2	ΔS^0 (298 K) J/mol.K	Regen Primary Energy MJ/kg-H_2	WTT Efficiency %	Comments
$NaBH_4$	-74.75	-57.75	57	386	21.3	AnH-AqH
	Hydrolysis Reaction			467	18.6	AqH-AqH
				500	17.7	An-Aq
				591	15.6	Aq-Aq
AlH_3	-32	6.6	131	323	24.0	TMAA no waste heat
	Thermolysis Reaction			210	31.0	50% waste heat
AB	-44.6	-33	39	485	18.1	Benzophenone
	Thermolysis Reaction			1319	8.0	Bayer
				789	12.4	PCUK
CBN	-41.8	-18.97	77	596	15.5	MeOH/$NaAlH_4$
	Thermolysis Reaction			217	30.5	Formic acid
LCH2	8.5	47.3-53.6	130.2	24	60.0	Trickle bed reactor
	Perhydro N-ethyl Carbazole			14	63.2	Electricity production



*RK Ahluwalia, TQ Hua and J-K Peng, "Fuel Cycle Efficiencies of Different Automotive On-Board Hydrogen Storage Options," IJHE 32 (2007) 3592-3602

WTT Efficiency Correlation

Analyzed a H_2 production, delivery and regeneration fuel cycle for NA NG and US electric grid: 68% SMR efficiency without credit for steam co-production, 77% with steam export.

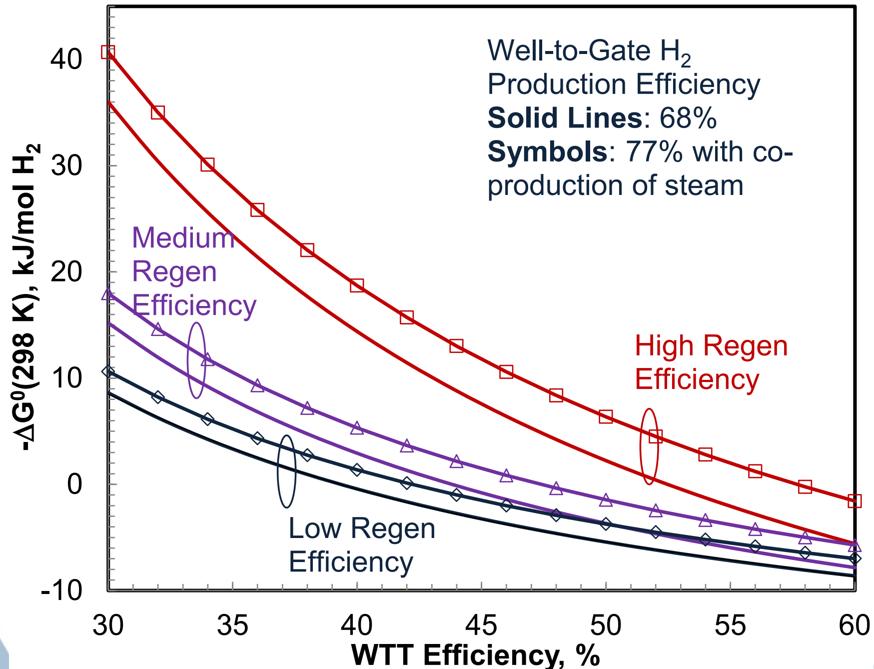
- WTT correlations for high, medium and low regeneration efficiencies

Materials with positive free energy of decomposition

- May meet the 60% WTT efficiency target if ΔG^0(298 K) > 1.6 kJ/mol.

Materials with negative free energy of decomposition

- Even with steam export, 60% WTT efficiency not possible
- With steam export, minimum ΔG^0(298 K) limited to -1.5 kJ/mol for 55% WTT efficiency and -6.4 kJ/mol for 50% WTT efficiency



Definitions of Free Energy and Enthalpy of Decomposition

$$AH_m = AH_n + (m-n)/2\ H_2$$

$$\Delta G = \left(\frac{2}{m-n}\right)[\Delta G_f(AH_n) - \Delta G_f(AH_m)]$$

$$NaBH_4 + 2\ H_2O = NaBO_2 + 4\ H_2$$

$$\Delta G = 1/4[\Delta G_f(NaBO_2) - \Delta G_f(NaBH_4) - 2\Delta G_f(H_2O)]$$

*60% efficiency target is for well-to-engine (WTE) efficiency, not WTT efficiency

Bounding Thermodynamic and Kinetic Properties

Desired thermodynamic properties of materials for which the WTT efficiencies may be between 50 to 60%

- Over the narrow range of desired ΔG^0(298 K), exothermic materials are unsuitable if ΔS is between the expected range 80 – 130 J/mol.K
- Materials that decompose above the FCS coolant temperature and require a burner may not be acceptable since the on-board system efficiency is quite low for ΔH between 20 and 40 kJ/mol-H_2

Desired kinetic properties of materials that decompose at 60 – 80°C

- Likely a catalytic process, otherwise the material would have short shelf life and may not meet the 0.05 g-H_2/h/kg stability target at room temperature
- Non-equilibrium decomposition kinetics that is independent of back pressure, otherwise the buffer tank would need to be refueled with gaseous H_2

		ΔS = 130 J/mol.K			ΔS = 105 J/mol.K			ΔS = 80 J/mol.K		
WTT Efficiency		60%	55%	50%	60%	55%	50%	60%	55%	50%
ΔG^0(298 K)	kJ/mol	1.6	-1.5	-6.4	1.6	-1.5	-6.4	1.6	-1.5	-6.4
ΔH	kJ/mol	40.3	37.2	32.3	32.9	29.8	24.9	25.4	22.3	17.4
P_{H2}(60°C)	atm	2.9	8.9	52.1	2.1	6.5	38.0	1.5	4.7	27.7
P_{H2}(70°C)	atm	4.4	13.2	73.3	3.0	8.9	49.4	2.0	6.0	33.3
P_{H2}(150°C)	atm	64.3	155.3	625.2	26.5	63.9	257.2	10.9	26.3	105.8

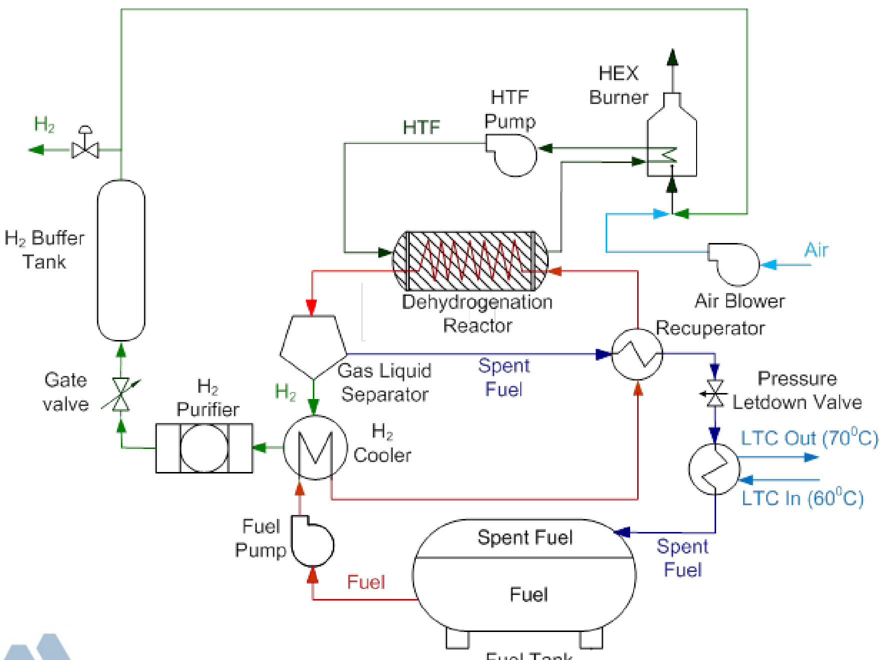
On-Board Chemical Hydrogen Storage System

Flow system to enable refueling of partially empty tanks

- Volume exchanged tanks for compactness
- Hydrogen buffer for start-up and fast transients
- Reactor operates at elevated pressure, reaction kinetics independent of back pressure, reactor size determined by reaction kinetics and heat transfer
- Fuel may be liquid, slurry or solution

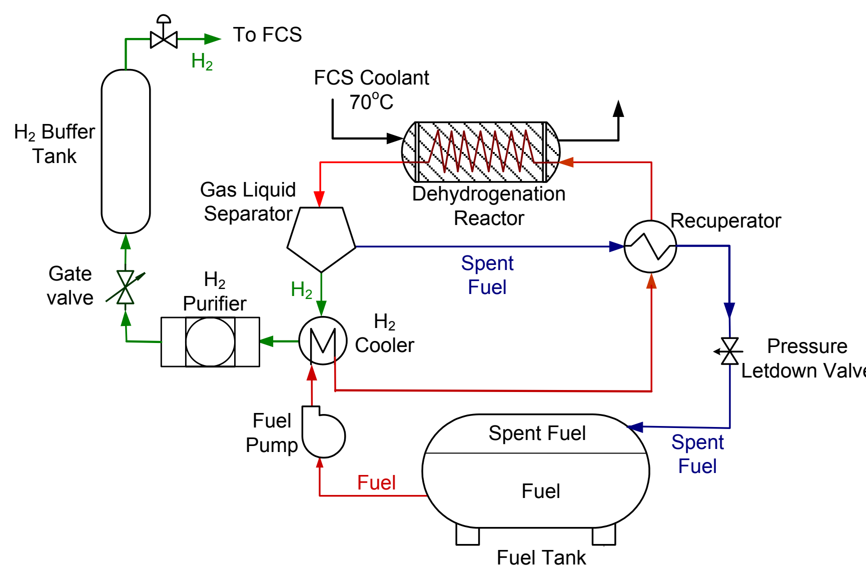
System with burner*

- 50-kW microchannel HEX burner
- HTF coolant separates burner & reactor



System without burner

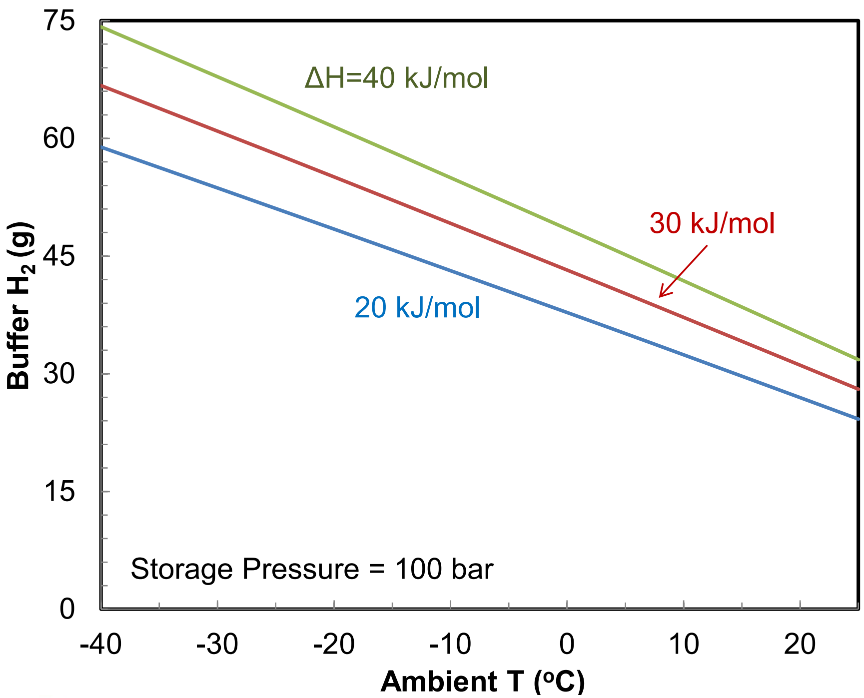
- Thermally integrated with FCS
- Mitigates FCS heat rejection problem

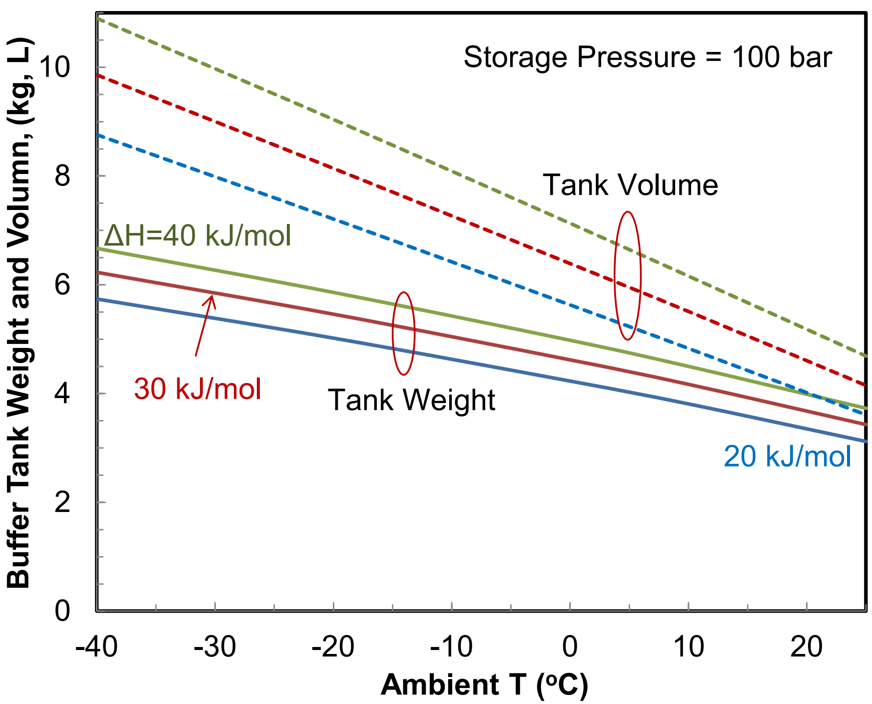


Storage System without Burner: Buffer H_2 Requirements

H_2 buffer capacity for FCS startup from -40°C*

- Buffer to supply H_2 until the fuel cell and the reactor reach the fuel decomposition temperature (70°C)
- Buffer replenished with excess H_2 released from fuel during normal operation when the stack coolant is at its peak temperature (80°C)
- Stack: 2 kW/kg specific weight, 0.5 kJ/kg.K average C_p
- Reactor: Thermal mass during startup includes weights of HX tubes, reactor walls, and coolant, 0.5 kJ/kg.K average C_p





RK Ahluwalia, JK Peng and TQ Hua, "Bounding Material Properties for Automotive Storage of Hydrogen in Metal Hydrides for Low-Temperature Fuel Cells," IJHE 39 (2014) 14874-14886.

Storage System without Burner: Baseline Material Targets

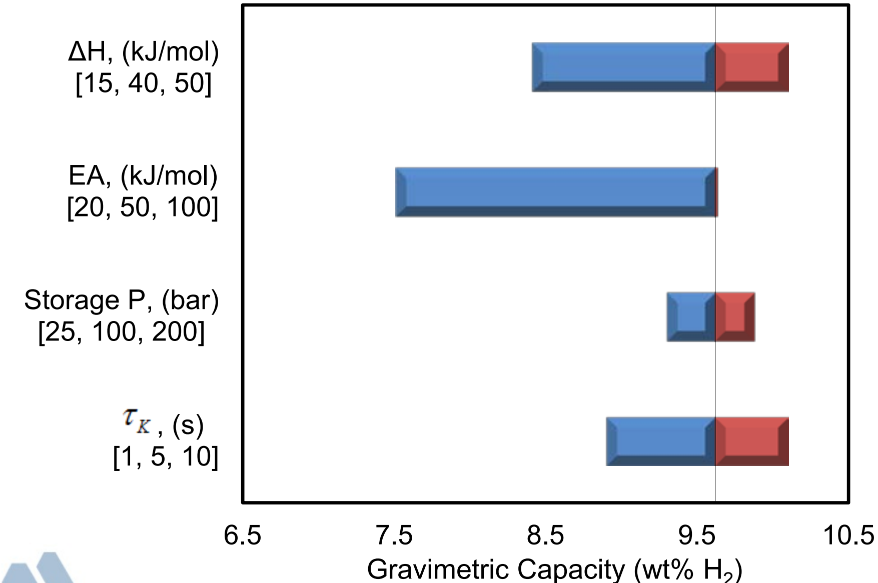
Thermodynamically mildly stable or unstable materials at room temperature that decompose at 70-80^oC, 100 bar backpressure

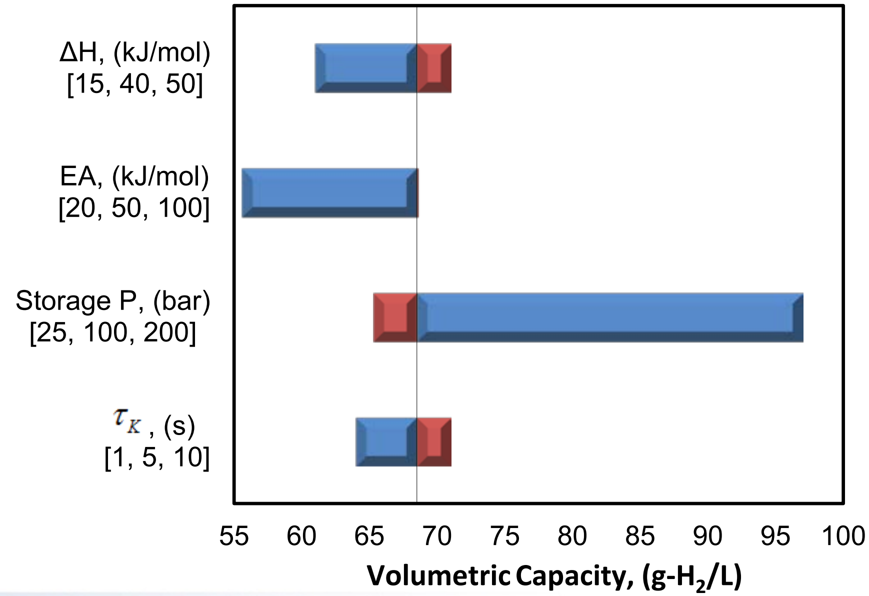
		Units	Reference Values	Range of Values	Comments and Relevant Targets
Chemical Storage Material	Free Energy of Decomposition	kJ/mol	1.6	-6.4 to 1.6	60% WTE efficiency
	Enthalpy of Decomposition	kJ/mol	40.0	20 to 40	90% on-board system efficiency
	Fuel Hydrogen Capacity	wt% H_2	9.6	8.4 - 9.6	5.5 wt% system gravimetric capacity
	Fuel Volumetric Capacity	g-H_2/L	68.5	61 - 71.5	40 g/L system volumetric capacity
	Decomposition Kinetcs	s	5	TBD	Time for 95% conversion at 70^oC
	Fuel Stability	g/h/kg-H_2	0.05		H_2 loss target
Operating Temperatures	Dehydrogenation Reactor	^oC	70	TBD	1.6 g/s minimum full flow of H_2
	Heat Transfer Fluid (HTF)	^oC	70	70 - 80	
	Spent Fuel Cooler	^oC	50	25 - 50	
Operating Pressures	Storage Pressure	bar	100	50 - 200	
	Minimum Delivery Pressure	bar	5		DOE target
H_2 Flow Rates	Refueling Rate	kg/min	1.5		Not relevant for liquid fuels
	Minimum Full Flow Rate	g/s	1.6		DOE target
Buffer H_2 Storage	Storage Pressure	bar	100	50 - 200	Start-up from -40^oC
	Buffer Storage Capacity	g-H_2	74	59 - 74	

Storage System without Burner: Sensitivity Analysis

On-going model testing and validation. As such, results are subject to uncertainties in shell-side heat transfer correlation

- ΔH: Determines reactor heat transfer area and fuel residence time. Reduces heat load on the FCS radiator (advantageous).
- Storage pressure: Determines the volume of the buffer. Volumetric material capacity target increases greatly if material decomposes at 25 bar back pressure.
- Activation energy (E_A): Fitting parameter.
- Isothermal conversion time (τ_K): Actual decomposition rate may be controlled by mass transfer (not yet considered in model) and heat transfer as τ_K is reduced.





FY2015 Collaborations

Physical Storage	PNNL Team: Liner properties at cryogenic temperatures (ST101)
Metal Hydrides	SRNL, UTRC: Material properties of metal hydrides, reverse engineering, acceptability envelope
Sorbents	SRNL, UM: Material properties of sorbents, reverse engineering, acceptability envelope (ST044, ST010)
Chemical Hydrogen	LANL, PNNL: Material properties of chemical hydrogen storage materials, reverse engineering, acceptability envelope (ST007)
Off-Board Fuel Cycle Efficiency	ANL (H2A Group), ANL (HDSAM)
Off-Board Cost	ANL (H2A Group), ANL (HDSAM)
On-Board Cost	SA
SSAWG	DOE, HSECoE (LANL, PNNL, SRNL, UM), OEMs,Tank Manufactures, UH, SA

- Argonne develops the storage system configuration, determines performance, identifies and sizes components, and provides this information to SA for manufacturing cost studies

Future Work

Physical Storage

- Apply ABAQUS model to support the on-going tank projects (graded carbon fiber composite structure, non-geodesic winding, alternate winding patterns and fibers, low-cost glass fibers, CF composites at cryogenic temperatures)
- Validate ABAQUS finite element model against experimental and field data for cold gas storage (collaboration with PNNL led project)
- Renew collaboration with LLNL to extend and validate ANL models to thin-walled high fiber fraction 700-bar pressure vessels at cryogenic temperatures (120 K)

Material Based Storage

- Analyze decomposition behavior and reactor heat transfer of chemical storage materials using LANL and PNNL data for AlH_3 and AB slurries as model fuels
- Analyze uptake and reactor heat transfer in powder and compacted sorbents using HSECoE data for Hex-Cell and MATI prototypes
- Determine favorable properties of unstable room-temperature metal hydrides
- Provide system-level support to new projects on material discovery

Document models and publish papers on material properties in IJHE

Project Summary

Relevance:	Independent analysis to evaluate on-board and off-board performance of materials and systems
Approach:	Develop and validate physical, thermodynamic and kinetic models of processes in physical and material-based systems Address all aspects of on-board and off-board targets including capacities, rates and efficiencies
Progress:	Determined the minimum pressure (32 bar) to avoid liner separation at near LN_2 temperatures (-190°C) in Type-4 tanks Evaluated liner failure modes at -190°C: stress concentration at liner/boss interface, pressure cycling induced fatigue failure Determined the WTT efficiency (48%), fuel cost penalty (5%), system cost reduction (20%) with cold gas storage option Reverse engineering to determine the desired properties of chemical storage materials: ΔG^0(298 K) > -6.4 kJ/mol, ΔH between 20 and 40 kJ/mol-H_2, 9.6 wt% H_2 and 68.5 g-H_2/L material capacities, decomposition temperature below 80°C
Collaborations:	SSAWG, HSECoE, Ford, LANL, PNNL, SA, SRNL
Future Work:	Propose, analyze and validate methods of reducing cost of CF wound storage tanks Validate AlH_3 and AB decomposition models using LANL and PNNL data, and sorption model using data for Hex-Cell and MATI prototypes from HSECoE

Reviewer Comments

Generally favorable reviews with the following comments/recommendations

- Additional assumption justifications and sensitivity analysis would be useful, such as recognizing tolerance band.
- Continue to pursue opportunities to validate results based on empirical testing and existing hardware.
- Emphasis should be placed on providing guidance on the requirements of future materials to meet the overall system targets
- Modeling of composite impact damage for compressed hydrogen storage tanks is encouraging and should be especially useful.
- Keep publishing results in appropriate peer-reviewed journals in a timely manner.

FY15 work scope consistent with above recommendations

√ Assumption justifications and sensitivity analysis were included in recent work on sorbent and chemical hydrogen storage materials

√ Ongoing work to validate sorbent and chemical hydrogen storage model results with test data being acquired by the HSECoE.

√ Guidance on material requirements of future materials was the main focus of reverse engineering work on chemical hydrogen, sorbents, and metal hydrides.

√ Results of compressed hydrogen storage tanks (liner, CF usage, impact damage) were discussed with PNNL for potential testing to address key issues.

√ Published two journal papers and another one being reviewed for publication.

Technical Back-Up Slides

Publications and Presentations

Journal Publications

R.K. Ahluwalia, J.K. Peng, and T.Q. Hua, “Bounding Material Properties for Automotive Storage of Hydrogen in Metal Hydrides for Low-Temperature Fuel Cells,” International Journal of Hydrogen Energy, 39 (2014) 14874-14886.

R.K. Ahluwalia, J.K. Peng, and T.Q. Hua, “Sorbent Material Properties for On-board Hydrogen Storage for Automotive Fuel Cell Systems,” accepted for publication in International Journal of Hydrogen Energy, 2015.

H.S. Roh, T.Q. Hua, R.K. Ahluwalia, and H.S. Choi, “Impact Damages on Type IV Hydrogen Storage Tanks for Fuel Cell Vehicles,” Submitted to International Journal of Hydrogen Energy, 2014.

Book Chapters

R.K. Ahluwalia, J.K. Peng, and T.Q. Hua, “Cryo-compressed Hydrogen Storage,” Compendium of Hydrogen Energy, Elsevier, submitted November 2014

Presentations

R.K. Ahluwalia, J.K. Peng, and T.Q. Hua, “Chemical Hydrogen Storage Material Requirements for Automotive Fuel Cells,” Storage System Analysis Working Group Meeting, Webinar, September 10, 2014.

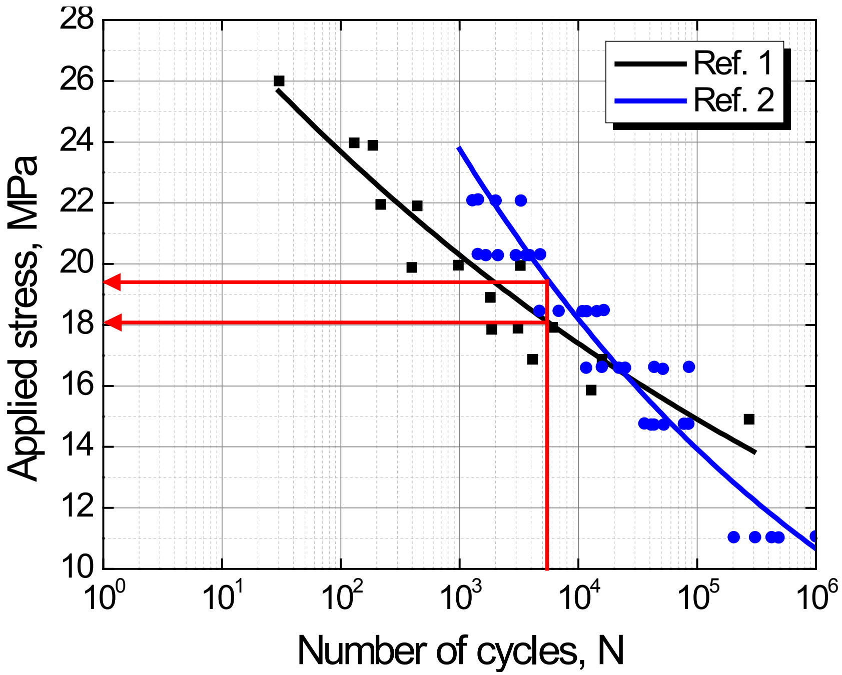
R.K. Ahluwalia, J.K. Peng, and T.Q. Hua, “Off-Board Considerations,” DOE Materials-Based Hydrogen Storage Summit, Golden, CO, January 27, 2015.

R.K. Ahluwalia, T.Q. Hua, J.K. Peng, and H.S. Roh, “System Level Analysis of Hydrogen Storage Options,” DOE Materials-Based Hydrogen Storage Summit PI Meeting, Golden, CO, January 28, 2015.

R.K. Ahluwalia, T.Q. Hua, J.K. Peng, and H.S. Roh, “System Level Analysis of Hydrogen Storage Options,” Hydrogen Storage Tech Team Meeting, Southfield, MI, February 19, 2015.

Fatigue Considerations

- In ambient temperature Type 4 tanks, the HDPE liner experiences compressive stress during pressure cycling, therefore fatigue is not an issue.
- At -190°C, pressure cycling induces tensile stress in the liner
  – Fatigue load (σ), $\sigma_{mean} = (\sigma_{max}+\sigma_{min})/2 = 30$ MPa, $R = \sigma_{min}/\sigma_{max} = 0.4$
- Need SN curves for HDPE at low temperatures to determine if fatigue is a concern
  – For 5500 pressure cycles at RT, maximum allowable stress for HDPE PE-100 grade is ~20 MPa



Test Conditions

Ref. 1

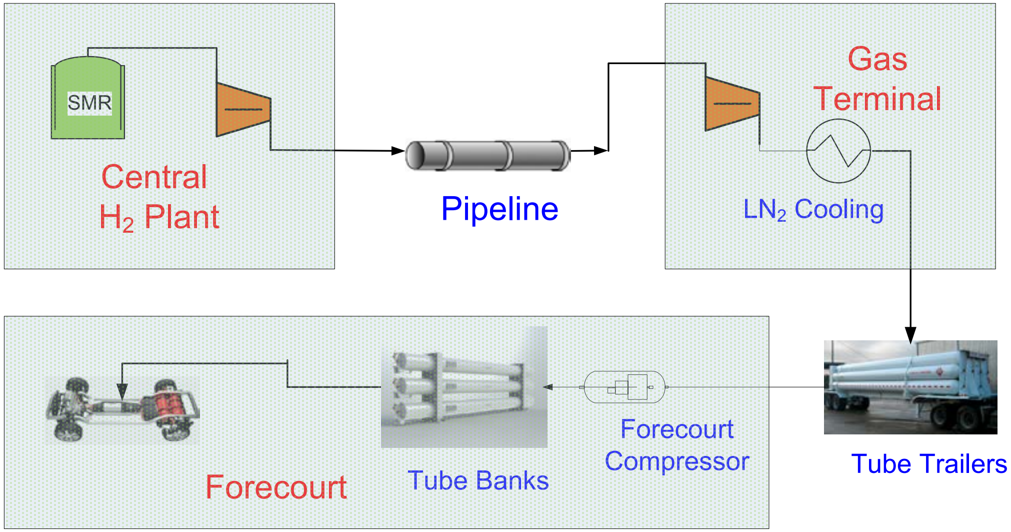
σ_{max} = 15 - 26 MPa (9 stress levels)
R=0, Frequency = 2 Hz

Ref. 2:

σ_{max} = 11 - 22 MPa (6 stress levels)
R=0.1, Frequency = 5 Hz

Ref. 1: A. Djebli et. al., Engineering, Technology & Applied Science Research, Vol. 4, No. 2, 2014, 600-604
Ref. 2: Rabia Khelif (Meccanica (2008) 43: 567–576)

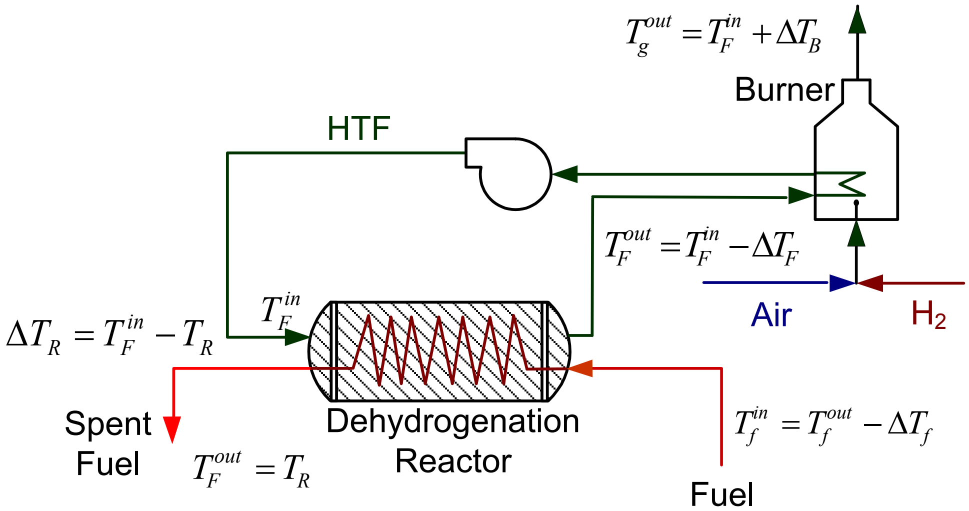
Off-board H_2 Cold Gas Delivery Analysis



- H_2 produced by SMR, transmitted via pipeline to gas terminal at city gate
- Compressed to 340 bar at gas terminal, cooled nominally to 90 K* using LN_2 and transported to forecourt by insulated Type 3 tube trailers
  - LN_2 production plant co-locates with gas terminal
- Compressed to 1.35X nominal storage pressure and stored in insulated Type 3 tube banks at forecourt
- HDSAM (2020 delivery scenario) analysis
  - Sacramento, 15% FCEV share, 115 stations, 1000 kg-H_2/day/station

*83 K actual temperature to account for heat gain in off-board storage tanks

System with Burner: Operating Temperatures and Efficiencies



Operating Temperatures

- T_R: Reactor temperature ($T_R = T_{f,out}$)
- ΔT_f: Fuel temperature rise ($\Delta T_f = T_{f,out} - T_{f,in}$)
- ΔT_F: Drop in HTF temperature across the reactor ($\Delta T_F = T_{F,in} - T_{F,out}$)
- ΔT_R: Reactor approach temperature ($\Delta T_R = T_{F,in} - T_{f,out}$)
- ΔT_B: Burner approach temperature ($\Delta T_B = T_{g,out} - T_{F,in}$)

Efficiencies

- η_R: Reactor efficiency, 1 - (Q_R / LHV of H_2 released)
- η_B: Burner efficiency
- η_d: Drive cycle efficiency
- η_{su}: Start-up efficiency
- η_s: Storage system efficiency

Q_R: **Reactor heat load**

Additional Material Targets

- Fuel should remain liquid and be pumpable over the range of operating temperatures (-40°C to T_{FC}).
- No solid phases should form as the fuel is decomposed.
- No gaseous products of decomposition other than H_2.

	Parameter	Reference Value	Comments
Physical Properties	Freezing Point	Below -40°C	
	Boiling Point	Above 120°C	Vapor pressure should be <1 mPa at 95°C
	Viscosity	TBD	Fuel pumpable to 100 bar at -40°C
Stability	Shelf Life	TBD	
	Toxicity and Safety	Non toxic	Compliant with applicable ES&H standrads
	H_2 Purity		SAE J2719 and ISO/PDTS 14687-2 specifications
Material Compatibity			Be compatible with materials rotinely used in automtive fuel systems
Off-Board Regenerability	WTT Efficiency	60%	Practcal industrial methods for regeneration
	Cycle Life	TBD	
	Cost	TBD	As per DOE targets