Hydrogen Storage Engineering
CENTER OF EXCELLENCE

Systems Engineering of Chemical Hydride, Pressure Vessel, and Balance of Plant for On-Board Hydrogen Storage

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DOE Fuel Cell Technology Program
Annual Merit Review

June 8, 2010
Technology Development Manager: Monterey Gardiner

DOE Hydrogen Program

U.S. Department of Energy
Energy Efficiency and Renewable Energy
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Project ID: ST005

Overview

- Timeline
  - Start: Feb. 2009
  - Project End: Jan. 2014
    - End Phase 1: 2011
    - End Phase 2: 2013
    - End Phase 3: 2014
- Budget
  - $6.2M Total (PNNL) anticipated
    - DOE direct funded
    - No cost-share required for National Lab
  - FY09: $600k
  - FY10: $1.5M
- Barriers
  - A. System Weight and Volume
  - B. System Cost
  - C. Efficiency
  - D. Durability
  - E. Charging/Discharging Rates
  - G. Materials of Construction
  - H. Balance of Plant (BOP) Components
  - J. Thermal Management
  - O. Hydrogen Boil-Off
  - S. By-Product/Spent Material Removal
- Partners

SRNL Savannah River National Laboratory
GM
Los Alamos National Laboratory
NREL National Renewable Energy Laboratory — Innovation for Our Energy Future
California Institute of Technology 1891
HRI UQTR
JPL
BASF The Chemical Company
Ford
Michigan
OSU Oregon State University
Lincoln Composites — A Member of Hexagon Composites Group
HSM Systems
Pacific Northwest National Laboratory
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Introduction: PNNL Scope in HSECoE

- Roles Supporting Engineering Center Structure
  - Technology Area Lead (TAL) for Materials Operating Requirements
  - Coordinate activities as the Technology Team Lead (TTL)
    - Bulk Materials Handling (Transport Phenomena)
    - Pressure Vessels (Enabling Technologies)
    - Manufacturing and Cost Analysis (Performance Analysis)
  - Liaison to VT Program projects and resources
- Technology Development and System Engineering Tasks
  - Solid Chemical Hydride System Design
  - Process Modeling & Engineering
  - Kinetics & Materials Characterization
  - Microarchitectures Device Development
  - Materials Reactivity & Compatibility
  - Containment and Pressure Vessel Design
  - Manufacturing & Cost Analysis

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Relevance: Hydrogen Storage

- Impact to FCT Program
  - Demonstrate high level of performance that meets DOE 2015 targets using solid chemical hydrogen storage
  - Apply materials discoveries and knowledge developed as part of the Materials Centers of Excellence
- Hydrogen Storage Community at Large
  - Develop and/or advanced modeling and simulation tools for the optimum design and engineering of on-board storage systems
  - Functional prototype systems available to OEMs
  - Engineering methodologies, analysis tools, and designs applicable to stationary storage and portable power applications
  - U.S. demonstration of on-board storage to advance state of the art globally

Approach: Objectives and Deliverables

- Technical Objectives of PNNL Scope
  - Design of chemical hydride hydrogen storage system & balance of plant (BoP) components
  - Reduce system volume and weight and optimize storage capability, fueling, and hydrogen supply performance
  - Mitigate materials incompatibility issues associated with hydrogen embrittlement, corrosion, and permeability
  - Demonstrate the performance of economical, compact, lightweight vessels for hybridized storage
  - Guide design and technology down selection through cost modeling and manufacturing analysis
- Program and annual Deliverables established
- Phased/gated progressions aligning with HSECoE go/no-go decisions

Focus is on Process Engineering, System Design and Functional Integration

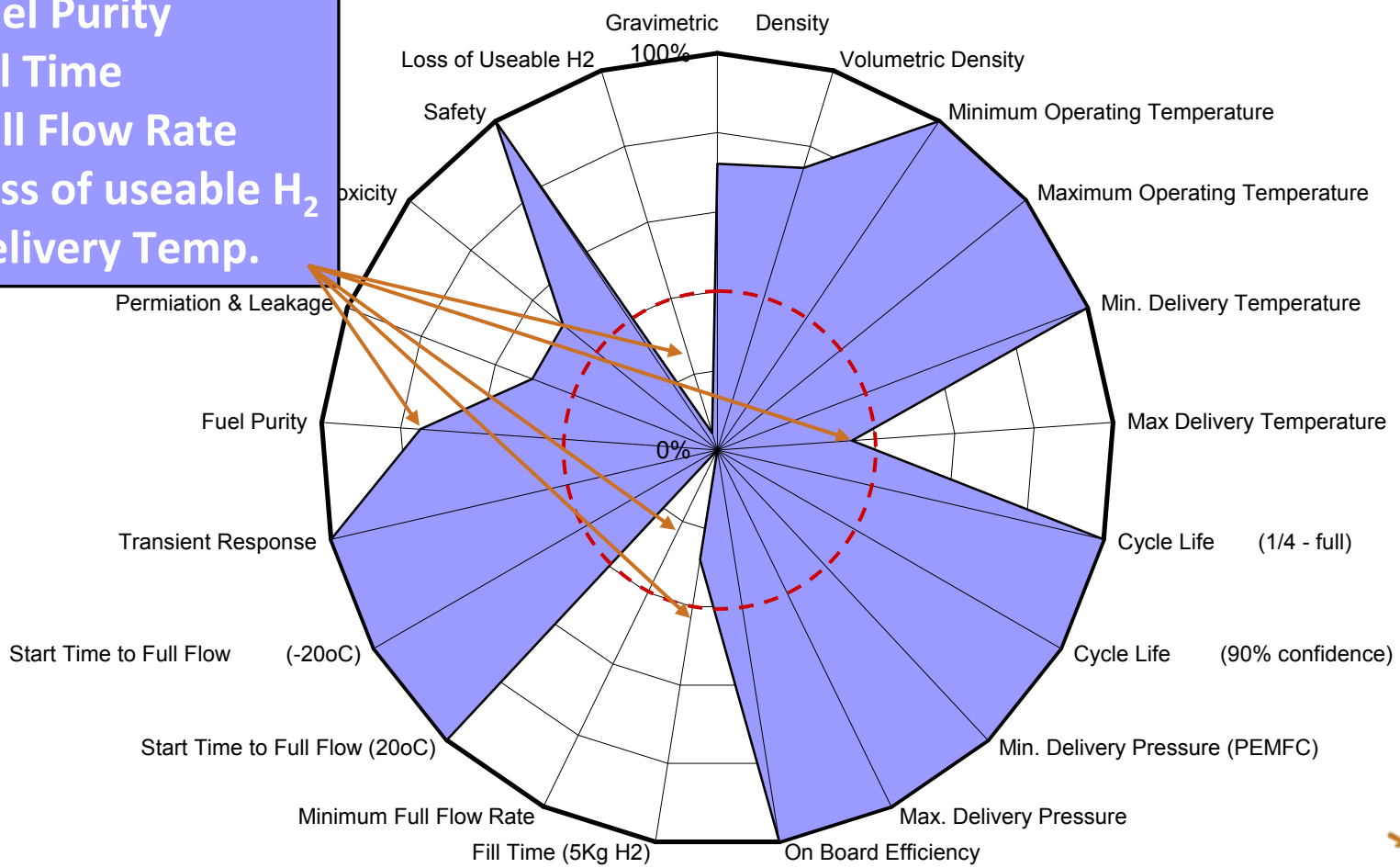
Accomplishment: Milestones FY10

Q1	Task 7	**Provide Rev.0 cost model, structure details and spreadsheet to Center partners for their evaluation.**
Q2	Task 1	**Complete preliminary design for fuel element transfer system (solids handling coupled to reactor).**
Q2	Task 2	**Complete COMSOL modeling of configurations**
Q2	Task 2	**Down select systems to be modeled for transient response**
Q3	Task 3	**Complete test station for monolithic fuel element and hydrogen release measurement**
Q3	Task 1	**Determine functional criteria and design rules based on modeling performance predictions and hydride system needs.**
Q3	Task 2	**Complete a conceptual design for a solid chemical hydride reactor that will provide input to the HSECoE's Phase 1 Go/No-go decision making process, and insight into the ability of such a system to meet the 2015 volumetric capacity target of 1.5 kWh/L.**
Q3	Task 3	**Determine bulk kinetics measurements and impact on performance.**
Q3	Task 6	**Complete modeling and establish pressure vessel design rules for use with prototypes.**
Q4	Task 4	**Complete assessment on the probability of integrating a heat exchanger within storage vessel.**
Q4	Task 5	**Complete identification of known materials compatibility issues and establish corrective action plan for component designs.**

Chemical Hydride System Status
Solid Ammonia-Borane: 2010 Targets

- 17 Targets Above 40%
- 4 Targets Undetermined or Below 40% Minimum

1. Fuel Purity
2. Fill Time
3. Full Flow Rate
4. Loss of useable H_2
5. Delivery Temp.



Source: Anton 2010 HSECoE program AMR

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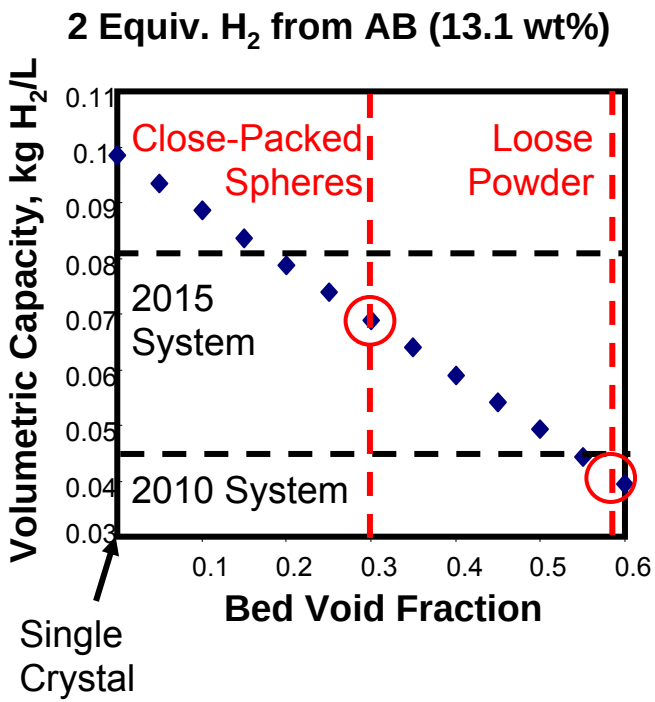
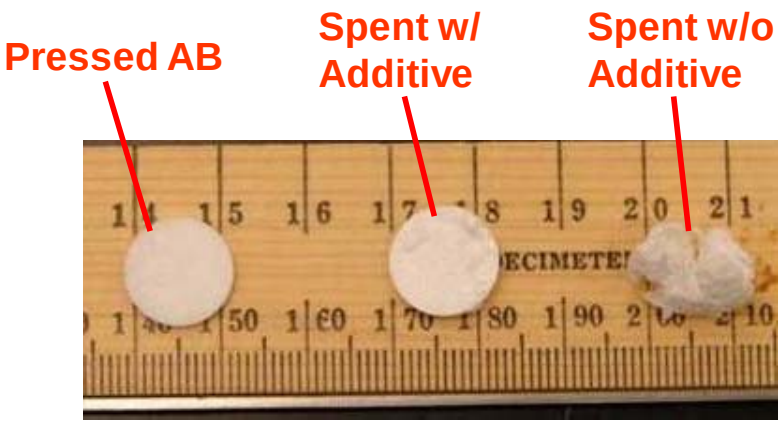
Primary Engineering Barriers for Chemical Hydride Systems

- Chemical Hydrides are not ‘reacted’ in the fuel tank
  - Solids handling engineering key part of any system concept
  - Exothermic reaction of most systems requires different thermal management solutions compared to MH or absorbents
  - AB thermolysis at <100°C; long term storage in hot climates?
- DOE Technical Targets:
  - BoP components and will add to
  - Performance impact of impurities needs a solution
  - Loss of Useable Hydrogen (g/hr)/kg H2 stored: 0.1 (2010) & 0.05 (2015); loss includes venting, if required
- Re-fueling vehicle logistics can be a challenge
- Ammonia Borane foams on reaction – potential limitation to practical engineering application

Engineered Form-Factor for Solid AB





- System targets are difficult for granulated materials
- AB foams when it releases hydrogen – not conducive to engineering
- Antifoaming approaches key
  - More than 50 additive formulations tested with 2-3 successful (CHCoE study)
  - Scaffold materials also demonstrate foam suppression at lower AB:scaffold loadings
  - Paves way for system with monolithic fuel & high volumetric density

Additive suppresses foaming and enables monolithic fuels

Source: PNNL CHCoE

Integrated System Design and Process Modeling for Solid Ammonia Borane

System Modeling Approach

- Ballast Tank
  - Provides H2 for start-up and transients
- No Heat Addition
  - Exothermic reaction heat warms incoming AB
- Issues/Assumptions
  - High heat transfer required between oil and AB in augers (heat/cool)
  - Extrapolation of kinetic data at 160°C to > 500°C
  - Modeling counterflow in Simulink
  - High Pressures in Ballast Tank—need for carbon fiber tank
  - No reaction in heated auger
  - Sticky AB during phase change
  - Impurity Borazine

BoP Equipment Equations/Assumptions

- Heated Auger
  - Psuedo Counterflow (co-flow section configured in counterflow)
  - Transient (includes metal thermal mass)
  - Assumes HT Oil → Metal → AB, No axial conduction
- Cooled Auger
  - Counterflow Heat Exchanger
  - Steady State (NTU-Effectiveness Method)
- Burner
  - Co-Flow
  - Transient (includes metal thermal mass)
  - Assumes HT Gas → Metal → Oil, No axial conduction
- Radiator
  - Cross Flow Heat Exchanger

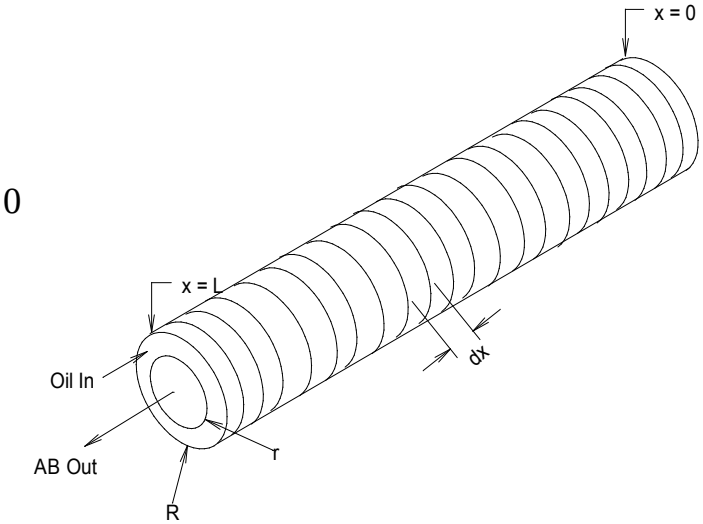
Example Simulink Component Modeling

Oil Energy Equation

$$\pi\left(R_{in}^{\ 2} - r_{out}^{\ 2}\right)\rho_{oil} C_{p,oil}\left(\frac{\partial T_{oil}}{\partial t} + u_{oil}\frac{\partial T_{oil}}{\partial x}\right) + 2\pi r_{out} h_{oil-metal}\left(T_{oil} - T_{metal}\right) = 0$$

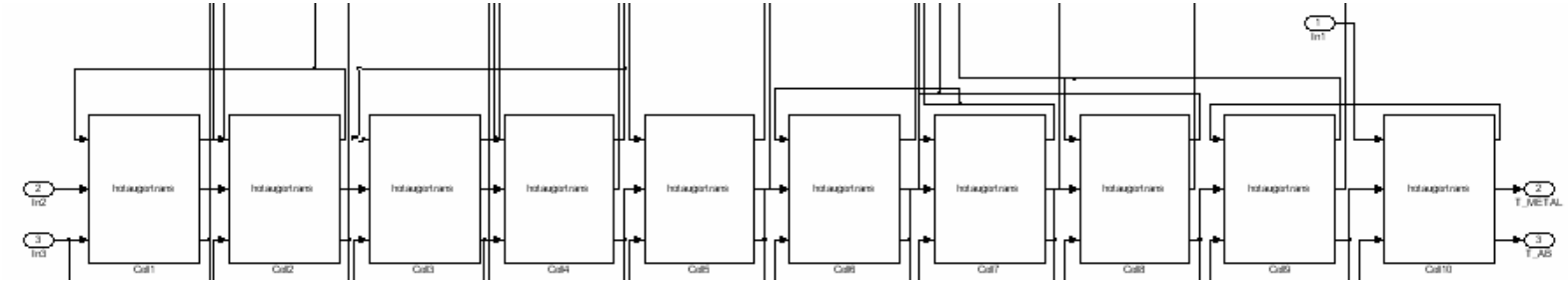
Metal Energy Equation

$$\pi\left(r_{out}^{\ 2} - r_{in}^{\ 2} + r_{auger}^{\ 2}\right)\rho_{metal} C_{p,metal}\left(\frac{\partial T_{metal}}{\partial t}\right) + 2\pi r_{out} h_{oil-metal}\left(T_{metal} - T_{oil}\right)$$
$$+ 2\pi(r_{in} + r_{auger})\varphi h_{metal-AB}\left(T_{metal} - T_{AB}\right) = 0$$



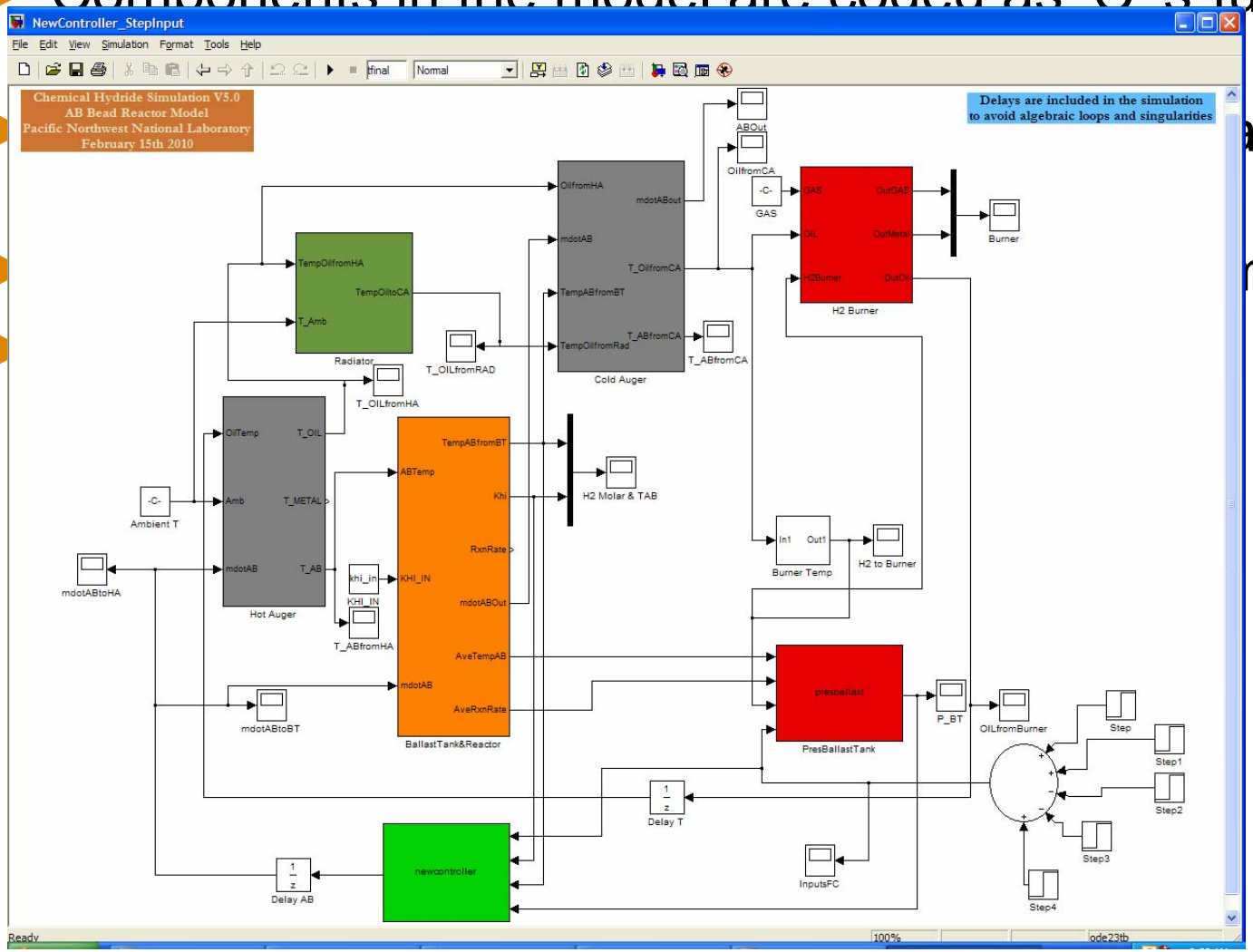
AB Energy Equation

$$\pi r_{in}^{\ 2}\rho_{bulk,AB} C_{p,AB}\left(\frac{\partial T_{AB}}{\partial t} + u_{AB}\frac{\partial T_{AB}}{\partial x}\right) + 2\pi r_{in}\varphi h_{metal-AB}\left(T_{AB} - T_{metal}\right) = 0$$



Integrated System Simulation

- Components in the model are coded as ‘C’ s-functions
- and ballast
- nent



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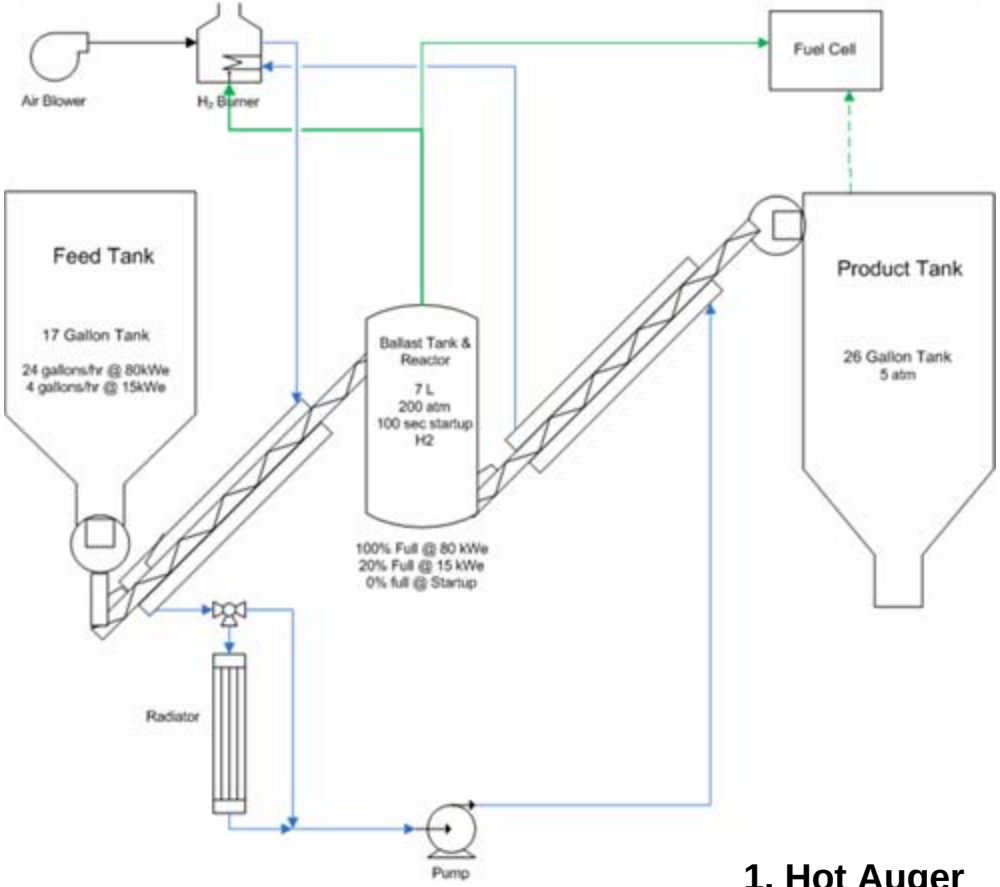
Baseline AB Bead Reactor System

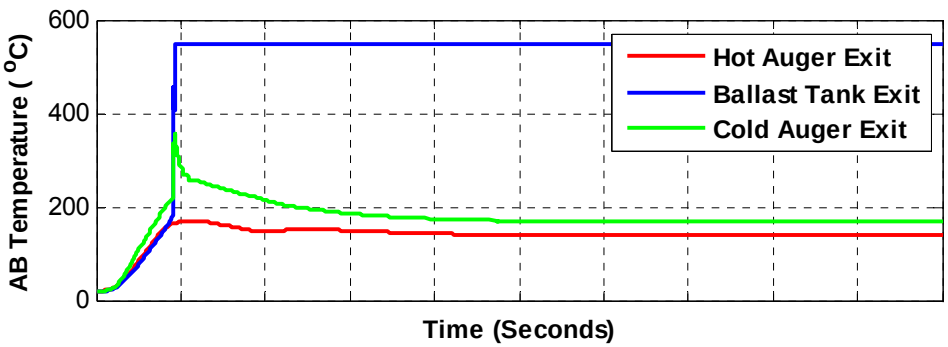


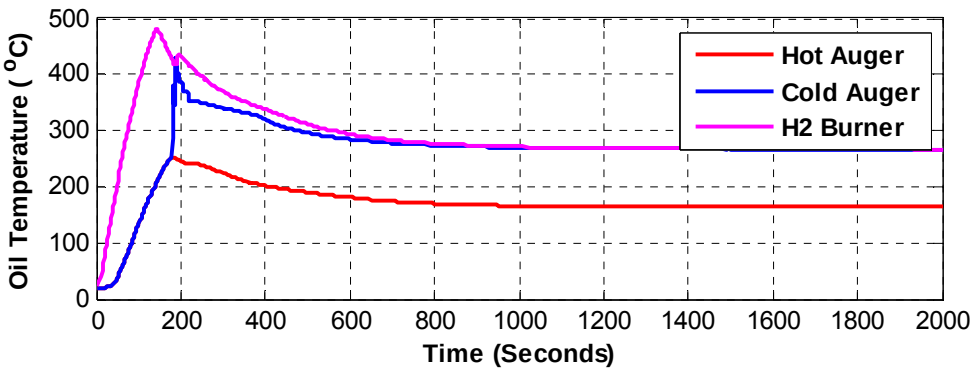
- Developing, refining system concepts
- Intrinsic kinetic models developed
- Developing reactor sub-models for use in system model
- Investigate auger / reactor heat transfer coefficients
- Determine "rheology", "stickiness" of reacting AB with and without additives (e.g., using DMA and/or rheometers)

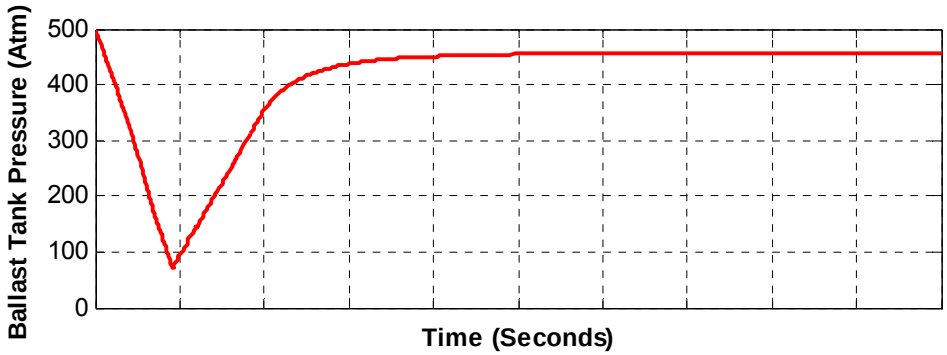
Main components in the reactor system:

1. **Hot Auger**
2. **Ballast Tank & Reactor**
3. **Cold Auger**
4. **Radiator**
5. **H_2 Burner**
6. **Control System**

Simulation Results: Start-Up from 20°C

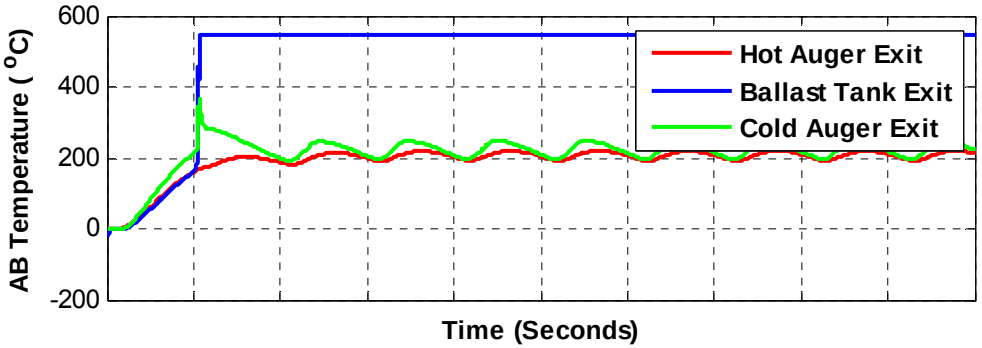


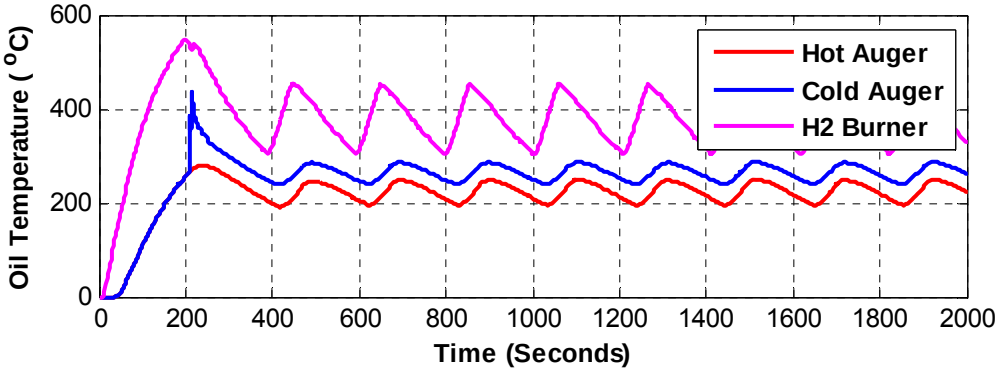


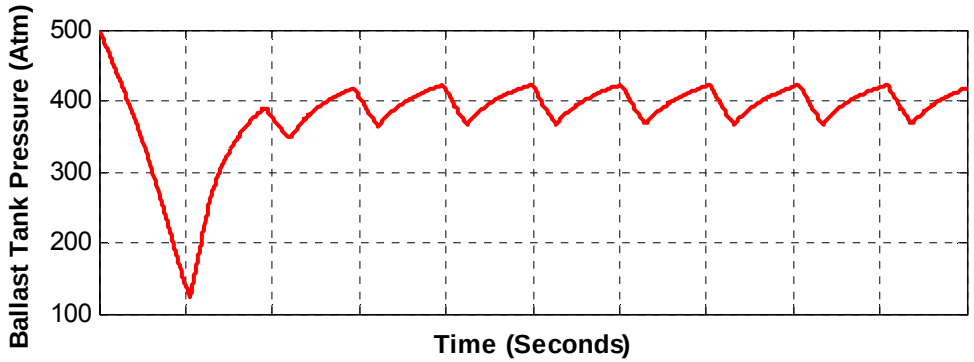


- Constant power 60 kWe
- AB begins to react at ~3 min
- Heat of reaction drives ballast tank reaction to maximum
- Reaction in ballast tank very small—will go away
- H_2 burner turns off at ~ 3 min
- Radiator not needed after hot auger, required for H_2 product
- Ballast Tank pressure drops to below 100 atm but rises again to 450 atm set point

Simulation Results: Start-Up from -20°C (cold)

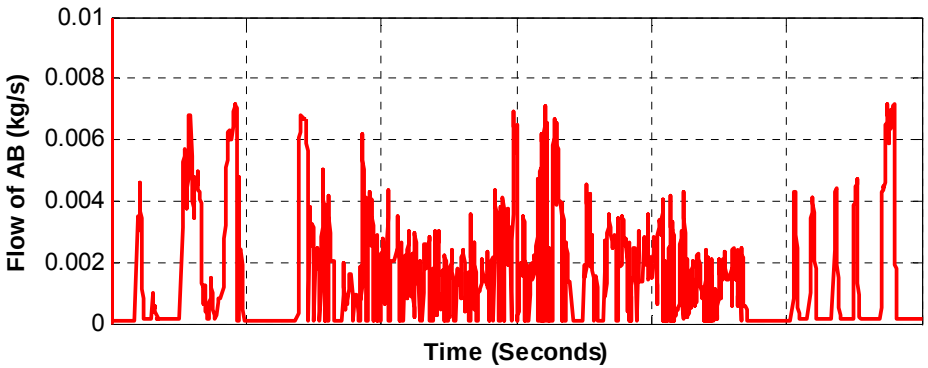


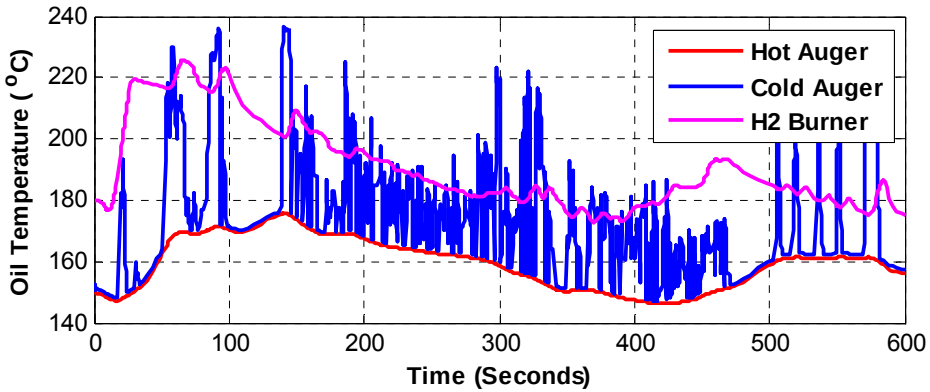


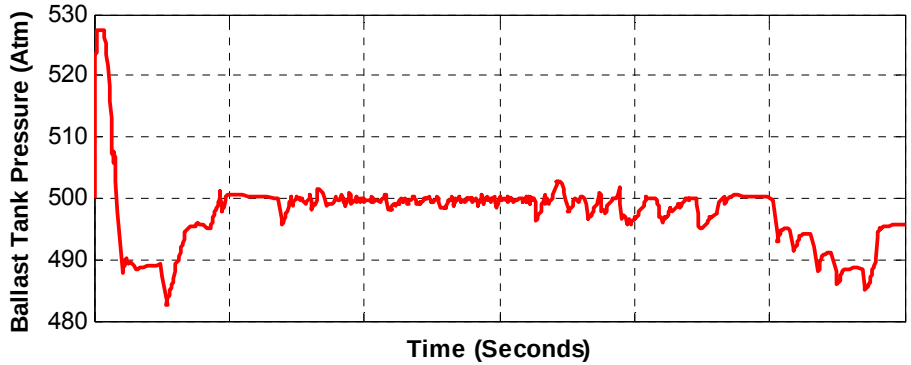


- Constant power 40 kWe
- AB begins to react at ~3.5 min
- Cold AB forces burner on after initial start-up
- Instability needs to be investigated
- Ballast Tank pressure drops to 100 atm but rises again to near 450 atm set point

Simulation Results: Drive Cycle after Warm-Up







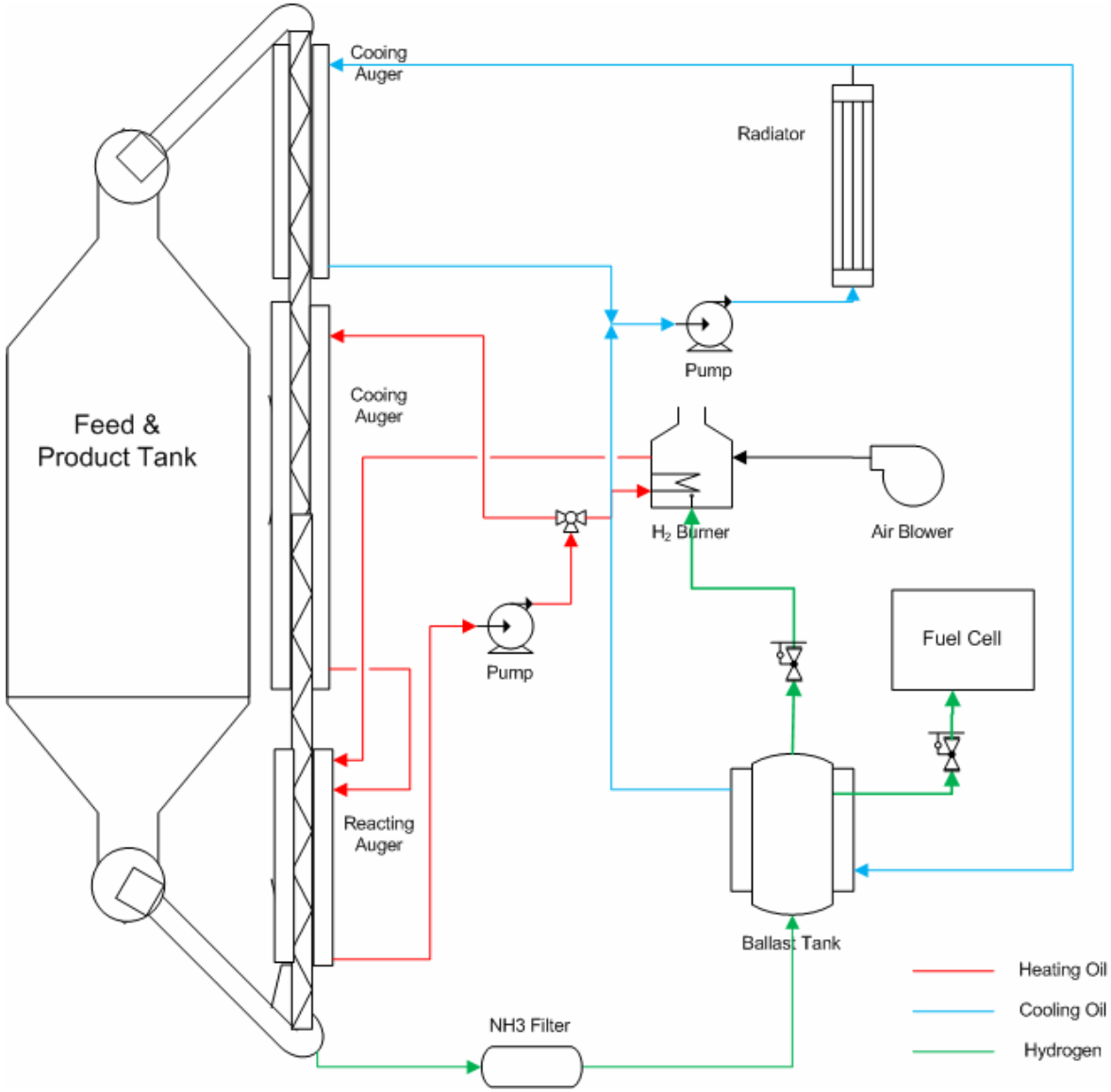
- US06 Drive Cycle with 0% Hybridization
- Pressure in Ballast Tank maintained ~ 500 atm
- Heated auger slowly cools at low flows
- H_2 burner turned on intermittently between 380 and 450 sec

System Weight and Volume Estimate

- Target: Total Mass 111 kg and Total Volume 178 liters

Component	Weight		Volume	
AB Storage	30.8	kg	0	L
Feed/Product Tanks	14	kg	140	L
Ballast Tank (carbon fiber)	29.7	kg	9	L
Hot Auger (steel)	10.8	kg	3.2	L
Cold Auger (steel)	20.2	kg	6.3	L
Burner/Blower	6.3	kg	5.7	L
Radiator	1	kg	1.8	L
NH_3 Filter	2.2	kg	2.7	L
Oil Piping/Pump/Tank	4.7	kg	3.5	L
Valves/Actuators	5	kg	3.5	L
Total	125	kg	176	L

Better Engineered Solution



- To address weight/volume constraints, a new design of the bead reactor is proposed
- Kinetics in the augers rather than ballast tank
- Combined Feed and Product Tank
- Better thermal control through multiple heat exchanger loops and through control logic.
- Hot hydrogen heats incoming AB feed

Materials Characterization

Accomplishments

- Materials Centers of Excellence recommended top storage materials
  - Based on multiple criteria
  - Available data and access to materials
- Materials properties of 12 materials posted on HSECoE Share point: MOR/Shared documents/Materials data base
  - Identified materials properties needed for modeling
  - Populated with literature and partner known and validated property data and kinetics
  - Gap analysis completed and plan established to augment data
- Screening criteria/Questionnaire created
  - Material must pass this rough assessment to be further considered
  - Provided to organizations who have a material of interest

HSECoE Materials Categories

	Tier 1 Developed Materials	*Tier 2* Developing Materials	Down-selected Materials
Adsorbents	AX-21	Pt/AC-IRMOF 8	MOF 177
	MOF 5		
Chamical Hydrides	$NH_3BH_{3(s)}$	$NH_3BH_{3(l)}$	
	AlH_3	$LiAlH_4$	
Metal Hydrides	$NaAlH_4$	$Mg(NH_2)_2+MgH_2+2LiH$	MgH_2
	$2LiNH_2+MgH_2$	$TiCr(Mn)H_2$	Mg_2NiH_4

- Developed Materials: System analysis is being performed on up-selected candidates and necessary engineering properties measured
- Developing Materials: Up-selected materials under performance evaluation and materials properties collected and measured if necessary
- Down-selected materials: Materials found to not improve system performance relative to up-selected materials, and thus not for further consideration

Storage Material Screening Criteria

Metal Hydrides

- Chemical formula and reversible reaction formula
- Capacity (wt% H_2 and kg H_2/L) as measured at what pressure (bar) and temperature (°C)
- Absorption: give tempe
- Desorption: give tempe
- Enthalpy, ΔH (J/mol): fo
- Crystal density (g/cm^3)
- Cost raw material + add
- Availability (g)

Chemical Hydrides

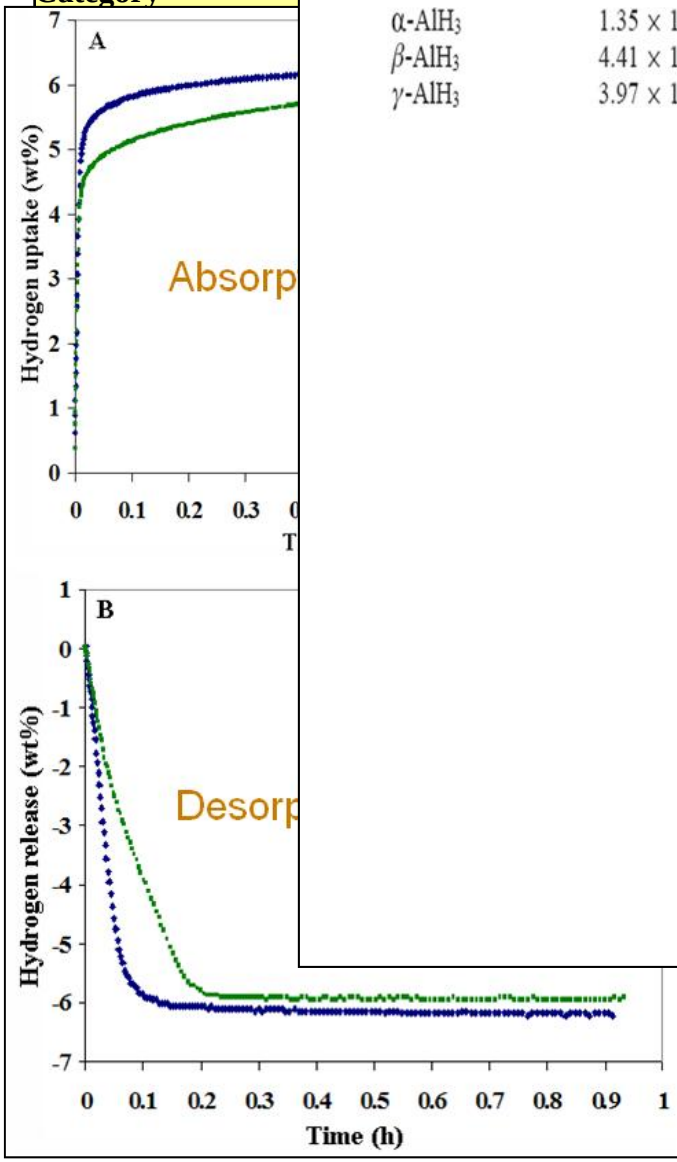
- Chemical formula and decomposition reaction formula
- Capacity (wt% H_2 and kg H_2/L) as measured at what temperature (°C)
- Desorption: give temperature (°C)
- Enthalpy of formation (J/mol)
- Crystal density (g/cm^3)
- Cost for raw material (precursor) (
- Availability (g)

Adsorbents

- Material and Synthetic Process
- Capacity as independently validated maximum Gibbs excess capacity (wt% H_2 and kgH_2/L) as measured at what pressure (bar) and temperature (°C). Provide isotherms at RT and 77K.
- Desorption: give temperature (°C) and rate (g H_2/s) to reach max desorption capacity
- Hydrogen uptake: give temperature (°C), pressure (bar) and rate (g H_2/s) to reach max adsorption capacity
- BET Specific surface area (m^2/g) and pore size distribution and/or bulk density (g/cm^3)
- Cost for raw material (precursor) and estimate for processing ($/g)
- Availability (g)

Exam

Category



J. Graetz, et al. J. Phys. Chem. B (2005) 109, 22181-22185

TABLE 1: Isothermal Decomposition Rate Constants (s^{-1}) for α-, β-, and γ-AlH_3[a]

polymorph	k(60 °C)	k(80 °C)	k(99 °C)	k(120 °C)	k(138 °C)
α-AlH_3	1.35×10^{-6}	9.14×10^{-6}	4.21×10^{-5}	2.80×10^{-4}	1.39×10^{-3}
β-AlH_3	4.41×10^{-6}	1.36×10^{-5}	5.99×10^{-5}	4.88×10^{-4}	2.46×10^{-3}
γ-AlH_3	3.97×10^{-6}	1.18×10^{-5}	3.94×10^{-5}	2.71×10^{-4}	7.98×10^{-4}

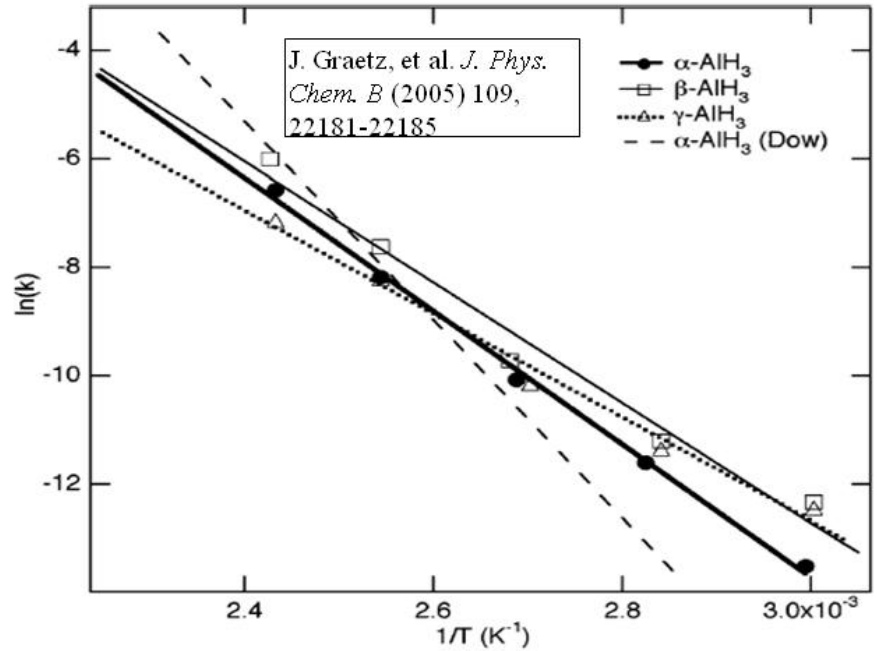


Figure 6. Arrhenius plot for large crystallites of α-AlH_3 (Dow)[4] and small crystallites of α-AlH_3, β-AlH_3, and γ-AlH_3. Reaction rates for the large crystallites of α-AlH_3 were measured at 135 °C ≤ T ≤ 160 °C and are extrapolated down to $T \sim 60$ °C.

Summary & Proposed Future Work

Collaborative Activities

Hydrogen Storage Engineering Center of Excellence	• Lincoln Composites - study of CF cost and pressure vessel design modeling • GM - design of structured media bed for MH • Ford – characterization of absorbent materials • UQTR - design and materials characterization of carbon absorbent • OSU - microarchetecture device concept development and thermodynamic analysis • UTRC - develop solutions for H_2 impurities filtering • LANL - AB system design and measure H_2 impurities • NREL - input for tank to wheels analysis and system cost models • SRNL - study AB reactivity and kinetics model development
SAWGG	• Participate in group discussions and analysis
Materials 'Reactivity' Program	• Khalil (UTRC) and Anton (SRNL) - understand reactivity properties of AB • Van Hassel (UTRC) - study impurities in H_2
Independent Analysis	• TIAX - provide design details for AB refueling cost and feasibility assessment, plus share cost parameters for system cost modeling

Summary of Accomplishments

- A representative *systems model of a AB based bead reactor system was developed* and successfully simulated in Matlab/Simulink environment.
- A COMSOL *transport model was developed for a bead and a block system*. The heat and mass transfer model used a simple reaction rate expression: (1) Bead reaction can occur within the auger that has been designed assuming a 200°C wall. (2) Heating the outside surface of a block can light off the reaction for the entire block.
- An improved *kinetic model has been developed and implemented* into the system model.
- *Hydrogen loss and impurities assessed for solid AB* as material is moved into and out of the pressurized reaction system.

Summary of Accomplishments (con't)

- Materials properties database established for HSECoE partners
- Screening criteria/Questionnaire created
- Engineering cost model structure established
- Studies and analysis of pressure vessels performed:
  - Metal hydride hybrid
  - Vessel material of construction sensitivity analysis
  - Liner material assessment
- Materials compatibility and reactivity studies started

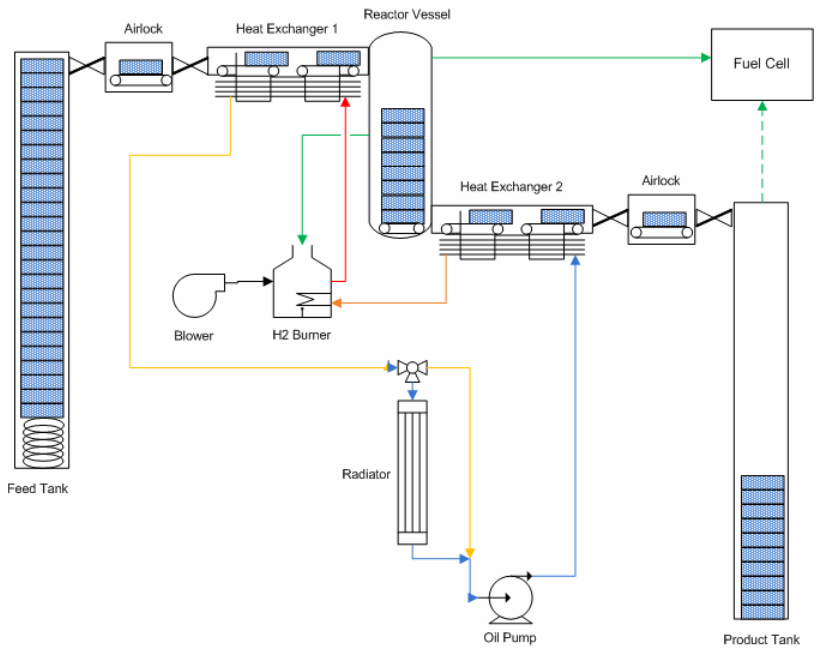
Future Work: Chemical Hydride System Design

- Future work includes implementation of the new bead reactor design in Matlab/Simulink and corresponding simulation analysis
  - Improve H2 Delivery Temperature
  - Increase Volumetric/Gravimetric Density
  - Include variable transport properties (ρ, Cp, k, zH2)
  - Address impurities and hydrogen losses in design
- Investigation of alternate materials for chemical hydride hydrogen storage.
- Implementation of the new kinetic model in Matlab/Simulink and corresponding simulation analysis
- Include temperature dependent transport properties into models as they become available. Modify kinetic model with higher temperature experimental data.

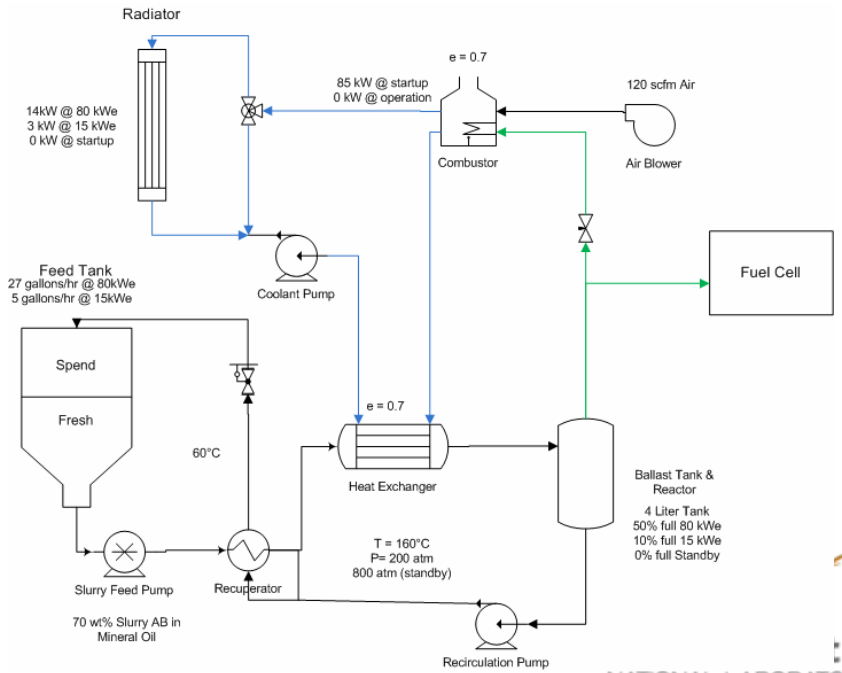
Future Systems to be Evaluated

- Materials to be Studied
  - Ammonia Borane ($NH_3BH_{3\,(s)}$) (Starting Material)
  - Alane (AlH_3)
  - Lithium Aluminum Hydride ($LiAlH_4$)
- Other System Configurations

Bulk Solids Configuration



Slurry Reactor Configuration



Future Work

- Complete system concept modeling efforts and provide initial component design for partner review
- Determine final reactor details and lock-in design
- Complete bulk kinetics modeling and validation studies
- Initiate heat exchanger modeling effort and provide initial component design for partner review
- Progression of cost model with system details and integrate component “catalog”
- Storage material bulk characterization

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Extra Details & Back-up Slides

Responses to Previous Year Reviewers' Comments

- FY2010 first full year for HSECoE activities
- 2010 is first AMR review – no previous reviewer comments

Publications and Presentations (FY2010)

Publications

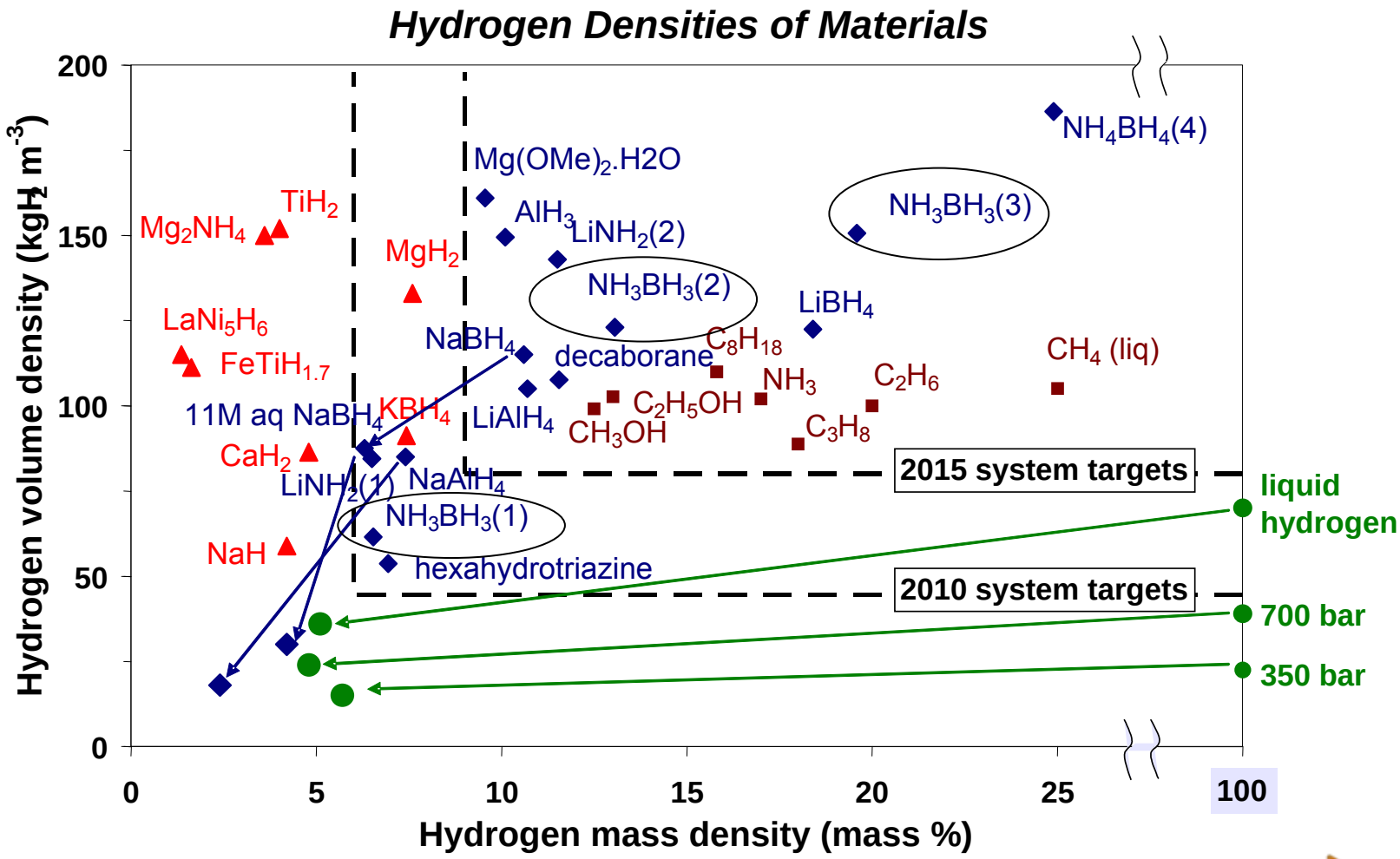
- Brooks KP, MN Devarakonda, SD Rassat, DA King, and DR Herling. 2010. "SYSTEMS MODELING OF AMMONIA BORANE BEAD REACTOR FOR OFF-BOARD REGENERABLE HYDROGEN STORAGE IN PEM FUEL CELL APPLICATIONS." In ASME 2010 Eighth International Fuel Cell Science, Engineering and Technology Conference.
- Brooks KP, MN Devarakonda, DA King, and DR Herling. 2010. "SYSTEMS MODELING OF AMMONIA BORANE BEAD REACTOR FOR OFF-BOARD REGENERABLE HYDROGEN STORAGE IN PEM FUEL CELL APPLICATIONS." Abstract submitted to ASME Fuel Cell Science, Engineering and Technology Conference, Brooklyn, NY.
- Holladay JD, KP Brooks, MN Devarakonda, SD Rassat, DA King, and DR Herling. 2010. "Ammonia Borane Bead Reactor System Model For Hydrogen Storage." Abstract submitted to 218th Meeting of The Electrochemical Soceity , Las Vegas, NV.

Presentations

- Ronnebro E. 2009. "Hydrogen storage materials properties for prototype system concepts." Abstract submitted to Materials Challenges in Alternative & Renewable Energy conference, Cocoa Beach, FL.
- Brooks KP, MN Devarakonda, and SD Rassat. 2010. "AB Systems Modeling for Off-Board Regenerable Hydrogen Storage Applications." Presented by Ewa Ronnebro (Invited Speaker) at Materials Challenges in Alternative & Renewable Energy 2010, Cocoa Beach, FL on February 23, 2010.

Background Information on Solid AB Thermal Stability

Ammonia Borane Shows Promise



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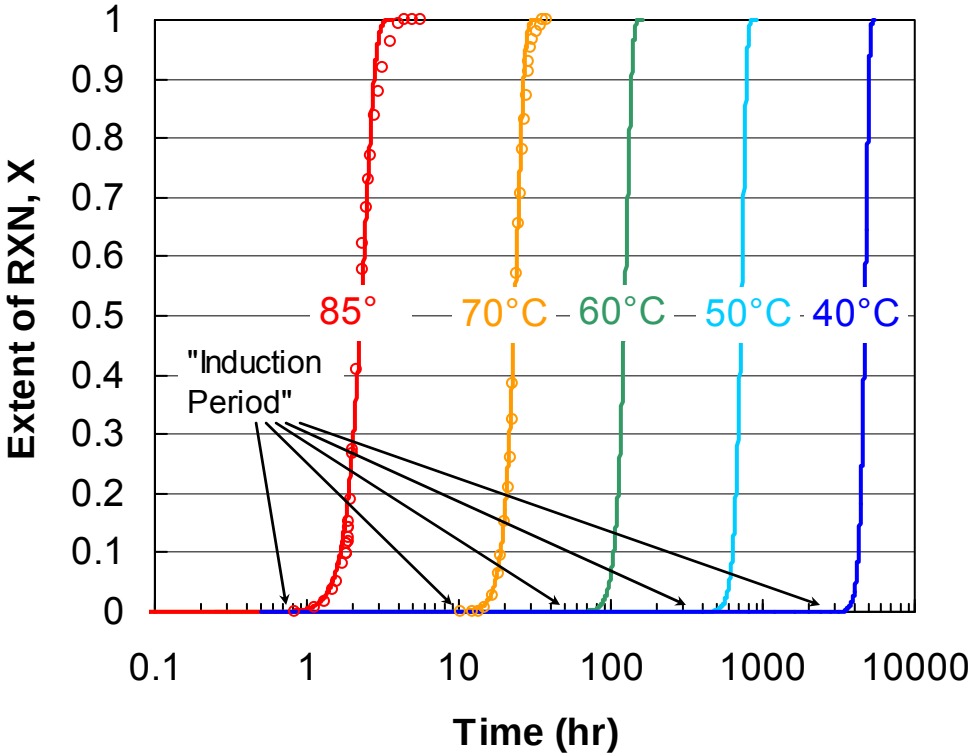
Courtesy of G. Thomas

AB Thermal Stability Calculations – Assumptions and Insight

- 1st equivalent only – Avrami kinetics
- 70-90 °C isothermal DSC data* used for initial fit of parameters
- Adiabatic assumed as a worst case
- Model AB bed properties
  - 1000 mol AB = 4 kg H_2 (2 H_2 equiv.)
  - 6.0 wt% H_2 in a storage unit including >50 wt% structure
  - No temperature gradients

Extrapolation of DSC Data to Lower Isothermal Temperatures



*Wolf et al., Thermochimica Acta 343, (2000) 19

Source: PNNL CHCoE

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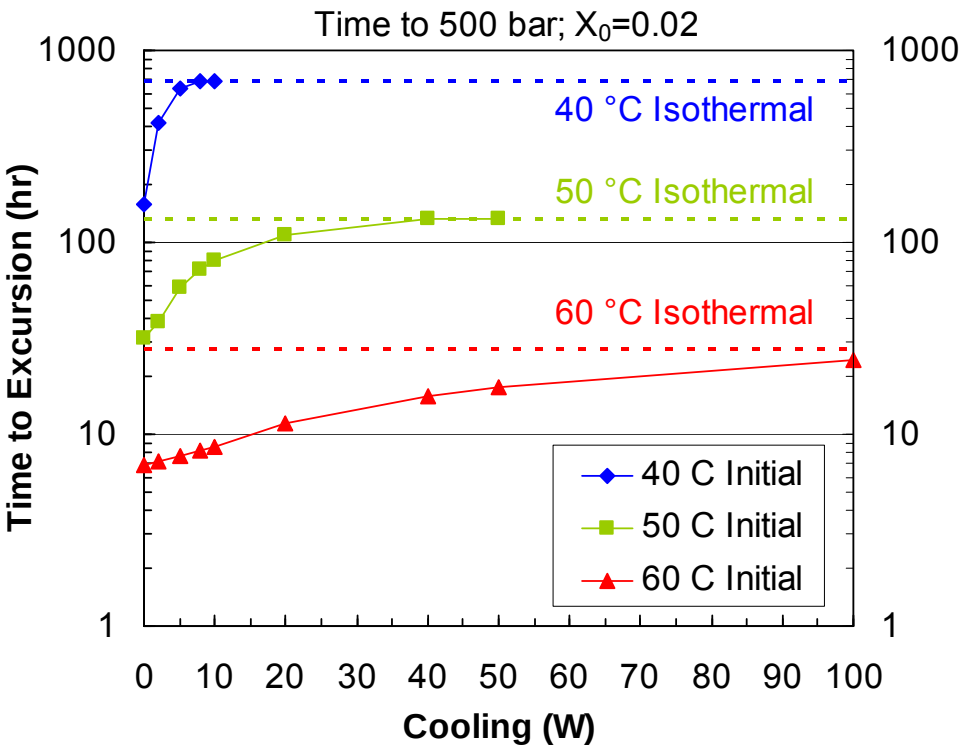
Heat Management to Stabilize Stored AB

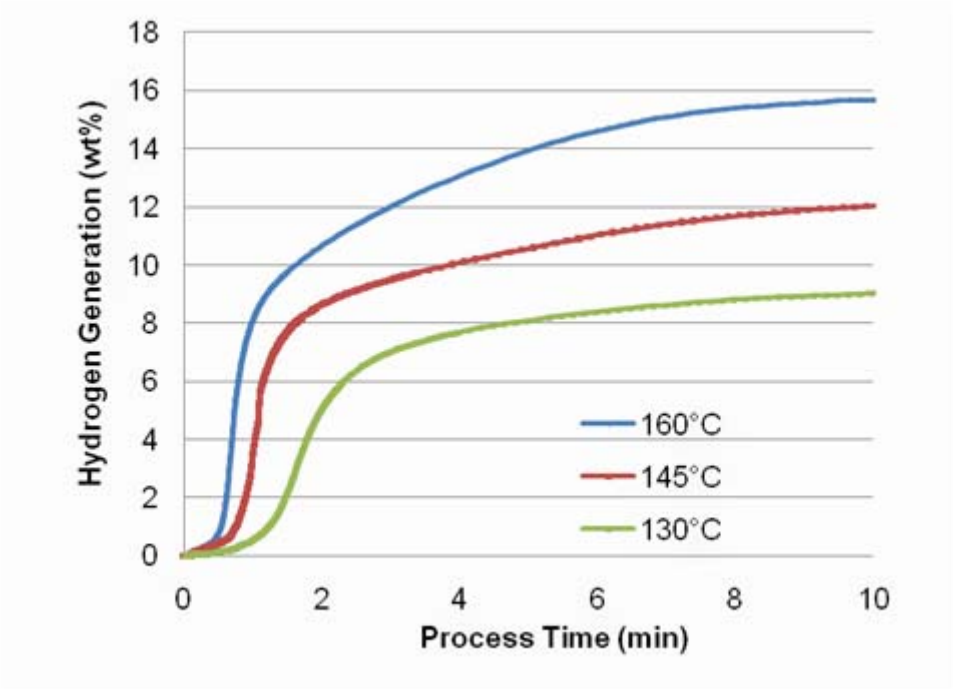


- Under adiabatic conditions, the AB bed temperature and reaction rate increases due to the heat evolved as H_2 is released (e.g., -22 kJ/mol)
- Small amounts of cooling and lower temperatures greatly increase the thermal stability of the packed AB bed (e.g., storage tank)
- Computationally, cooling was not allowed to decrease T below the initial value

Source: PNNL CHCoE

Solid CH Kinetics Model Development

Initial Kinetics Model



- $AB \rightarrow AB^* \leftrightarrow P + 3H_2$
- Rate Equations
  - $r_{AB} = -k_1 y_{AB}$
  - $r_{AB}^* = (k_1 y_{AB} - k_2(y_{AB}^* - K_{eq}(y_{AB,initial} - y_{AB} - y_{AB}^*))$
  - $r_{H2} = 3(k_2(y_{AB}^* - K_{eq}(y_{AB,initial} - y_{AB} - y_{AB}^*))$
    - where $k_1 = A_1 e^{-E1/RT}$ and $k_2 = A_2 e^{-E2/RT}$
- Species Equations

$$\frac{\partial y_{AB}}{\partial t} = r_{AB} - \frac{\dot{m}_{AB,out}}{\rho_b A}\frac{\partial y_{AB}}{\partial x}$$

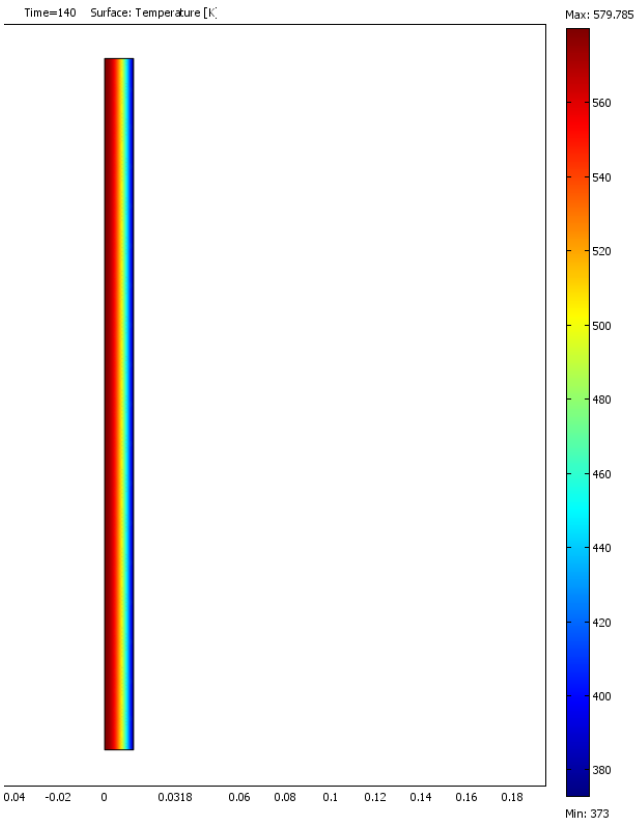
$$\frac{\partial y_{H_2}}{\partial t} = r_{H_2} + D_{H_2}\frac{\partial^2 y_{H_2}}{\partial^2 x}$$

- Heat Equation

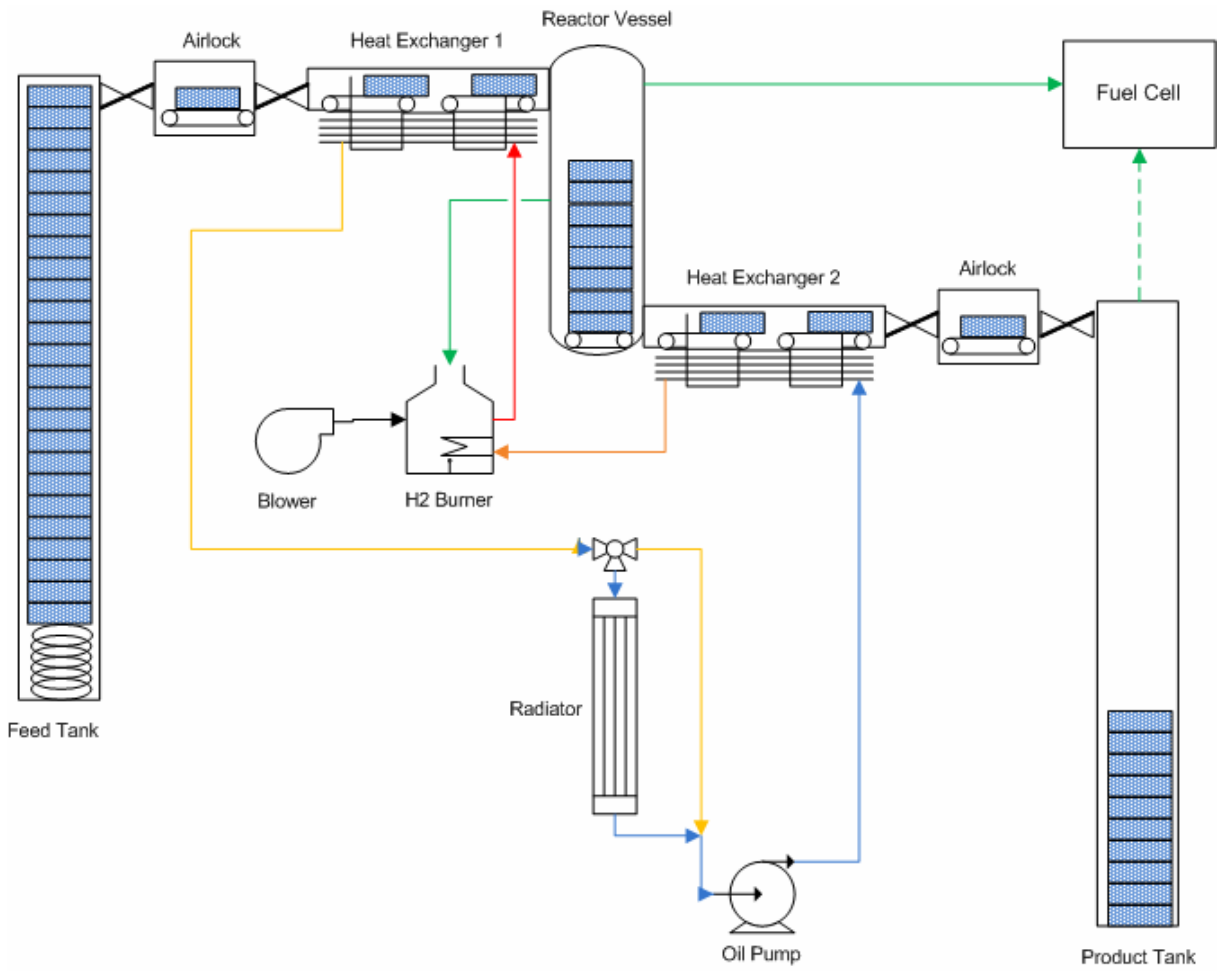
$$\rho_b C_p \frac{\partial T}{\partial t} = \Delta H_{rxn} r_{H_2} - \frac{C_p \dot{m}_{AB,out}}{A}\frac{\partial T}{\partial x}$$

Heat Transfer/Reaction in Packed Bed (Auger)

- Auger Properties
  - 1” Diameter, 5 ft long
  - Residence Time 36 sec @ 80 kWe
- Outer Surface Heating
  - 100°C → Reaction initiates at 130 sec, duration ~ 10 sec, T_{max} = 317°C
  - 200°C → Reaction initiates at 34 sec, duration ~ 10 sec, T_{max} = 570°C
- Lessons Learned
  - Auger length reasonable if 200°C oil temperature
  - Reaction very rapid and results in high temperature
  - Must not exceed ~ 700°C or boron nitiride is formed ($\Delta T_{adiabatic}$ = 482°C)



Solid “Block” of AB System Design Concept



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Heating Outside of AB Block

- 1-D model ½” thick AB (L,W >> ½”)
- Heat outer 0.04”, inner remains at 20°C
- Although bulk temperature is low, reaction initiates

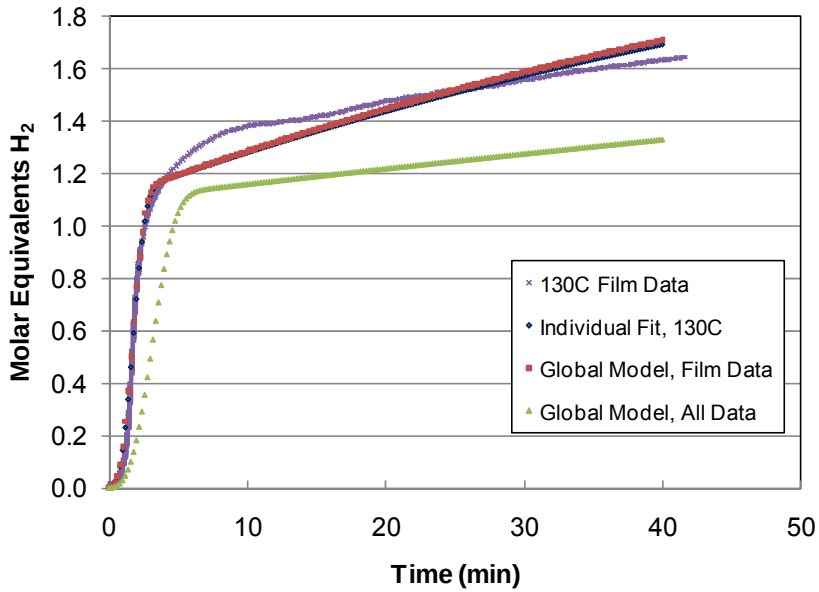
Heated Section Temp (°C)	Ave Bulk Temp (°C)	Reaction Time (s)
100	33	160
200	50	120
300	67	90

Improved AB Kinetic Model

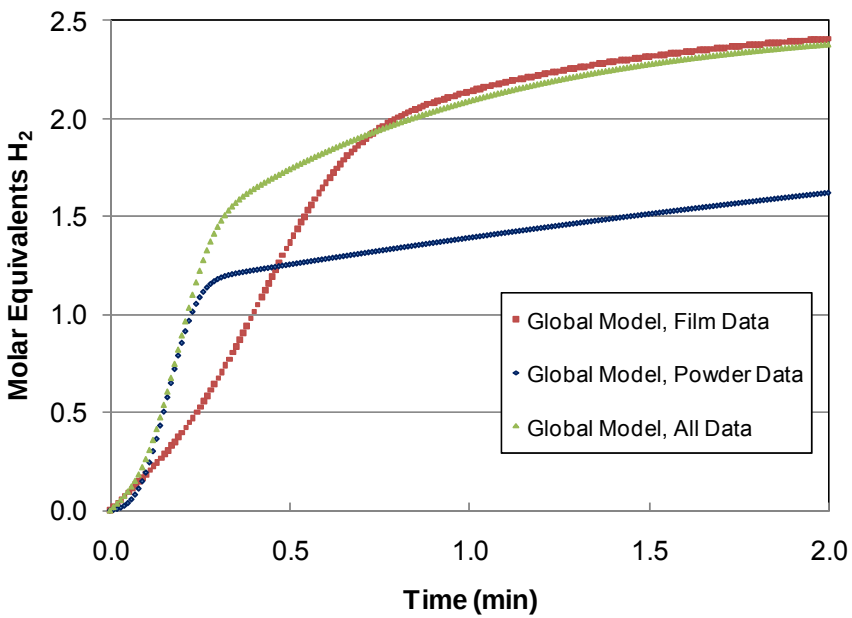
- Ammonia Borane reaction kinetics represented by Avrami kinetics:

$$\chi = 1 - \exp\left\{-\left[k(t-\tau)\right]^n\right\}$$

0 for $t \leq \zeta$



Predicted H_2 Release at 130°C



Predicted H_2 Release at 180°C

$$\chi_{tot} = 1.1\left\{1 - \exp\left[-(k_1 t)^3\right]\right\} + 1.4\left\{1 - \exp\left[-(k_2 t)\right]\right\}$$

Note: Experimental data maximum only 160°C

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Reaction Rate Calculation in Ballast Tank

- Approach
  - For a given conversion (χ) and temperature (T), obtain t* (psuedo-reaction time) from look-up table.

$$\chi_{tot} = 1.1\left\{1-\exp\left[-\left(k_1 t\right)^3\right]\right\} + 1.4\left\{1-\exp\left[-\left(k_2 t\right)\right]\right\}$$

  - Calculate the derivative of χ with respect to t* to obtain reaction rate for isothermal case.

$$\frac{d\chi}{dt^*} = R_{rxn} = 3.3 k_1^3 t^{*2} \exp\left[-\left(k_1 t^*\right)^3\right] + 1.4 k_2 \exp\left[-\left(k_2 t^*\right)\right]$$

  - Use R_{rxn} to calculate χ for new time and position step

$$\frac{\partial \chi}{\partial t} = -u_{AB}\frac{\partial \chi}{\partial x} + R_{rxn}$$

  - Calculate new temperature (T) from energy equation

$$\rho_{bulk,AB} C_{p,AB} \frac{\partial T_{AB}}{\partial t} = \frac{\Delta H_{rxn} R_{rxn} \rho_{bulk,AB}}{MW_{AB}} - \frac{C_{pAB}\dot{m}_{AB,in}}{A}\frac{\partial T_{AB}}{\partial x}$$

Hydrogen Loss and Purity Issues with AB

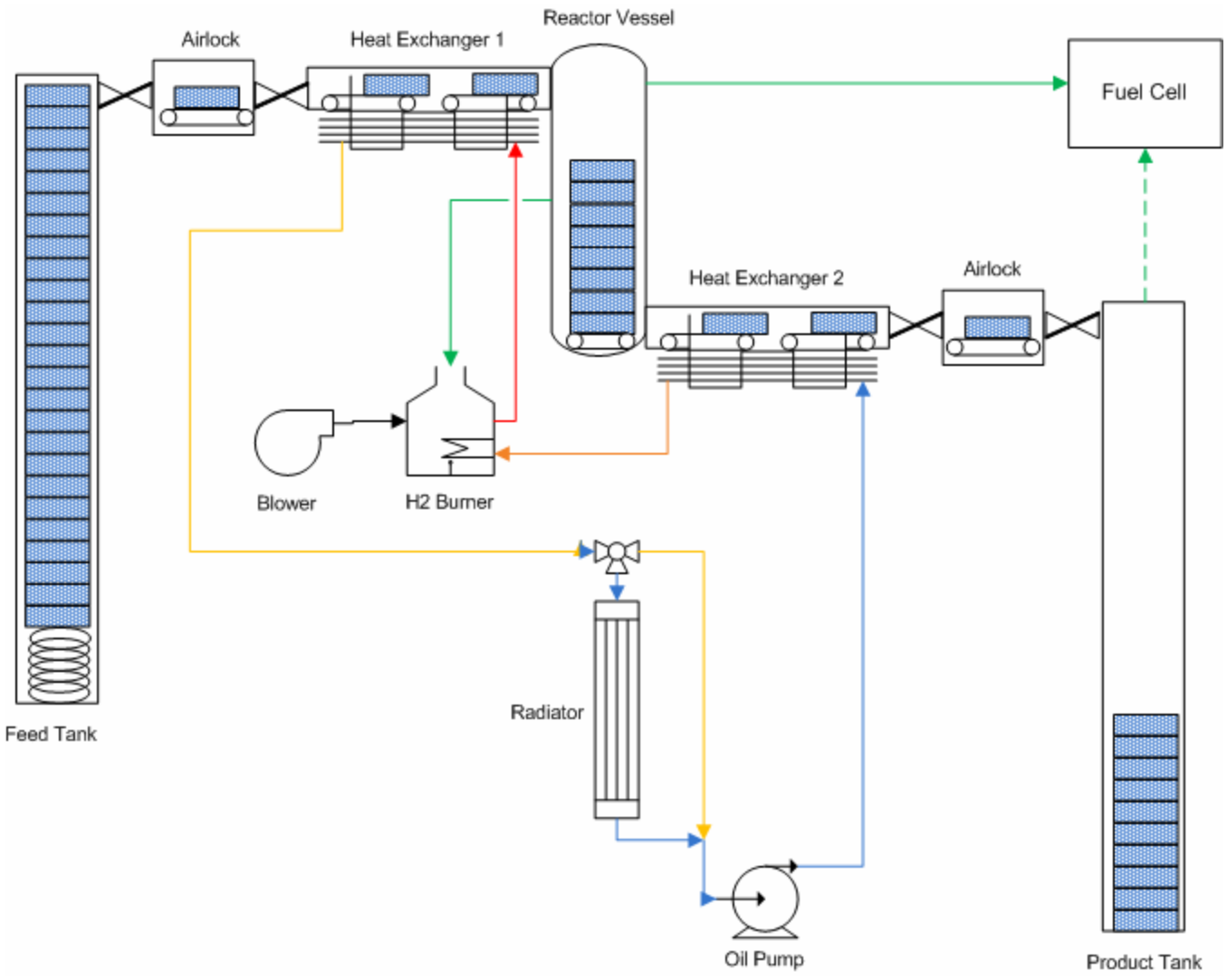
- Moving material between pressurized and unpressurized parts of the system
  - H_2 loss increases with system pressure
  - Air infiltration constant with gap size

System Pressure	Beads Random Packing		PEZ Block 1/8" Gap	
	H_2 Loss	Purity impact from Air	H_2 Loss	Purity
(atm)	($gH_2/hr*kgH_2$)	(%)	($gH_2/hr*kgH_2$)	(%)
5	0.9	99.93%	1.0	99.91%
10	1.7	99.93%	2.1	99.91%
50	8.7	99.93%	10.3	99.91%
100	17.4	99.93%	20.6	99.91%
500	86.9	99.93%	103.0	99.91%

(Assuming ideal gas law, 2.5 equivalents produced)
(Block is assumed to be 3" x 3" x 1/2" thick)

Approach to Solid CH System Modeling

Bulk Solids Reactor



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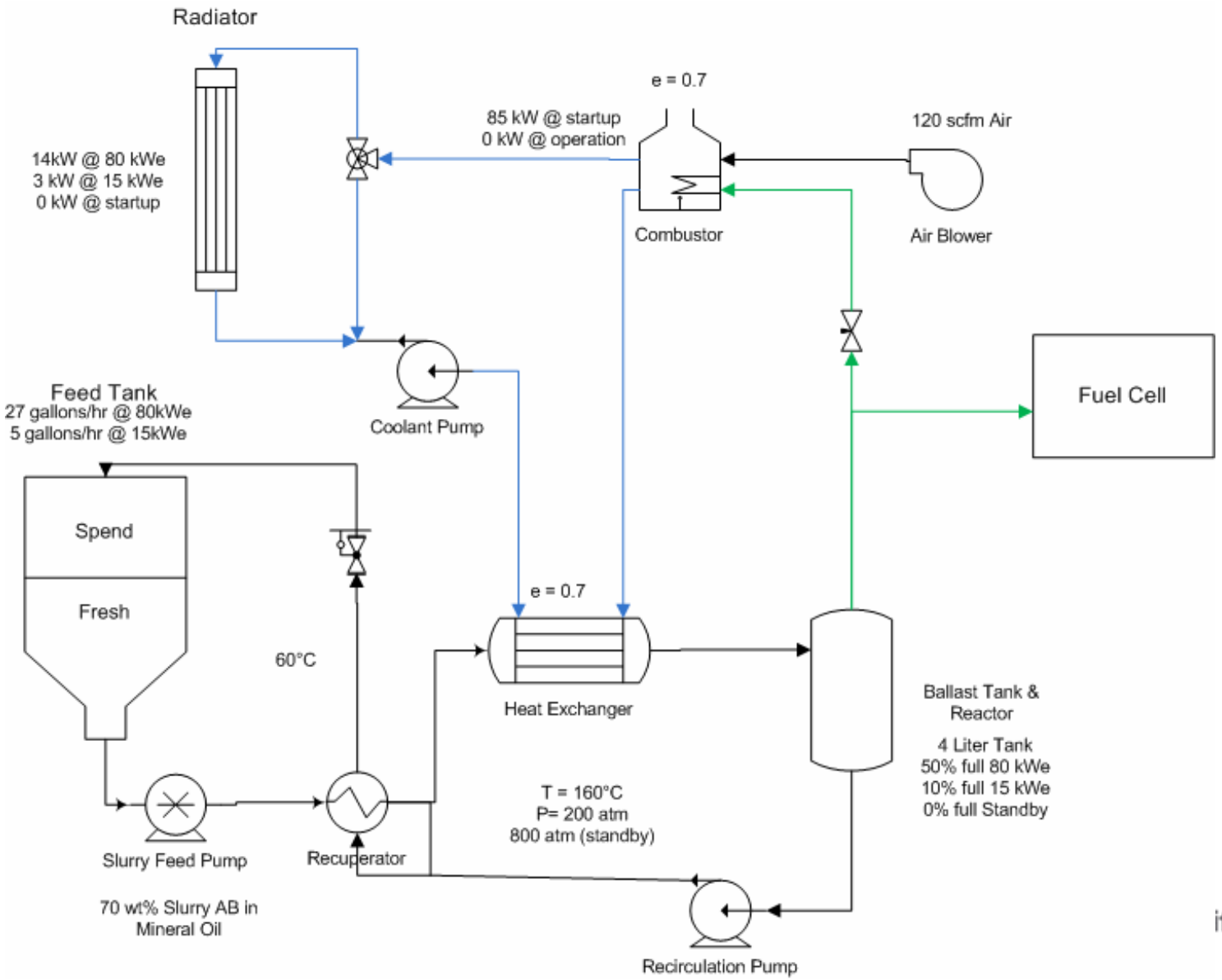
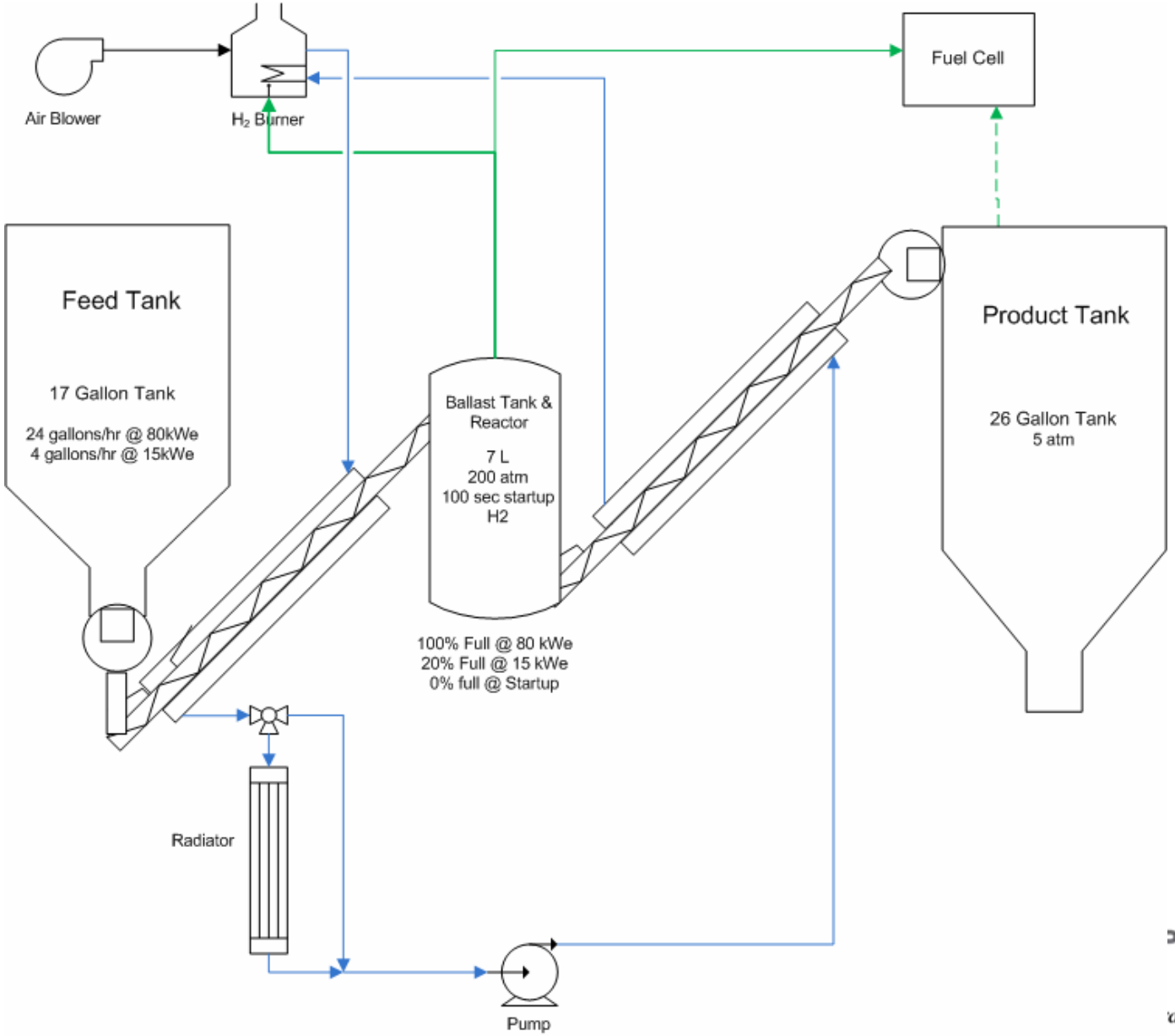
Slurry Reactor



Powder/Beads/Extrudate Reactor



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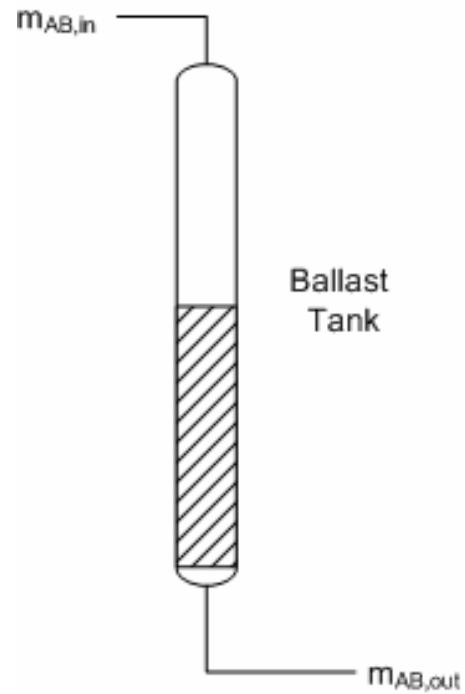
Ballast Tank Equations



- $AB \rightarrow AB^* \leftrightarrow P + 3H_2$
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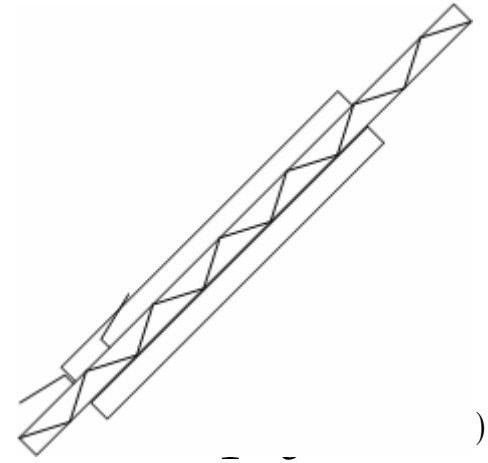
  - $r_{H2} = 3(k_2(y_{AB}^* - K_{eq}(y_{AB,initial} - y_{AB} - y_{AB}^*)))$
    - where $k_1 = A_1 e^{-E1/RT}$ and $k_2 = A_2 e^{-E2/RT}$
- Species Equations

$$\frac{\partial y_{AB}}{\partial t} = r_{AB} - \frac{\dot{m}_{AB,out}}{\rho_b A}\frac{\partial y_{AB}}{\partial x} \qquad \frac{\partial y_{AB}^*}{\partial t} = r_{AB}^* - \frac{\dot{m}_{AB,out}}{\rho_b A}\frac{\partial y_{AB}^*}{\partial x} \qquad \frac{\partial y_{H_2}}{\partial t} = r_{H_2} + D_{H_2}\frac{\partial^2 y_{H_2}}{\partial^2 x}$$

- Heat Equation

$$\rho_b C_p \frac{\partial T}{\partial t} = \Delta H_{rxn} r_{H_2} - \frac{C_p \dot{m}_{AB,out}}{A}\frac{\partial T}{\partial x}$$

Heated/Cooled Auger



- Heat Transfer Equations

$$NTU = \frac{UA}{C_{P,AB}\dot{m}_{ABin/out}}$$

$$C_r = \frac{C_{pAB}\dot{m}_{AB,in/out}}{C_{p,oil}\dot{m}_{oil}}$$

$$\varepsilon = \frac{\quad}{1 - C_r e^{(-NTU(1-C_r))}}$$

$$q_{HA} = \varepsilon C_{P,AB}\dot{m}_{ABin}\left(T_{oil,hot} - T_{ambient}\right)$$

$$q_{CA} = \varepsilon C_{P,AB}\dot{m}_{ABin}\left(T_{BT} - T_{oil,cool}\right)$$

$$T_{oil,HA} = T_{oil,hot} - \frac{q_{HA}}{C_{p,oil}\dot{m}_{oil}}$$

$$T_{oil,CA} = T_{oil,cool} + \frac{q_{CA}}{C_{p,oil}\dot{m}_{oil}}$$

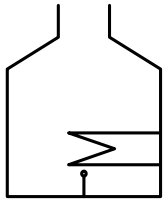
$$T_{AB,HA} = T_{ambient} + \frac{q_{HA}}{C_{p,AB}\dot{m}_{AB,in}}$$

$$T_{AB,CA} = T_{AB,BT} - \frac{q_{CA}}{C_{p,AB}\dot{m}_{AB,out}}$$

Ancillary Equipment

- Burner

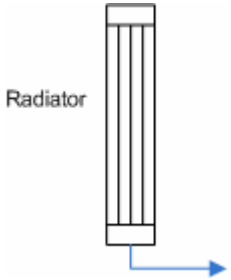
$$C_{P,oil}\dot{m}_{oil}\left(T_{oil,hot}-T_{oil,CA}\right)=\dot{m}_{H_2,burn}\Delta H_{rxn,H_2}\varepsilon_{burner}$$



- Radiator

$$C_{P,oil}\dot{m}_{oil}\left(T_{oil,HA}-T_{oil,cool}\right)=UA\Delta T_{lm}$$

$$\Delta T_{lm}=\frac{\left(T_{oil,HA}-T_{oil,cool}\right)}{\ln\left(\dfrac{T_{oil,HA}-T_{ambient}}{T_{oil,cool}-T_{ambient}}\right)}$$



Materials Compatibility

Storage Media Relationship to Reactivity and Compatibility

Materials Operating Requirements

D. Herling, PNNL

- Materials Centers of Excellence Collaboration – SRNL, LANL, NREL
- Reactivity & Compatibility – UTRC
- Adsorption Properties – NREL
- Metal Hydride Properties – SRNL
- Chemical Hydride Properties – LANL
- Media Structure - GM

Chemical Hydride Properties – LANL

Metal Hydride Properties – SRNL

Adsorption Properties – NREL

Media Structure - GM

Reactivity & Compatibility – UTRC, PNNL

ET-Pressure Vessels & Containment– PNNL

Bulk Materials Handling

H_2 Storage Materials

	Prototypical Material *(initial systems foci)*	Developed Materials *(performance analysis)*	Potential Materials *(further assessment needed)*
Adsorbents	**AX-21** *(UQTR/ANL/GM/UTRC)*	**MOF 5** *(Ford)* **MOF 177** *(Ford)* **IRMOF 8** *(Ford)*	**Duke PEEK** *(NREL)* **UMO AC** *(NREL)* **LLNL AeroGel** *(NREL)* **Pt/AC-IRMOF 8** *(NREL)*
Chamical Hydrides	**$NH_3BH_{3(s)}$** *(PNNL/UTRC)*	**$NH_3BH_{3(l)}$** *(LANL)* **AlH_3** *(SRNL)* **$LiAlH_4$** *(PNNL)*	**N-Ethyl Carbazole** *(LANL)*
Metal Hydrides	**$NaAlH_4$** *(UTRC/Sandia)*	**$LiNH_4+MgH_2$** *(SNL)* **$2Mg(NH_2)_2+MgH_2+LiH$** *(SRNL)*	

Material Operating Requirements

Adsorbents	AX-21 *(UQTR)*	Operating Temperature 77K Material Form Pellet/Powder
Chemical Hydrides	$NH_3BH_{3(s)}$ *(PNNL)*	Operating Temperature 160C Material Form Pellet/Solid
Metal Hydrides	$NaAlH_4$ *(UTRC)*	Operating Temperature <200C Material Form Pellet/Powder

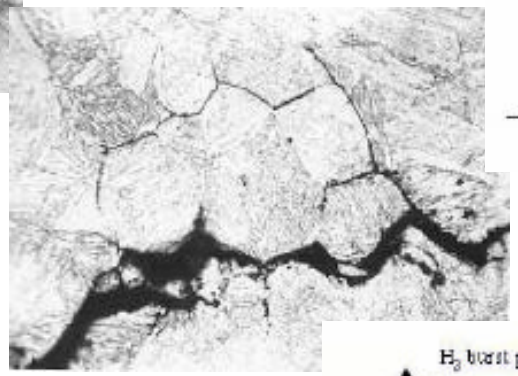
Material Hydrogen Effects

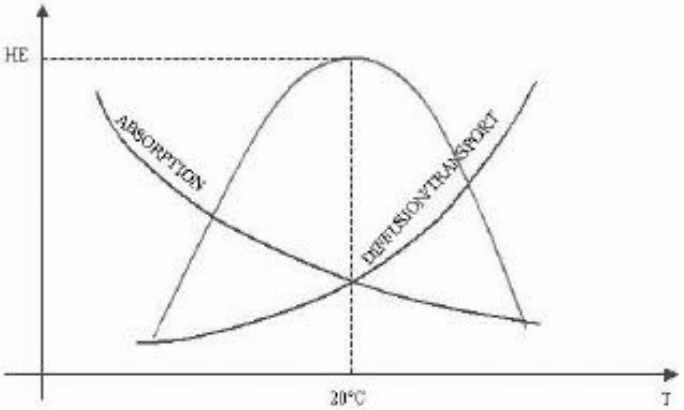
- Hydrogen Embrittlement
  - Internal
  - External
- Hydrogen Attack
- Hydrogen Permeability
- Temperature considerations are very important

Hydrogen Embrittlement

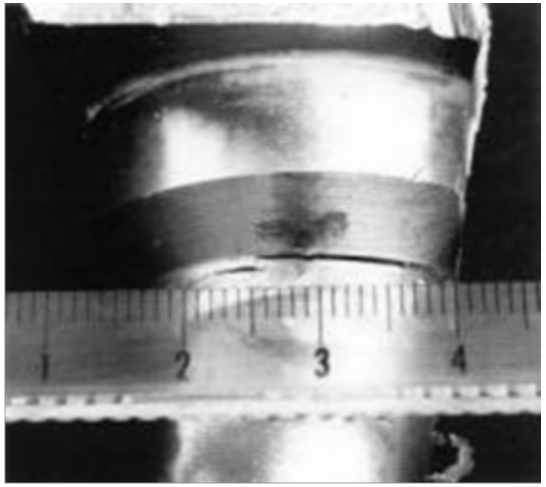
Microvoids
(internal corrosion pits)

Intergranular Crack

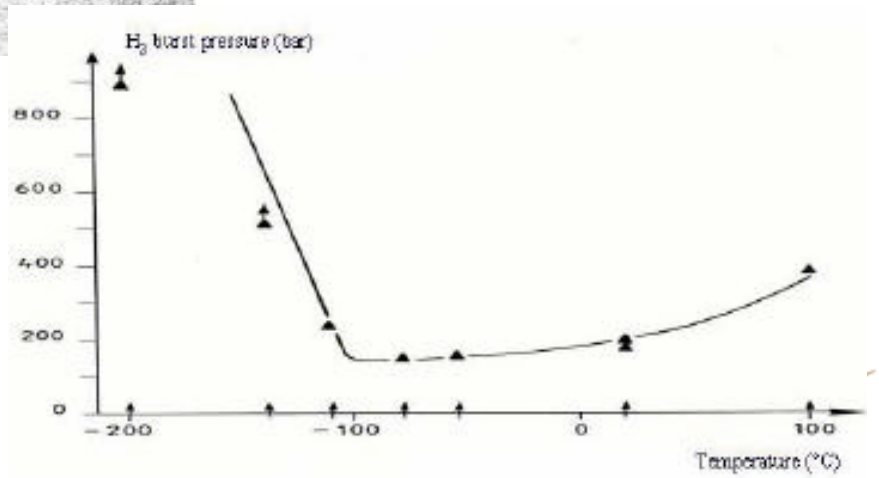




Temperature Effects



Stainless
Pipe
Hydrogen
Crack



Barthélémy, H., *COMPATIBILITY OF METALLIC MATERIALS WITH HYDROGEN REVIEW OF THE PRESENT KNOWLEDGE*, Air Liquide 2006

Difference in Materials Relative to Hydrogen Embrittlement

- The materials which can be used without any specific precautions are :
  - Brass and most of the copper alloys
  - Aluminum and aluminum alloys (some high strength aluminum alloys are known to be sensitive to hydrogen embrittlement)
  - Cu-Be (this material is particularly interesting because of its very high mechanical properties and good fatigue resistance e.g. spring or membrane)
- The materials which are known to be very sensitive to HE are :
  - Ni and high Ni alloys (contrary to steels, unacceptable HE behavior may remain even at rather high temperature)
  - Ti and Ti alloys

Hydrogen Attack

- Hydrogen attack increases when temperature and pressure increase. In addition, the higher the Cr and Mo content, the better the binding of carbon, which reduces risks of HA by decarburization or formation of methane
- Hydrogen attack increases when the level of mechanical stresses increase

Polymers

- Limited data on most polymers
- HDPE is common, but current storage materials exceed the working temperature range
- Higher temperature material candidates under consideration
- Diffusion is highly dependent on the degree of crystallinity
- Higher density materials with lower free-volumes also have lower diffusion rates
- Hydrogen impurities and mixed gases can have an effect on different polymers compatibility

Recommendations on Communication Compatibility and Reactivity Group

- The “scope”, i.e. the hydrogen pressure, the temperature and the hydrogen purity,
- The “material”, i.e. the mechanical properties, chemical composition and heat treatment,
- The stress level of the equipment, vessels, or containment
- The surface defects and quality of finish, and
- The welding procedures
- Component database for all pressure vessels, containments, and BOP.
  - Tubing
  - Valves
  - Heat exchangers
  - Pumps
  - others

Containment & Pressure Vessel

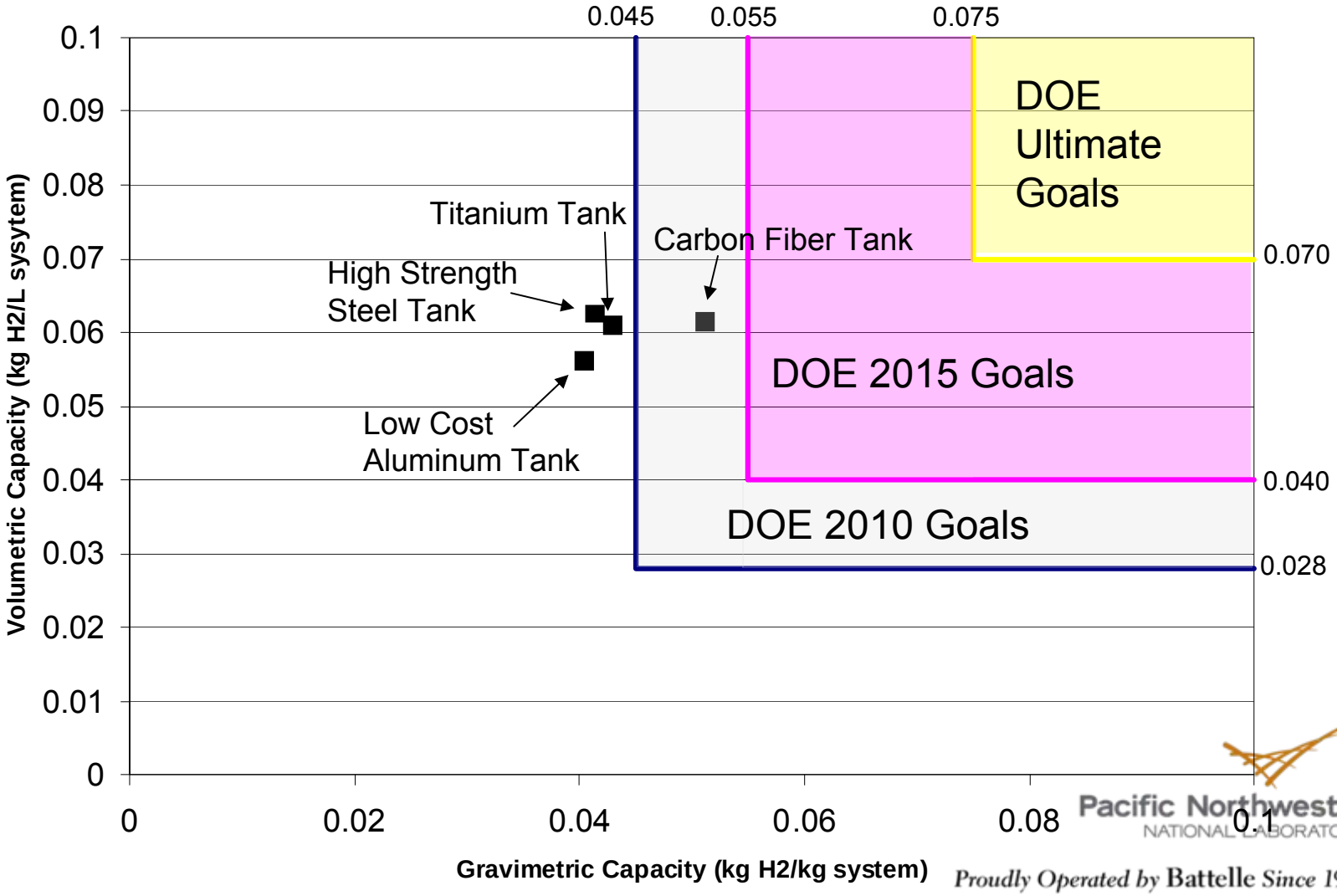
Tier 1 Material Operating Requirements

	Adsorbents AX-21 *(UQTR/GM/UTRC)*	Chemical Hydrides $NH_3BH_{3(s)}$ *(PNNL/UTRC)*	Metal Hydrides $NaAlH_4$ *(UTRC/Sandia)*
Operating Temperature	70K LH_2 77K LN 100K LH_2	160C	<200C
Material Form	Pellet/Powder	Pellet/Solid	Pellet/Powder
Vessel Requirements	Subambient	Thermal control/Ballast Tank	Thermal control
Issues	Cryogenic material requirements Thermal control H_2 Permeability	Materials handling Storage material impurities Balance of plant	Material handling Gas diffusion (O_2)
	Each design must meet the DOE goals		

NaAlH4 Initial Tank Design

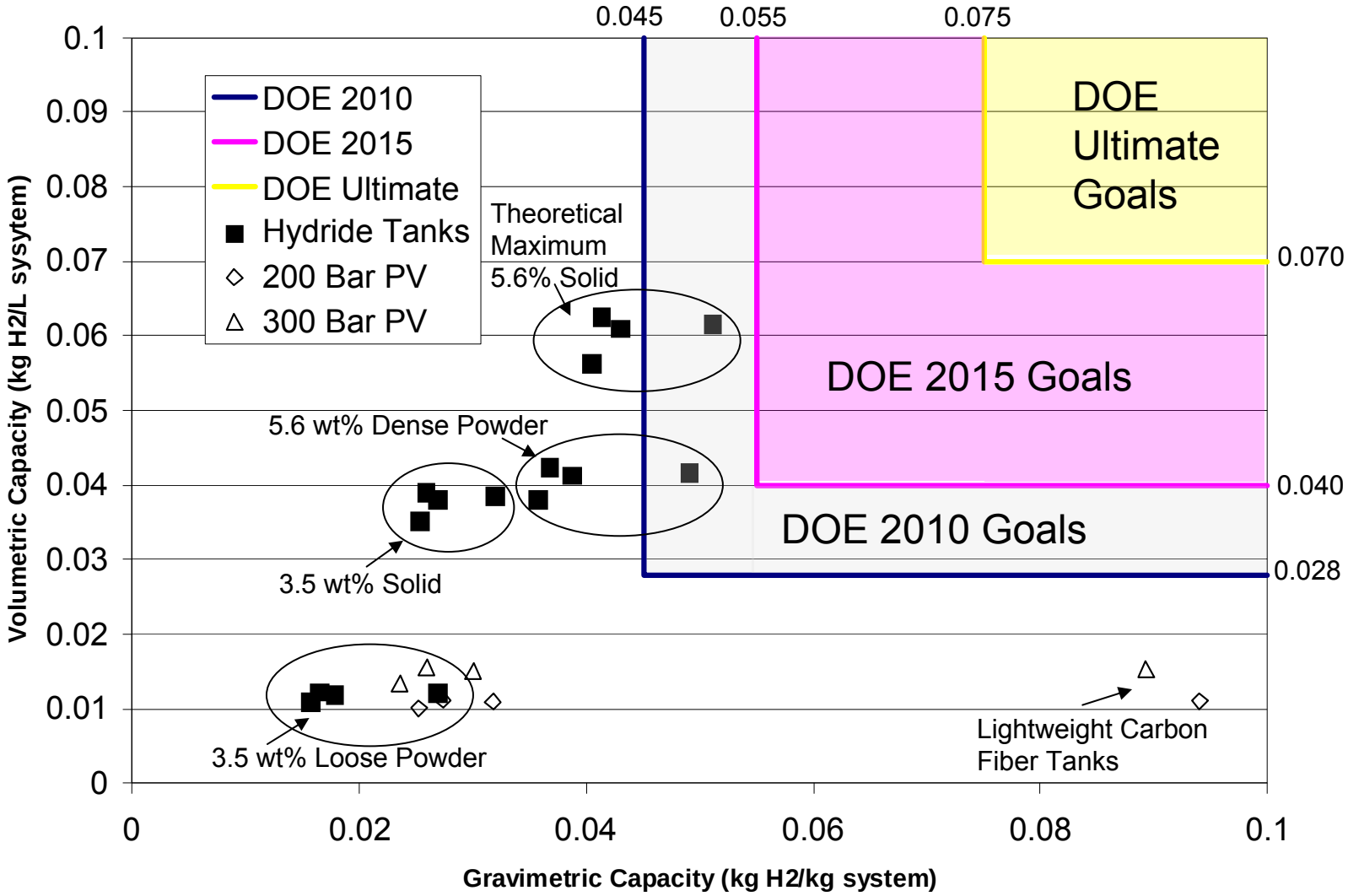
Assumptions: 5.6 wt%, 200 Bar, 95% Solid hydride inside tank, Maximum theoretical performance of hydride.

Not Included: Liner, Insulation, Temperature Control Systems, etc.



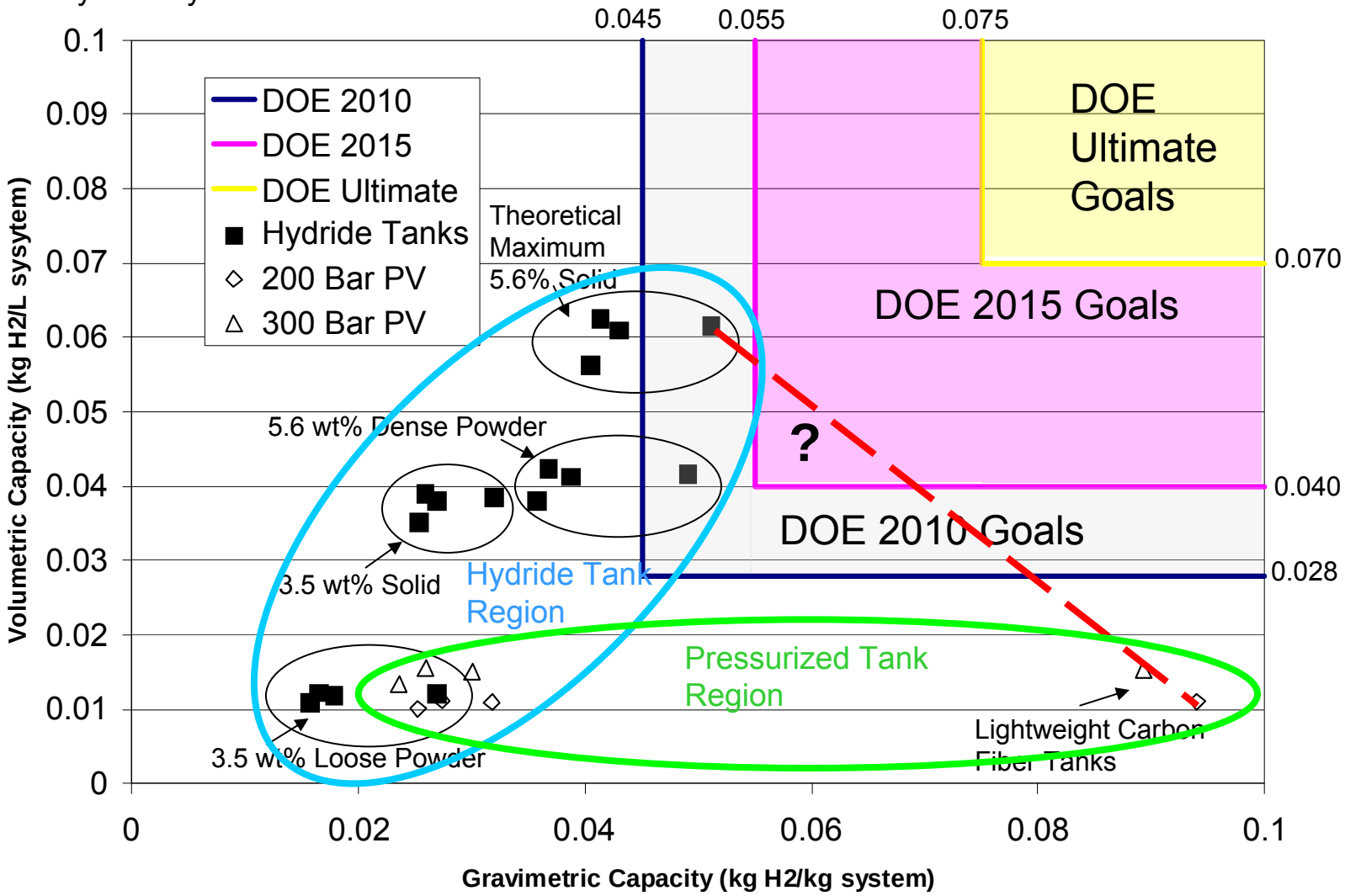
NaAlH4 Design Performance Estimates

Four sets of hydride performance assumptions. The worst set is less desirable than comparable pressurized tanks.



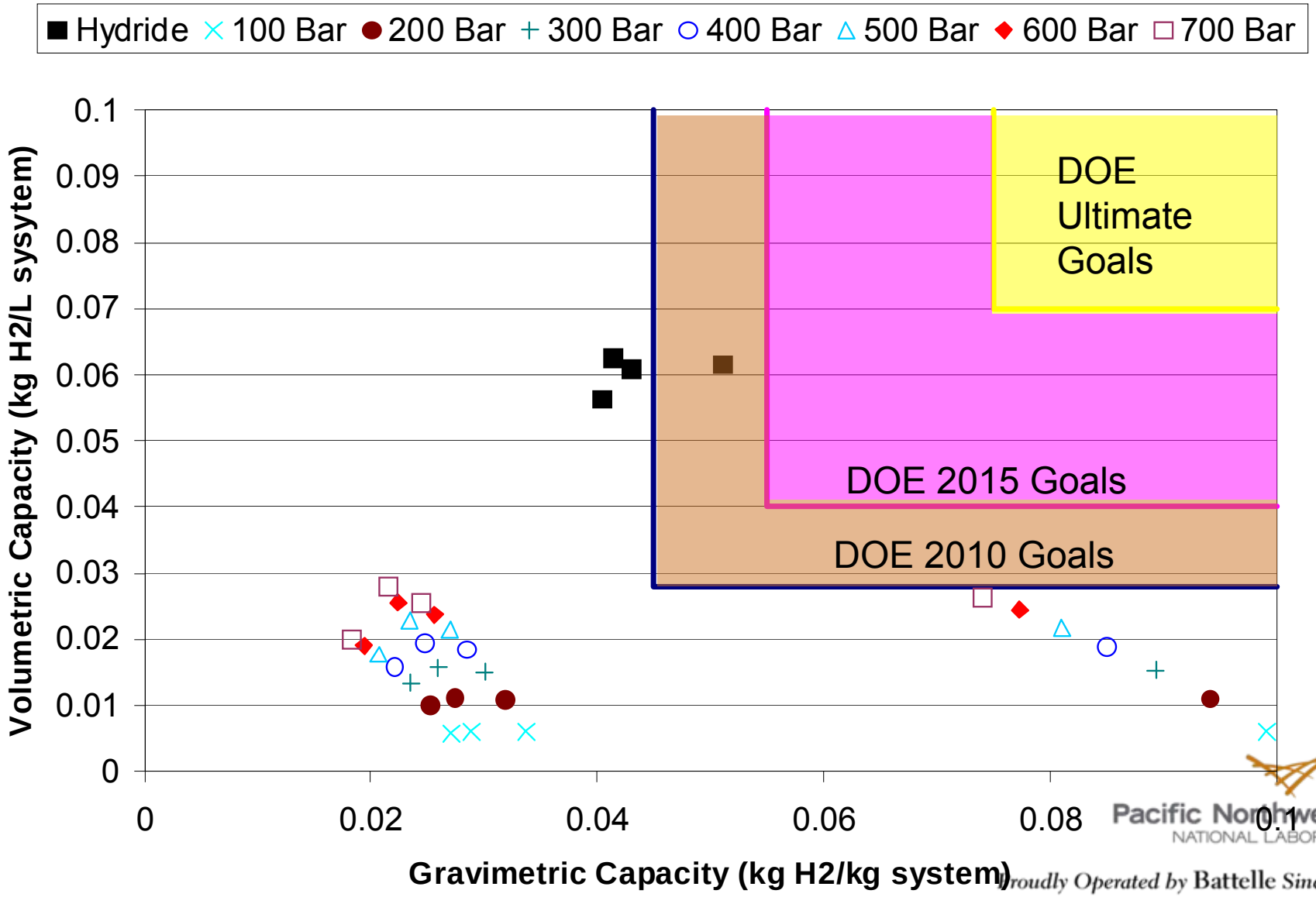
Possible Hybrid Tank to Meet 2015 Goal?

If a hydride tank can achieve a high volumetric capacity, there could be a way to meet the 2015 goal with a two-tank system, or one hybrid tank that combines pressurized gas storage with a partial hydride system.



Pressure Tanks Compared to Hydride Goals

Note: Temperature is assumed to be 100C



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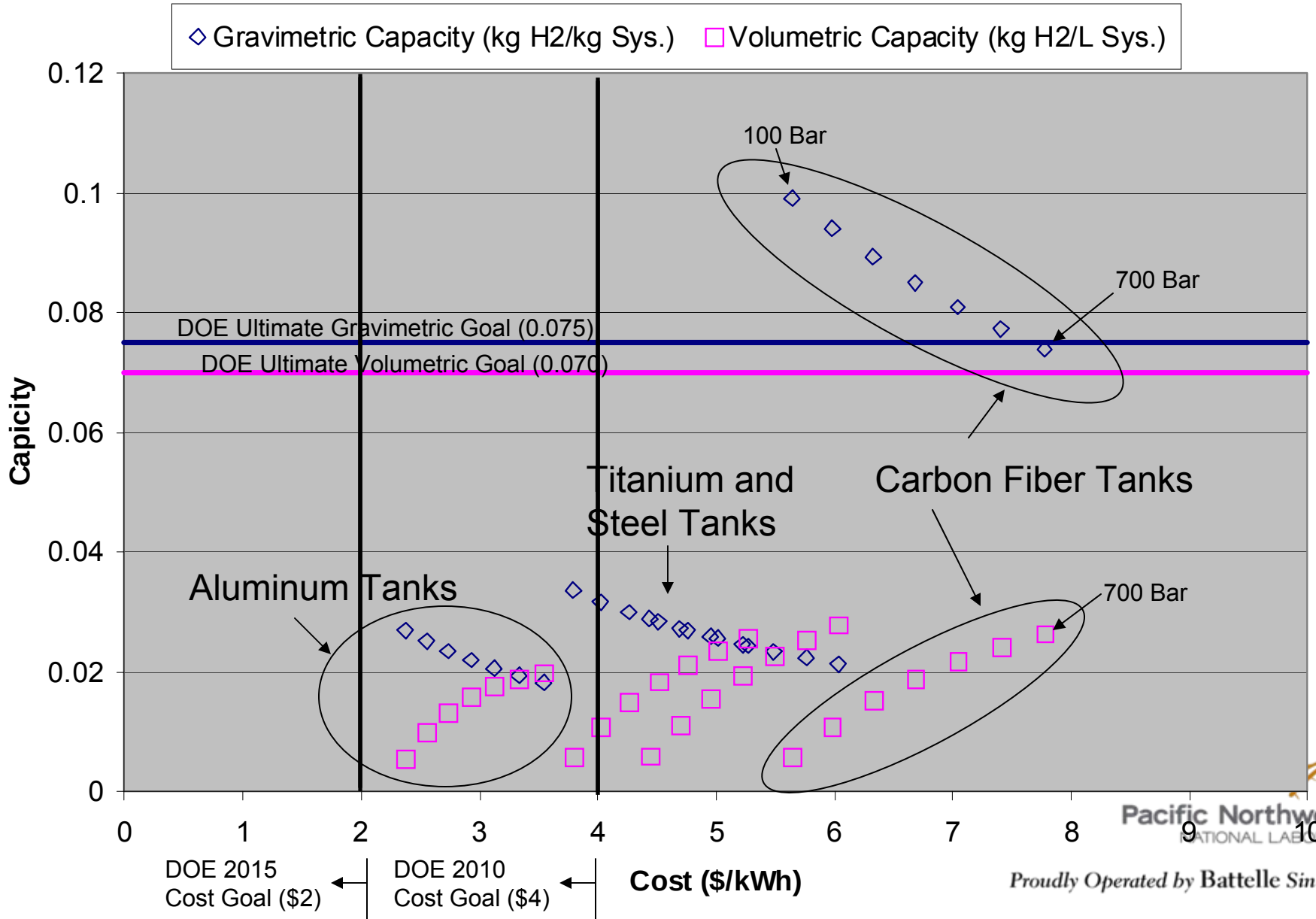
Combined Tank Performance, 100-700 Bar

Note: Temperature is assumed to be 100C



Temperature Example: 700 Bar Carbon Fiber Tank

Temp (°C)	Cost ($/kWh)	Gravimetric Capacity (kg H2/kg sys.)	Volumetric Capacity (kg H2/L sys.)
0	6.220	0.091	0.033
50	7.000	0.081	0.029
100	7.775	0.074	0.026

Critical Commonalities of the Pressure and Containment Task Vessels

- Thermal management
- Safety-material compatibility, etc.
- Low cost
- Lightweight
- Volumetric capacity
- On-board vs. off-board recharging

Trends

- Lower temperature is better.
  - High temperature reduces material strength.
  - High temperature lowers hydrogen gas density.
- Higher pressure is better.
  - Gains in gas density are greater than need for thicker tank.
  - Higher hydrogen density is needed or DOE's ultimate volumetric goal is unobtainable.
- Carbon fiber has greatest potential to meet all goals.
  - But high temperature requirements lead to unacceptable costs because of resin expense.

Conclusions

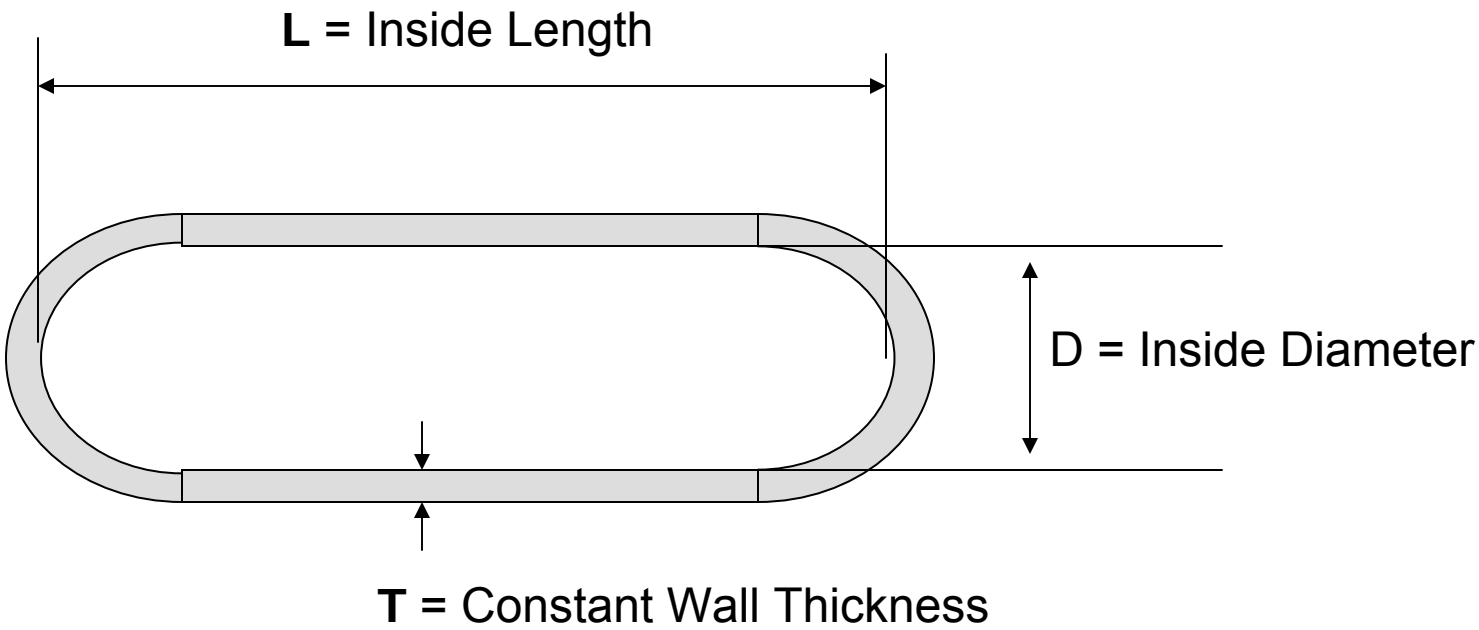
- Note: Storage Enhancement due to metal hydride will drastically affect the results.
- Carbon fiber is the lowest-weight option in all scenarios, but looks cost-prohibitive at 300C.
- High-strength titanium and steel are heavier but lower-cost options.
- Aluminum is the lowest-cost option of them all, but the weight is a detraction.
- Low-strength steel and magnesium do not compare well to the others in cost or weight.

Preliminary Calculations for Hybrid Metal Hydride Tank On-Board Storage

Introduction

- These calculations investigate a range of values for the design of a pressurized hydrogen storage vessel.
- Since the details of the internal structure are not yet known, this study focuses on a constant internal volume to contain 5.6 kg of hydrogen at a specified temperature and pressure.
- Metal hydrides can increase the actual storage capacity by up to a factor of 6, so the effective storage capacity of the tanks in this study is expected to be between 5.6 kg and 33.6 kg.

Geometry of Simple Tanks



Internal volume is chosen based on hydrogen density at the specified temperature and pressure to hold 5.6 kg.

L/D = 3, so dimensions are determined by volume requirement.

T is defined such that peak hoop stress equals material yield strength, including a safety factor of 2.0 for metals or 2.35 for composites.

Carbon Fiber Composite Assumptions

- Toray 700S
  - 370 ksi composite strength, 60% volume fraction
- Translation Efficiency
  - 90% translation efficiency for 2900 and 290 psi
    - Quantum reports 83% @ 5 ksi and 63% @ 10 ksi
- Hoop Design Strength:
  - 222 ksi (370*2/3*.90)
- Reducing Volume Fraction of Fiber is not Economical.
  - Reduced volume fraction was considered, but is not effective.

Pressure Effect Assumptions

Calculated from: *Revised Standardized Equation for Hydrogen Gas Densities for Fuel Consumption Applications* (NIST, 2008)

	20 bar (290 psi)	**200 bar (2900 psi)**
Hydrogen Gas Density @ 100 C	1.29 g/L	12.8 g/L
Hydrogen Gas Density @ 300 C	0.840 g/L	7.92 g/L
Internal Storage Volume for 5.6 kg of H2 @ 100 C	4353 L	475 L
Internal Storage Volume for 5.6 kg of H2 @ 300 C	6665 L	707 L

Temperature Effect Assumptions

	100 C Yield Strength (ksi)	300 C Yield Strength (ksi)	% Strength Reduction
Steel	60	54	10%
Steel (High Strength)	250	225	10%
Titanium	120	80	33%
Titanium (High Strength)	165	110	33%
Carbon Fiber Composite	222	222*	100%
Aluminum	80	40	50%
Magnesium	18	10	45%

*Strength remains the same, but resin cost increases substantially.

Cost Assumptions

Material	Cost: $/lb	Cost Source
Steel (60 ksi)	0.4	2006 Estimate
Steel (250 ksi)	2	2006 Estimate
Titanium (120 ksi)	2	2006 Estimate
Titanium (165 ksi)	2	2006 Estimate
Carbon Fiber (100C)	9.4	Current*
Carbon Fiber (300C)	74	Current*
Aluminum	1	2006 Estimate
Magnesium	2	2006 Estimate

*See next slide for carbon fiber composite material cost breakdown

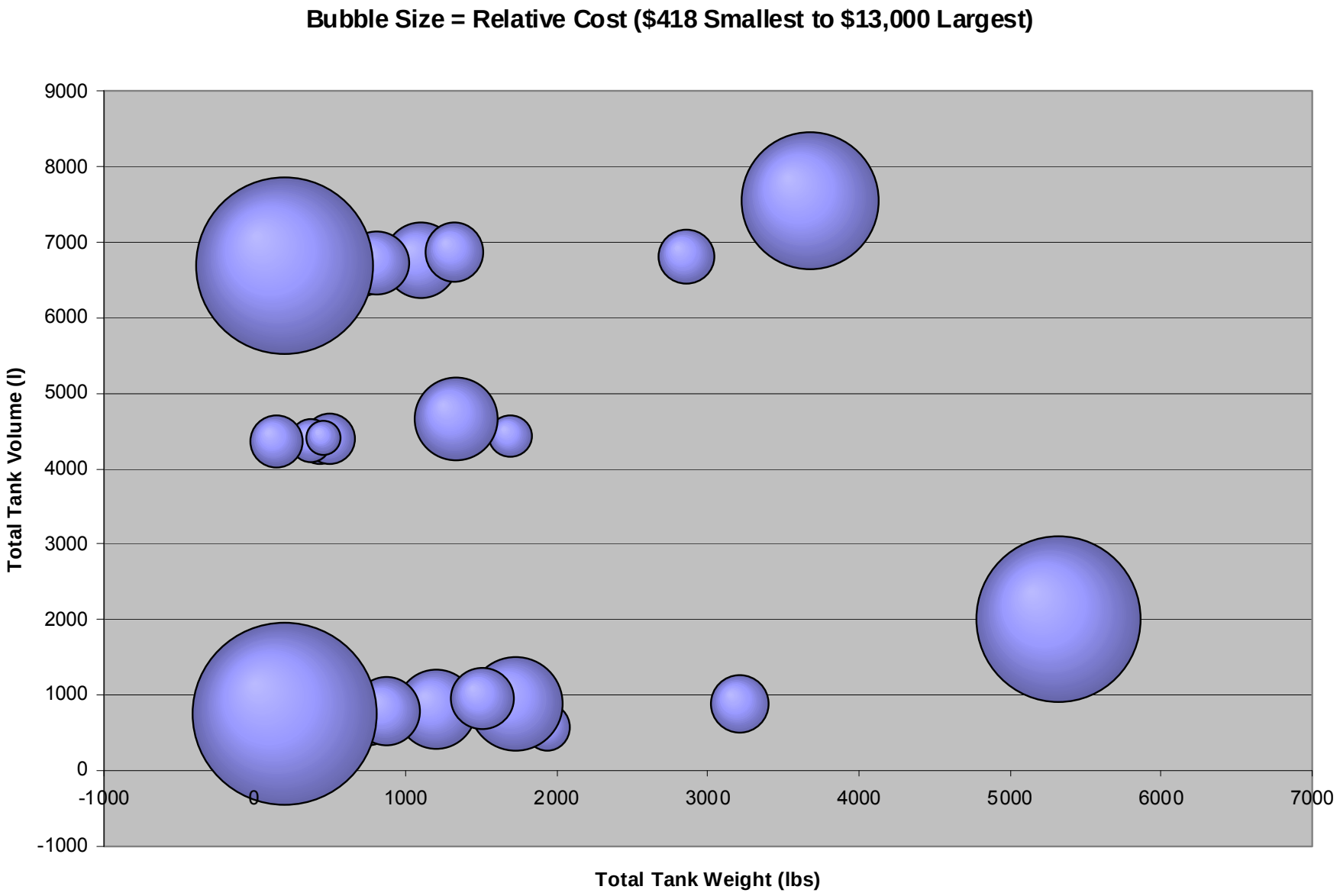
Detailed Composite Cost Determination

- Toray 700S Fiber
  - 13 $/lb
  - .0650 lb/in3 (1.8 g/cc)
- 100 C Resin
  - Non-specific Resin
  - 2 $/lb
  - .0477 lb/in3 (1.32 g/cc)
  - E=6.9E5 Pa
- 100 C composite
  - 60% fiber volume fraction
  - .05808 lb/in3
  - 67.1% wf fiber, 32.9% wf resin
  - **9.4 $/lb**
- 300 C Resin
  - RP-46 (specific resin)
  - 199 $/lb
  - .0477 lb/in3 (1.32 g/cc)
  - E=6.9E5 Pa
- 300 C composite
  - 60% fiber volume fraction
  - .05808 lb/in3
  - 67.1% wf fiber, 32.9% wf resin
  - **74 $/lb**

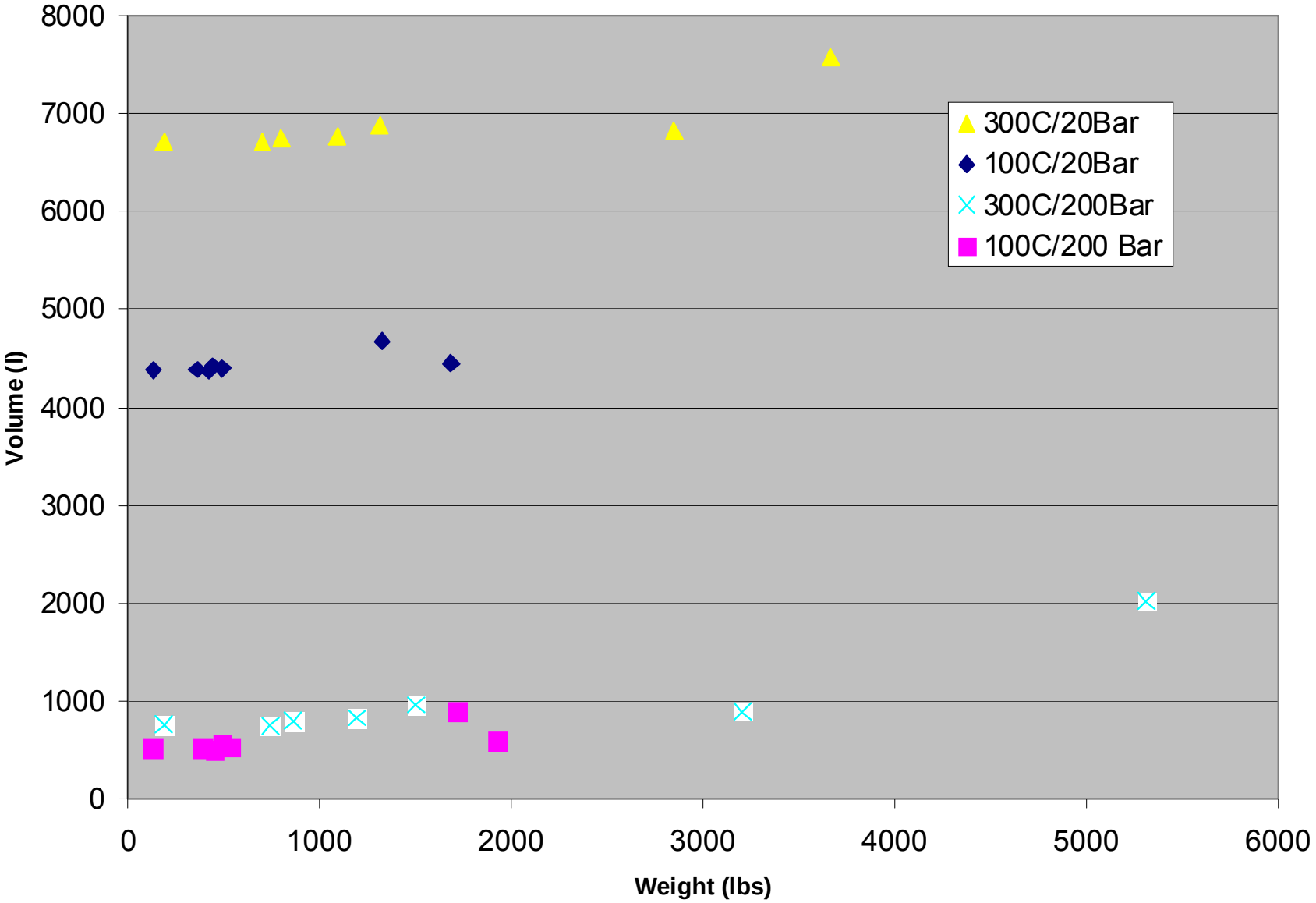
General Loading Assumptions

- Safety Factor of 2.0 for metals, 2.35 for carbon fiber
- 25% overpressure: ignored
  - If necessary, it affects all designs equally
- 5mm HDPE liner: ignored
  - Assumed it affects all designs equally
- 1mm Glass fiber overwrap: ignored
  - Non functional
- Pressure Loads: 20 Bar (290 psi), 200 Bar (2,900 psi)
- Hydrides will increase storage capacity by 6x-1x
  - This is not reflected in results
  - 20 Bar results look unattractive when this is not accounted for

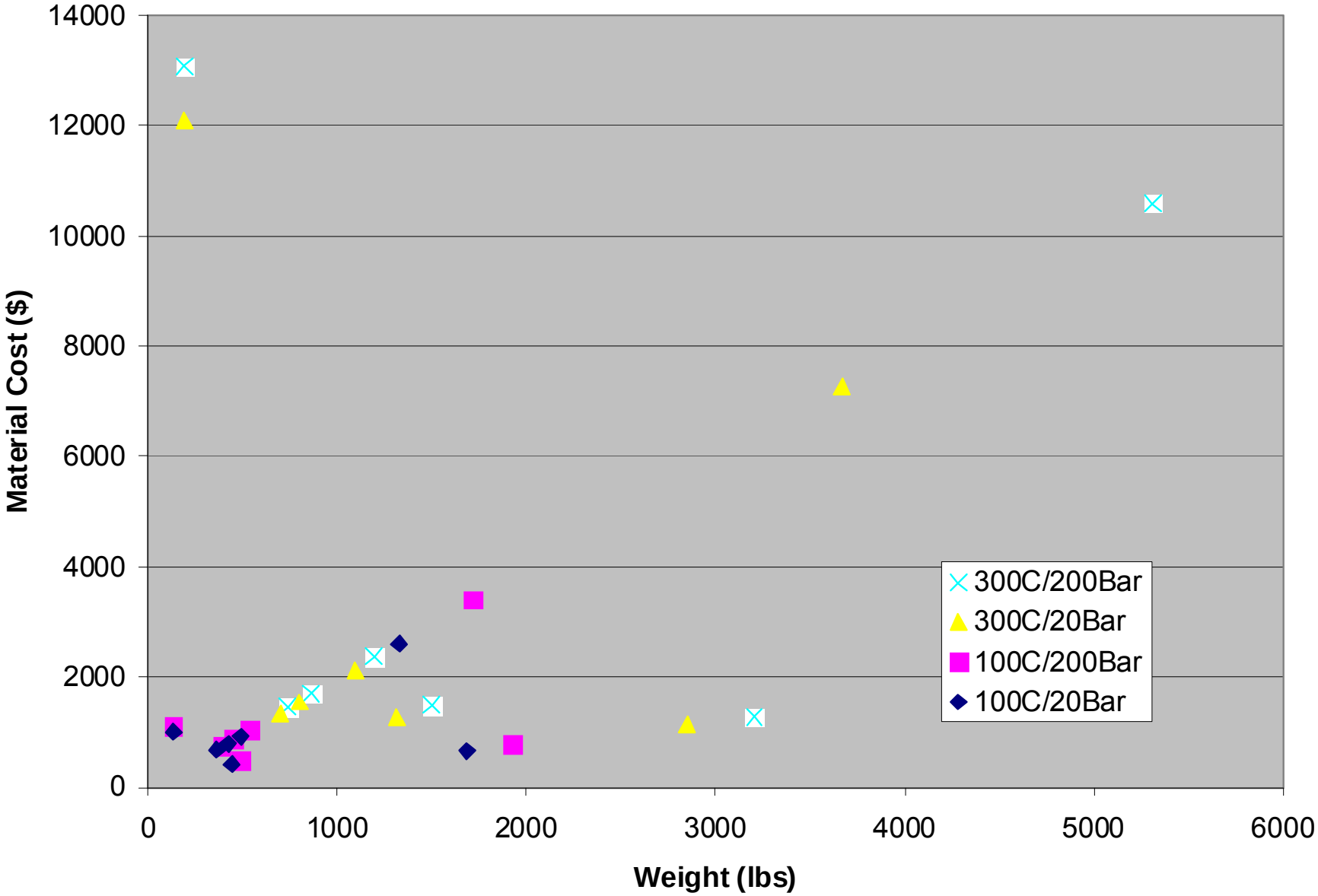
All Results: Bubble Chart



All Results: Volume/Weight Comparison



All Results: Cost/Weight Comparison



Below 1000 lbs and $1500

	Total wt (lbs)	Total Volume (L)	Material cost	Temp	Press
Carbon Fiber	134	509	1116	100 C	200 Bar
Carbon Fiber	136	4383	1004	100 C	20 Bar
Titanium (165)	366	4387	674	100 C	20 Bar
Titanium (165)	391	514	751	100 C	200 Bar
Steel (250)	425	4376	792	100 C	20 Bar
Aluminum	447	4424	418	100 C	20 Bar
Steel (250)	454	500	876	100 C	200 Bar
Aluminum	492	556	476	100 C	200 Bar
Titanium (120)	492	4400	927	100 C	20 Bar
Titanium (120)	536	528	1042	100 C	200 Bar
Steel (250)	702	6704	1347	300 C	20 Bar
Steel (250)	741	749	1452	300 C	200 Bar

100°C Results

	Total wt (lbs)	Total Volume (L)	Material cost ($)	Temp	Press
Carbon Fiber	134	509	1116	100 C	200 Bar
Carbon Fiber	136	4383	1004	100 C	20 Bar
Titanium (165)	366	4387	674	100 C	20 Bar
Titanium (165)	391	514	751	100 C	200 Bar
Steel (250)	425	4376	792	100 C	20 Bar
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Steel (250)	454	500	876	100 C	200 Bar
Aluminum	492	556	476	100 C	200 Bar
Titanium (120)	492	4400	927	100 C	20 Bar
Titanium (120)	536	528	1042	100 C	200 Bar
Magnesium	1327	4675	2597	100 C	20 Bar
Steel (60)	1686	4448	663	100 C	20 Bar
Magnesium	1717	897	3402	100 C	200 Bar
Steel (60)	1930	585	766	100 C	200 Bar

300°C Results

	Total wt (lbs)	Total Volume (L)	Material cost ($)	Temp	Press
Carbon Fiber	192	757	13080	300 C	200 Bar
Carbon Fiber	192	6711	12099	300 C	20 Bar
Steel (250)	702	6704	1347	300 C	20 Bar
Steel (250)	741	749	1452	300 C	200 Bar
Titanium (165)	803	6744	1550	300 C	20 Bar
Titanium (165)	864	794	1697	300 C	200 Bar
Titanium (120)	1095	6774	2133	300 C	20 Bar
Titanium (120)	1197	829	2364	300 C	200 Bar
Aluminum	1315	6885	1286	300 C	20 Bar
Aluminum	1501	961	1486	300 C	200 Bar
Steel (60)	2850	6827	1129	300 C	20 Bar
Steel (60)	3205	891	1276	300 C	200 Bar
Magnesium	3668	7569	7280	300 C	20 Bar
Magnesium	5311	2022	10591	300 C	200 Bar

DOE Goal Considerations

- System Gravimetric and Volumetric Capacity targets are compared to set of potential designs.
- With ideal assumptions, a hydride enhancement factor greater than 1.0 is necessary to meet 2010 and higher targets.
- Assuming a 6.0 hydride enhancement factor, and ideal assumptions, a few designs meet the Ultimate Target

Maximum Potential Goals
6x Hydrogen Storage Efficiency
No Significant Insulation

System	State	kWh/ kg	kWh/ L	$/kWh net	Weight GOAL	Volume GOAL	Cost GOAL
Steel (250 ksi)	100 C, 200 Bar	2.19	2.24	0.78	2015	2015	>2015
Aluminum (80 ksi)	100 C, 200 Bar	2.04	2.01	0.43	2015	2015	>2015
Titanium (165 ksi)	100 C, 200 Bar	2.49	2.18	0.67	2015	2015	>2015
Carbon Fiber	100 C, 200 Bar	5.81	2.20	1.00	Ultimate	2015	>2015
Carbon Fiber	300 C, 200 Bar	4.47	1.48	16.68	Ultimate	2015	FAIL

Maximum Potential Goals
6x Hydrogen Storage Efficiency
Significant Insulation: Materials Unaffected by Temperature

System	State	kWh/ kg	kWh/ L	$/kWh net	Weight GOAL	Volume GOAL	Cost GOAL
Steel (250 ksi)	300 C, 200 Bar	1.54	1.50	1.16	2010	2015	>2015
Aluminum (80 ksi)	300 C, 200 Bar	1.43	1.35	0.63	FAIL	2015	>2015
Titanium (165 ksi)	300 C, 200 Bar	1.77	1.46	1.00	2010	2015	>2015
Carbon Fiber	300 C, 200 Bar	4.47	1.48	1.48	Ultimate	2015	>2015

Weight Goal

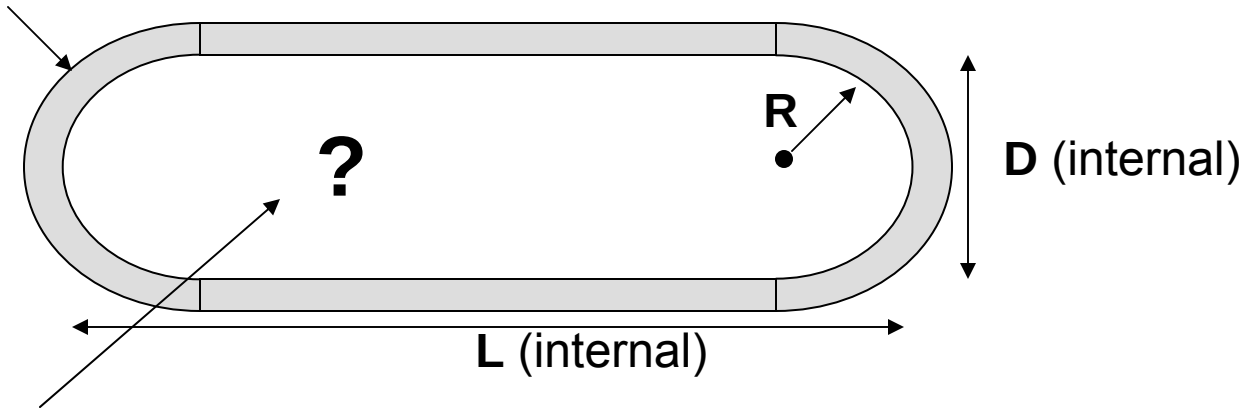
- Weight goal depends largely on tank material, metal hydride material, and system components.
- These scoping calculations only consider tank shell material, not the hydride and not the system components.
- The calculations show that many materials have the potential to meet the 2015 goal, but only carbon fiber can meet the ultimate goal.
- Tank shell material strength and density are the key contributors to tank weight.

Volumetric Goal

- There is no way to meet the ultimate volumetric goal with the current assumptions.
- Possible fixes:
  - Increase hydrogen storage efficiency above 6x
  - Increase pressure above 200 Bar
- There are potential options for meeting 2015 goal, but they have no hope of going higher.
- This is fundamental and NOT related to tank material

Tank Structure Scoping Analyses: Two Key Terms

Tank Shell: The outer casing of the proposed hydrogen tank is considered apart from the other system components. The function of containing the internal pressure dictates many requirements for the rest of the system. The assumed shape is cylindrical with hemispherical ends. The standard L/D ratio is 3, but others were considered (and made little difference).



Hydride System: In these calculations, the specific hydride system is treated as an unknown. Liners, insulation, valves, pipes, hydride material, and any other components other than the tank shell are all lumped together under this term. A pressure range of 20-200 Bar and a peak temperature range of 100C to 300C is considered, under the assumption that the hydride system will function in this range.

Methodology

- Tank Shell internal radius is determined by volume requirement for 5.6 kg of hydrogen gas at a given temperature, pressure, and hydride absorption factor.
  - Choosing an L/D ratio leaves R as the only variable.
- Tank Shell wall thickness is based on allowable hoop strength, which is based on material strength and a safety factor of 2 for metals and 2.35 for composites.
  - Thickness = Pressure*Radius/Hoop Stress Allowable
- Weight, volume, and cost are determined from Tank Shell volume.
  - Although the Hydride System particulars are not yet known, these results are useful in determining the system's potential to meet DOE targets.

Carbon Fiber Composite Assumptions

- **Toray 700S**
  - 370 ksi composite strength (60% volume fraction)
  - 90% translation efficiency for 2900 and 290 psi
    - Quantum reports 83% @ 5 ksi and 63% @ 10 ksi
  - Wrap 2/3 fibers hoop, 1/3 axial
  - Hoop Design Strength = 222 ksi (370 ksi*2/3 *.90)
- **Cost**
  - Carbon Fiber = 13 $/lb (1.8 g/cc)
  - 100C Resin (generic) = 2 $/lb (1.32 g/cc)
  - 300C Resin (RP-46) = 199 $/lb (1.32 g/cc)
- **Composite**
  - 222 ksi hoop design strength
  - .058 lb/in3 (1.61 g/cc)
  - Cost at 100C = 9.4 $/lb
  - Cost at 300C = 74 $/lb

Results: Maximum Potential DOE Target Goals

Assumptions: 6x hydrogen storage efficiency (hydrogen density is 6x gaseous density at given temperature and pressure). Tank shell material strength or material cost is based on peak temperature. Insulation is not assumed.

System	State	kWh/ kg	kWh/ L	$/kWh net	Weight GOAL	Volume GOAL	Cost GOAL
Steel (250 ksi)	100 C, 200 Bar	2.19	2.24	0.78	2015	2015	>2015
Aluminum (80 ksi)	100 C, 200 Bar	2.04	2.01	0.43	2015	2015	>2015
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Carbon Fiber	100 C, 200 Bar	5.81	2.20	1.00	Ultimate	2015	>2015
Carbon Fiber	300 C, 200 Bar	4.47	1.48	16.68	Ultimate	2015	FAIL

Results: Target Goals at Elevated Temperature

Assumptions: 6x hydrogen storage efficiency (hydrogen density is 6x gaseous density at given temperature and pressure). Tank shell material strength or material cost is based on low temperature. Perfect insulation is assumed such that the tank shell temperature peak is only 100C. Additional weight of insulation system is not included.

System	State	kWh/ kg	kWh/ L	$/kWh net	Weight GOAL	Volume GOAL	Cost GOAL
Steel (250 ksi)	300 C, 200 Bar	1.54	1.50	1.16	2010	2015	>2015
Aluminum (80 ksi)	300 C, 200 Bar	1.43	1.35	0.63	FAIL	2015	>2015
Titanium (165 ksi)	300 C, 200 Bar	1.77	1.46	1.00	2010	2015	>2015
Carbon Fiber	300 C, 200 Bar	4.47	1.48	1.48	Ultimate	2015	>2015

Results Compared to DOE Target Potentials

- Carbon fiber, steel, titanium, and aluminum tanks all have some potential to meet the 2015 Gravimetric, Volumetric, and Cost goals.
  - However, adding realistic hydride system components could eliminate any or all of the designs from serious contention.
- Only carbon fiber tanks have the potential to meet the Ultimate Gravimetric goal.
  - It would take a change in the basic assumptions to allow steel, titanium, or aluminum to meet this target goal.
  - Again, adding realistic hydride system components could eliminate any or all of the designs from serious contention.
- None of the tanks have the potential to meet the Ultimate Volumetric goal.
  - Increasing the hydride efficiency (above a 6x factor) or increasing pressure (above 200 Bar) is necessary.
- The Ultimate cost goal has not been set by DOE, but all tank shells under consideration could exceed the 2015 goals.

Hydride System Requirements

- The Tank Shell calculations give us some minimum requirements for the Hydride System.
- To meet Ultimate gravimetric goal the hydride must have an effective weight percent of:
  - At least 8.6 wt% H_2 [hydrogen wt./(system wt.-tank shell wt.)]
- To meet the Ultimate volumetric goal the effective hydrogen density must be:
  - At least 74.4 g H_2 /l
  - This is greater than 6x density of H2 @ 100C, 200 Bar
- To meet the 2015 cost goal the hydride system cost (full system excluding tank shell) must be:
  - Less than $1/kWh
  - Ultimate DOE goal is not yet established

Cost Modeling & Manufacturing Analysis

Accomplishments

- Spreadsheet of On-Board Storage Cost
  - Provides some details on the manufactured costs of specific components
  - Provides costs of purchased items
  - Manufacturing cost for system
  - Use of preexisting data including TIAX analysis results
    - Sodium Borohydride
    - Sodium Alanate (Both UTRC [more detail], TIAX [less detail but probably 2005$]
    - AX-21 (Not much detail)

Accomplishments (cont'd)

- Received conceptual designs
  - Ammonia Borane
    - No clear specifications, but BOM list
  - Metal Hydride
    - Going to revist their previous estimate
  - Adsorbent
- Clear from analysis of TIAX values that previous targets were unobtainable
  - Exception 2010 cost target met by Sodium Borohydride
  - Progress formulas applied appear to have provided best possible numbers
- Cost of hydrogen media carrier alone: hydride, AX-21
  - TIAX estimates close to previous cost targets
  - UTRC example for NaAlNH4 was higher

Previous Cost Estimates

Table 1 - TIAX and UTRC Cost Estimates for AX-21 and Metal Hydrides

On-board Storage Source		AX-21 TIAX	MH TIAX	MH UTRC	MH UTRC
Useable H2	kg	5.6	5.6	5.0?	5.0?
Carrier Media	$	640	1,155	1,250	2,500
Tank	$	755	647	300	600
Major BOP	$	370	240	310	520
Other BOP	$	625			
System Assemby	$	510	70	183	336
Hydrogen	$	18			
Total	$	2,918	2,112	2,043	3,956
Targets					
Media Cost	$/kWh	3.43	6.19	7.51	15.02
Total	$/kg	521.07	377.14	408.60	791.20
Total	$/kWh	15.65	11.33	12.27	23.76

Cost Model Requirements & Assumptions

- Engineered Cost Model
  - Allows user to change variables and see where most improvement can come
  - Cost Targets TBD
    - Storage System cost -- discounted 2003$
    - (& fuel cost) – discounted 2005$
      - with GDP Implicit Price Deflator
  - Only on-board storage – not off-board regeneration
- High degree of transparency
  - Needs to provide estimated cost currently
    - Include a Bill of Materials (BOM) cost database
  - Apply progress ratios

Cost Model Requirements (cont'd)

- Provide predicted future price with high production
  - Provide an ability to change progress values
  - Provide estimates based on assumed units per year?
    - Previous results used 500,000 units per year as high volume
    - UTRC used 1,000,000 units
  - Manufacturing costs of the storage material (not trivial)
    - No clear path to commercialization
- Provide an ability to transform on-board storage estimates
  - From one size to a slightly different sized on board storage system
- Issue: How much flexibility in the model to estimate systems
  - Three very different versions of Ammonia Borane

Bill of Materials

- Detailed component specifications being defined
  - Quantity and specification
    - The more details on the specification, the better the estimate
      - For example, the type of carbon steel (SAE No. 1005 through 1095?)
      - Ammonia Borane
        - Fill-tank bladder specifications
        - Tubing – specifications, material, welded, connection specifications
  - Specifics on ambient temperature each component must operate, specific duty item is undertake.
    - Example, valves
      - Electronic, input size, output size, specific brand could give required specifications
    - Example, Step motor
      - Input condition (voltage, current); Drive Condition, Full step, Dynamic torque, Unipolar or Bipoloar, any ramp up/acceleration; Environmental Condition (humidity, Ambient temperature, pressure, condensation) Motor Life(# of motor shaft revolutions)

Cost Modeling Next Steps

- Complete detailed estimates for each system
- Determine the scope of ultimate change for each system
- Develop scaling functions for main manufactured components
- Develop manufacturing cost estimate for manufactured costs
- Develop approach for instituting progress ratios to develop high output costs
- Determine approach for valuing high production estimates for carrier media