Analyses of Hydrogen Storage Materials and On-Board Systems

Project ID #
ST20

DOE Merit Review
May 17, 2006

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Reference: D0268

Timeline

- Start date: June 2004
- End date: Sept 2009
- 28% Complete

Barriers

- Barriers addressed
  - A. Cost
  - C. Efficiency
  - G. Life Cycle and Efficiency Analyses

Budget

- Total project funding
  - DOE share = $1.5M
  - No cost share
- FY05 = $200k
- FY06 = $275k

Partners

- Team: GTI, Prof. Robert Crabtree (Yale), Prof. Daniel Resasco (U. of Oklahoma)
- Feedback: National Labs, Developers, Stakeholders

Objectives

This project provides an independent cost assessment of the hydrogen storage technologies being developed for the DOE Grand Challenge.

Objective	Description	Technology Focus		
		2005	2006	2007
On-Board Assessment	Develop system-level designs and estimate the cost, weight, and volume for the on-board storage system	• Sodium Alanate	• Sodium Borohydride • Activated Carbon*	• HC Carrier • TBD
Off-Board Assessment	Evaluate designs and cost inputs and estimate the refueling cost and Well-to-Tank energy use and GHG emissions for the fuel chain	-	• Sodium Borohydride • Magnesium Hydride* • Sodium Alanate	• HC Carrier • TBD
Overall	Help guide DOE and developers toward promising R&D and commercialization pathways by evaluating the status of the various on-board hydrogen storage technologies on a consistent basis	• Sodium Alanate	• Sodium Borohydride	• HC Carrier • TBD

* Review of developer inputs only. Did not perform a detailed, independent assessment.

A consistent, Well-to-Wheels (WTW) assessment requires an evaluation of both the on-board and off-board performance and cost.

Approach	Material/Component Performance	System-Level Performance	Cost

On-Board Assessment	• Material wt %
	• P, T requirements
	• Thermo, kinetics
		• Storage system weight and volume
		• Vehicle efficiency (e.g. mi/kg H_2)
		  • Powertrain weight
		  • Thermal, power requirements
			• Storage system factory cost:
			  • Material
			  • Subsystems
			  • Balance of plant
			  • Process

Off-Board Assessment	• Regeneration efficiency • Material wt % • Thermo, kinetics	• Reprocessing/ production, delivery & forecourt requirements • WTT energy and GHG emissions (MJ, g/kg H_2)	• Capital & operating costs • Equivalent H_2 selling price ($/kg)
Overall	NA	• WTW energy and GHG emissions (MJ, g/mile)	• Ownership cost ($/mile)

Our on-board cost and performance estimates are based on detailed technology assessment and bottom-up cost modeling.

Performance/ Tech Assessment

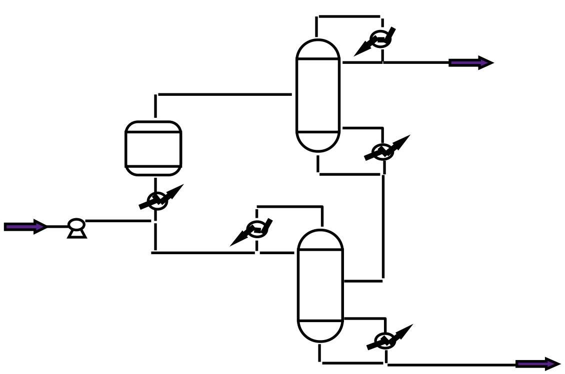
- Literature Search
- Outline Assumptions
- System Design and Configurations
- Process Models
- Developer Input

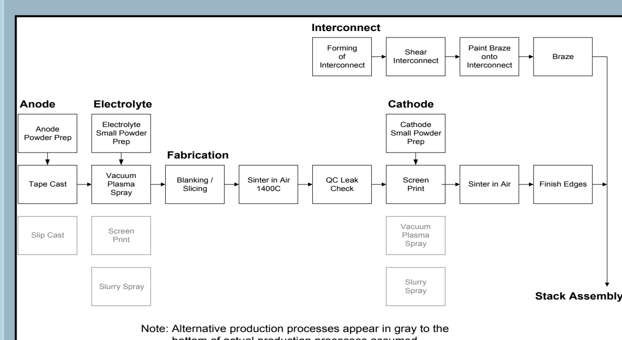
Cost Model and Estimates

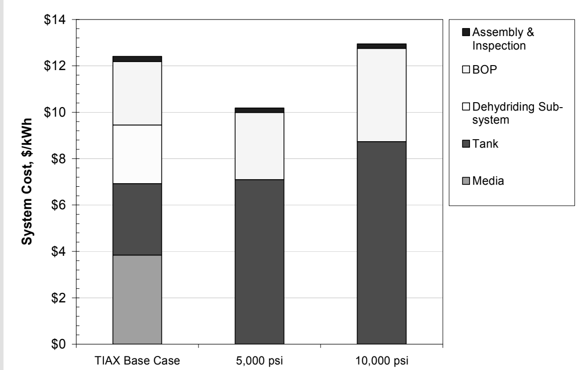
- Document BOM
- Specify Manufacturing Processes and Equipment
- Determine Raw Material Costs

Overall Model Refinement

- Developer and Industry Feedback
- Revise Assumptions and Model Inputs
- Sensitivity Analyses





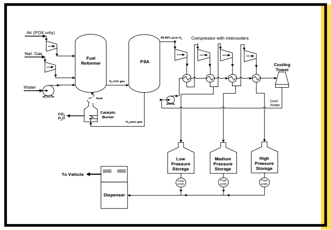


BOM = Bill of Materials

Approach Off-Board Assessment

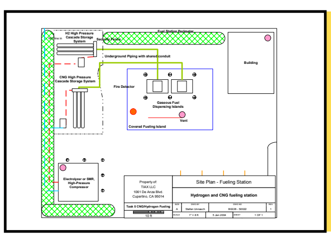
The off-board assessment makes use of existing models to calculate cost and performance for each technology on a consistent basis.

Conceptual Design



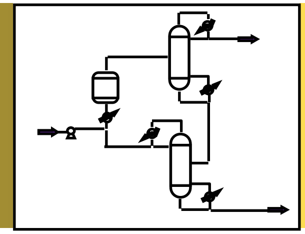
- System layout and equipment requirements

Site Plans



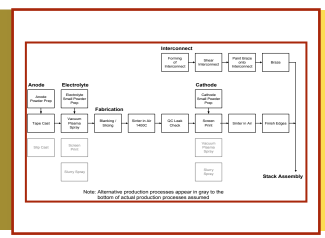
- Safety equipment, site prep, land costs

Process Simulation



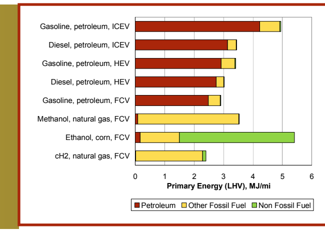
- Energy requirements
- Equipment size/ specs

Capital Cost Estimates



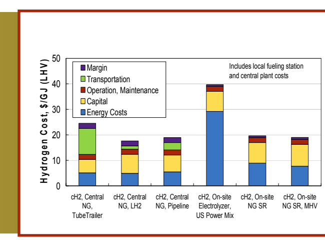
- High and low volume equipment costs

GREET Model



- WTT energy use
- WTT GHG

H2A Model



- Equivalent hydrogen selling price

We have evaluated certain aspects of six H_2 storage technologies. Today's presentation will focus on the on-board $NaBH_4$ system.

Analysis To Date		cH_2 *	Alanate	$NaBH_4$	HC carrier	MgH_2	Carbon
On-Board	Review developer estimates	√	√	√			√
	Develop process flow diagrams and system energy balances	√	√	√			
	Independent performance assessment (wt, vol)	√	√	√			
	Independent cost assessment	√	√	√			
Off-Board	Review developer estimates	√		WIP	WIP	WIP	
	Develop process flow diagrams and system energy balances	√		WIP		WIP	
	Independent performance assessment (energy, GHG)	√		WIP			
	Independent cost assessment	√		WIP			
Overall	WTT analysis tool[1]	WIP					
	Solicit input on TIAX analysis	√	√	WIP			
	Interim report		WIP				

* Detailed, independent assessment conducted for DOE under other contracts.
[1] Working with ANL and H2A participants on separate WTT analysis tools.

(grey box) = Not part of current SOW
WIP = Work in progress

Progress Tank Design Assumptions

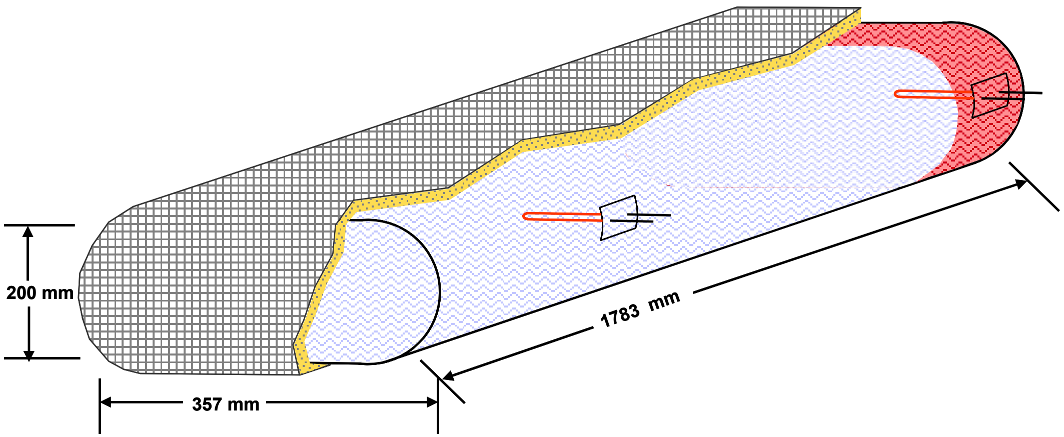
We made a number of system-level design assumptions based primarily on literature review and discussions with developers and stakeholders.

System Element	Design Parameter	Value	Basis
Media	H_2 Storage Capacity	5.6 kg	ANL drive-cycle modeling, midsized vehicle
	$NaBH_4$ H_2 Capacity (theoretical)	21.3 wt%	Based on hydrolysis of sodium borohydride with water: $NaBH_4 + 4H_2O \rightarrow NaB(OH)_4 + 4H_2$ (weight of water not included)
	$NaBH_4$ Concentration in Water	26 wt%	MCell: conversation w/ Wu and Mohring
	Solution Stabilizer	3 wt% NaOH	MCell: Zhang, et al (NHA '04)
	$NaBH_4$ solution density	1.04 kg/L	MCell: correspondence w/ Wu and Mohring
	Metaborate solution density (saturated)	1.25 kg/L	MCell: correspondence w/ Wu and Mohring
	Freeze Point of Metaborate	~ -12 ^{o}C	TIAX estimate of water freeze point suppression due to concentration of metaborate ions
Storage Tank	Wetted Material	Polypropylene / Stainless Steel	Rohm&Haas: web site
	Borate Separator Material	Polypropylene	Rohm&Haas: web site
	Maximum Tank Heat Input	20 W	TIAX tank heat loss model w/ ~.02 m insulation to maintain -12^{o}C in -40^{o}C ambient

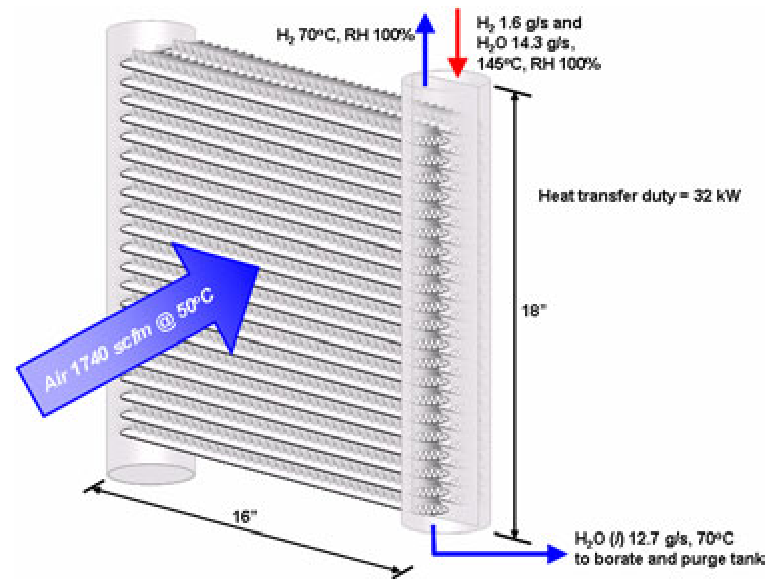
* Additional system design assumptions are in the Backup Slides section.

The system-level design assumptions were used to develop individual component specifications and designs.

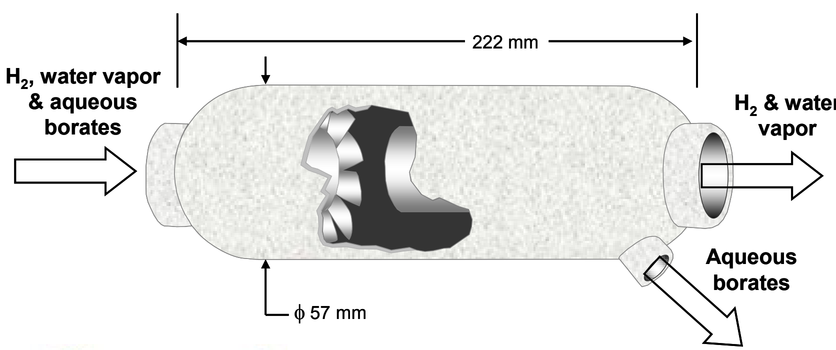
Storage Tank



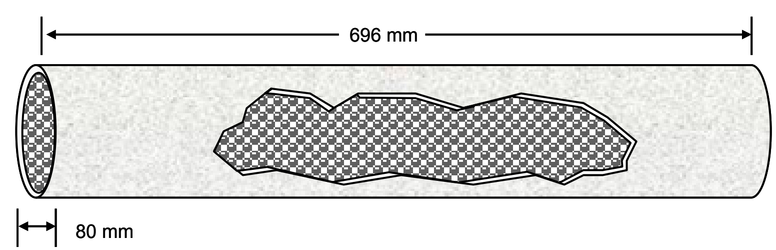
Condenser



Liquid Separator



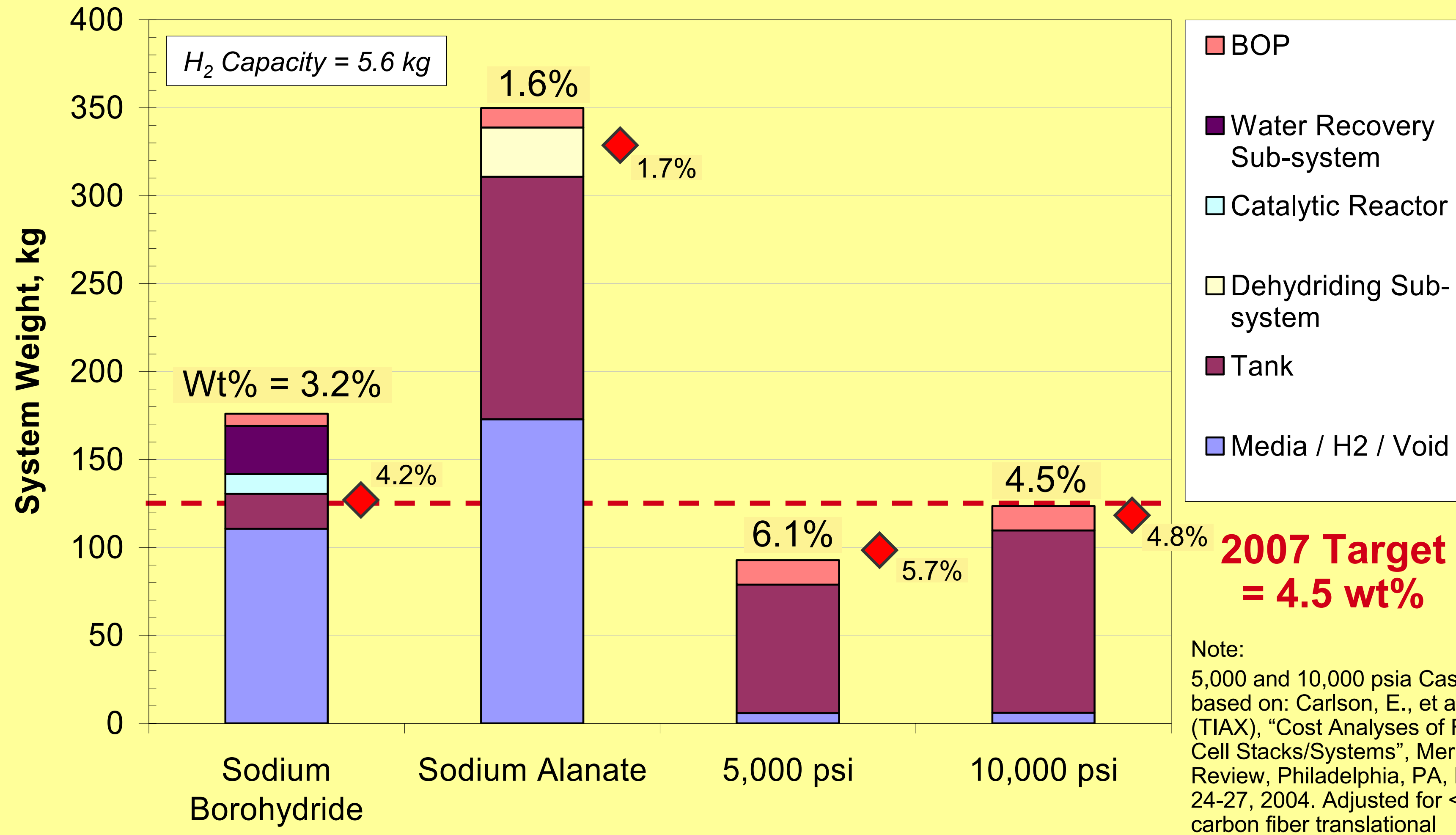
Reactor



Feedback from national labs, developers, and stakeholders was solicited at numerous meetings since the last Merit Review.

Audience/ Reviewer	Date	Location	TIAX Presentation Content
DOE Merit Review	May 05	Crystal City VA	On-board $NaAlH_4$
Safe Hydrogen, DOE, NREL	Jun 05	Telecon	Prelim Off-board MgH_2
H_2 Delivery Tech Team Mtg.	Jul 05	Telecon	On-board $NaAlH_4$, Prelim On-board and Off-board $NaBH_4$ (no cost)
Millennium Cell, DOE	Jul 05	Telecon	Prelim On-board $NaBH_4$
Rohm and Haas	Jul 05	Telecon	Approach (discussion only)
DOE, LLNL, ANL	Jul 05	Telecon	On-board cH_2 and $NaAlH_4$
Safe Hydrogen	Aug 05	Cambridge MA	On-board $NaBH_4$, Prelim Off-board $NaBH_4$ and MgH_2
MH COE System Analysis Mtg.	Sep 05	Telecon	On-board $NaAlH_4$, Prelim BOP cost reductions
H_2 Storage Tech Team Mtg.	Sep 05	Washington DC (video conf.)	Prelim On-board $NaBH_4$, Prelim BOP cost reductions
CH COE System Analysis Mtg.	Oct 05	Argonne IL	Prelim On-board $NaBH_4$
Fuel Cell Seminar	Nov 05	Palm Springs CA	Prelim On-board $NaBH_4$
Storage System Analysis Mtg.	Nov 05	Palm Springs CA	On-board $NaAlH_4$, Prelim On-board $NaBH_4$
FreedomCAR & Fuel Partnership Analysis Workshop	Jan 06	Washington DC	On-board $NaAlH_4$, Prelim On-board $NaBH_4$, Prelim Off-board $NaBH_4$ and MgH_2
H_2 Storage Tech Team Mtg.	Apr 06	Detroit MI	Revised On-board $NaAlH_4$ and $NaBH_4$

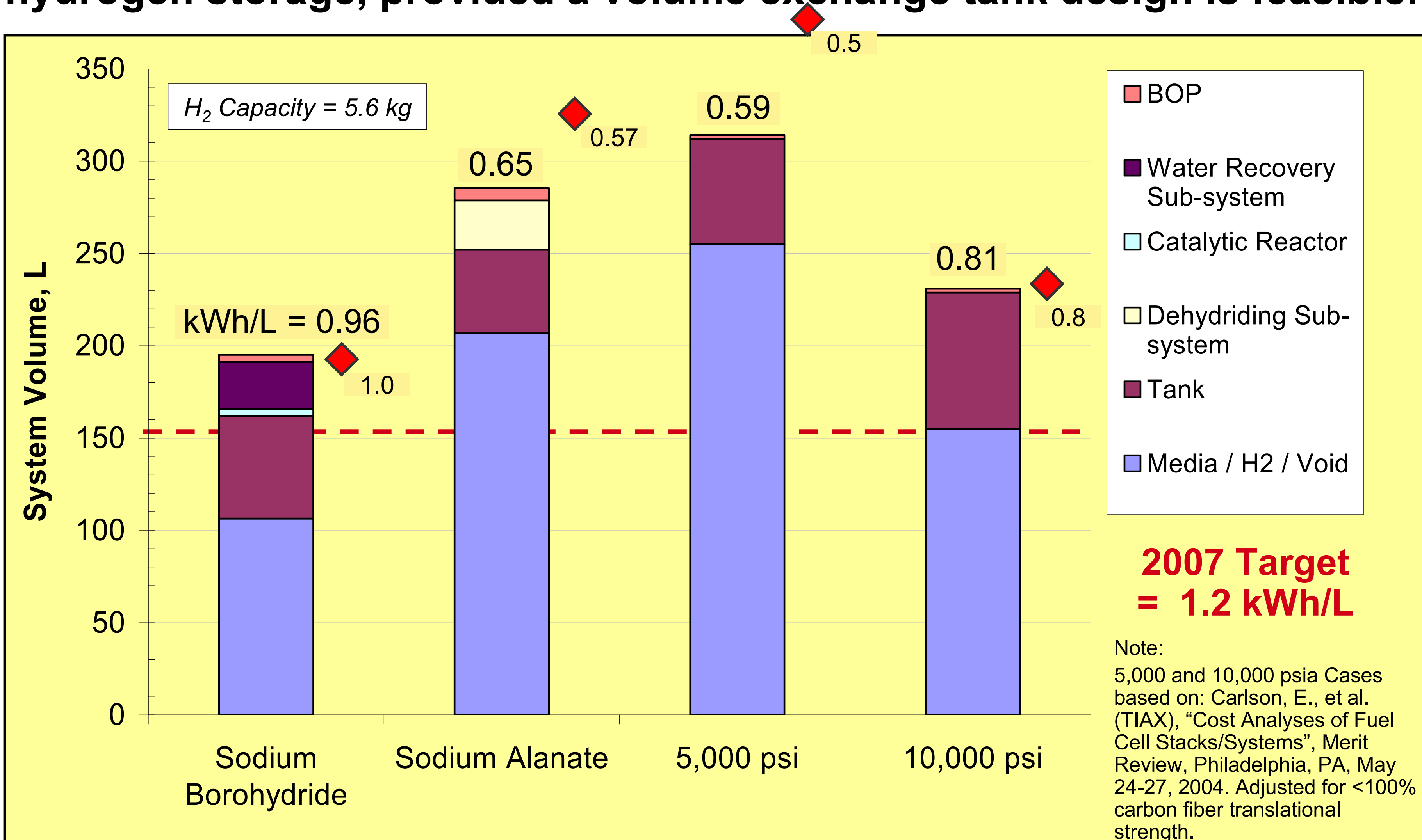
The current designs for the sodium alanate and sodium borohydride systems will likely be heavier than compressed hydrogen storage.



Note:
5,000 and 10,000 psia Cases based on: Carlson, E., et al. (TIAX), “Cost Analyses of Fuel Cell Stacks/Systems”, Merit Review, Philadelphia, PA, May 24-27, 2004. Adjusted for <100% carbon fiber translational strength.

◆ Represents current status according to developers

The sodium borohydride system could be smaller than compressed hydrogen storage, provided a volume exchange tank design is feasible.



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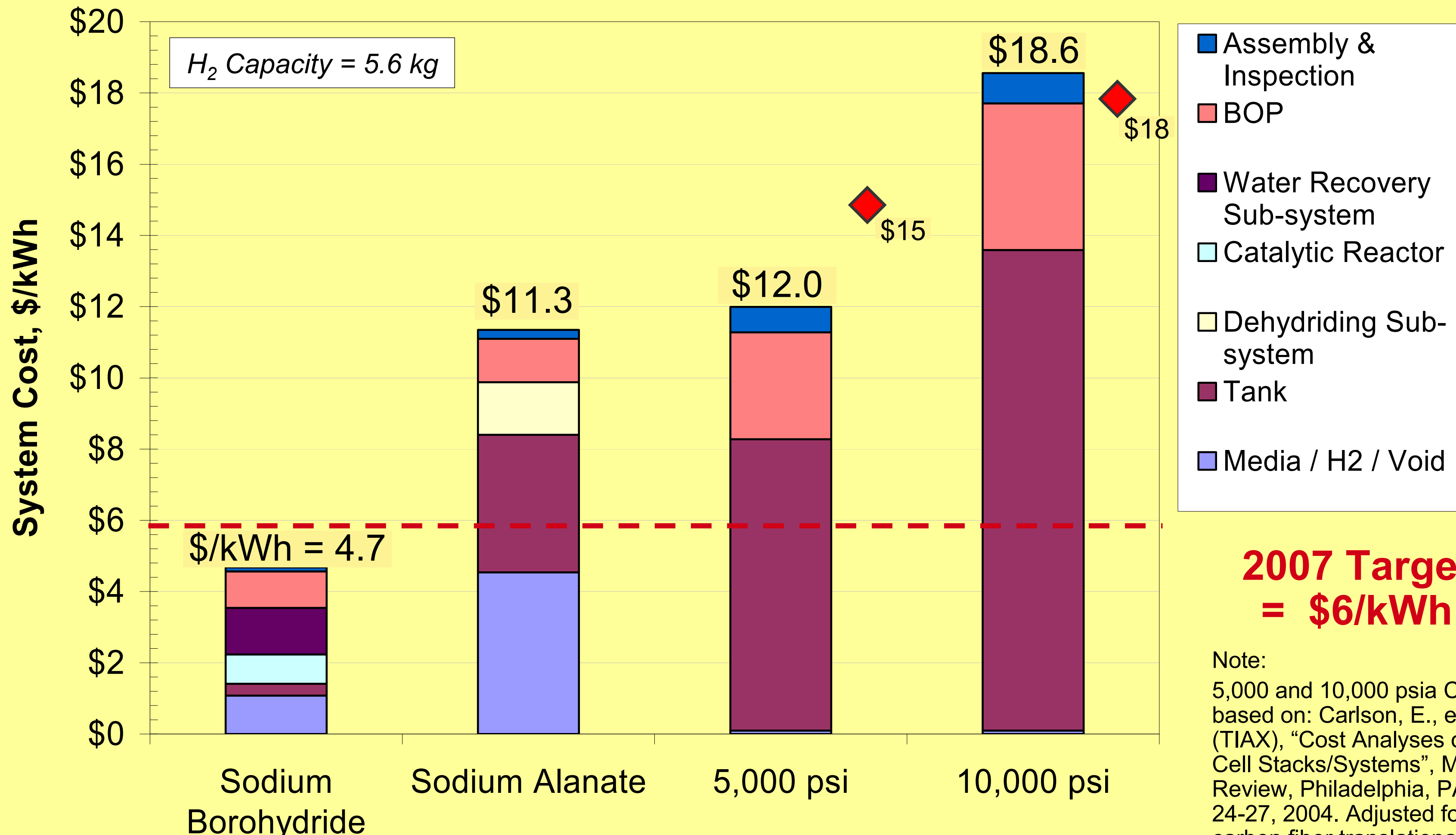
◆ Represents current status according to developers

Although the factory cost of the $NaBH_4$ system will be lower than the compressed hydrogen and alanate systems, fuel costs may be higher.



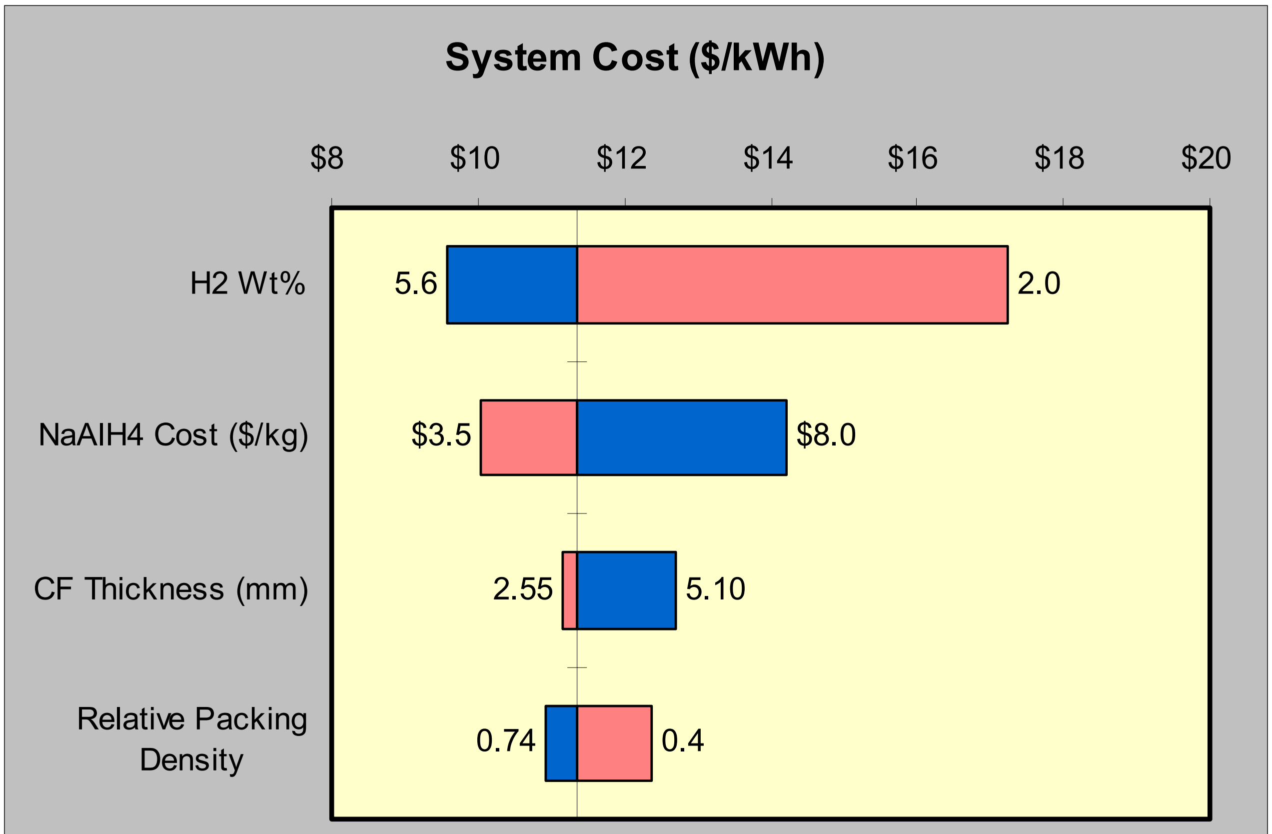
2007 Target = $6/kWh

Note:
5,000 and 10,000 psia Cases based on: Carlson, E., et al. (TIAX), "Cost Analyses of Fuel Cell Stacks/Systems", Merit Review, Philadelphia, PA, May 24-27, 2004. Adjusted for <100% carbon fiber translational strength.

◆ Represents current status according to developers (assuming high volume manufacturing)

Single- and multi-variable sensitivity analyses are used to estimate the dependence and sensitivity of cost on/to the critical cost drivers.

Single-Variable Sensitivity Analysis: Example – Sodium Alanate Factory Cost



Base Case = $11.3 / kWh

As we finalize the sodium alanate and sodium borohydride cases, our findings show they will not meet the 2007 weight and volume targets.

Storage Parameter	Units	2007 Target	Sodium Alanate	Sodium Borohydride
Specific energy (mass)	kWh/kg (kg H_2/kg)	1.5 (0.045)	0.53 (0.016)	1.06 (0.032)
Energy density (volume)[1]	kWh/L (kg H_2/L)	1.2 (0.036)	0.65 (0.019)	0.96 (0.029)
Storage system cost	\$/kWh (\$/kg H_2)	6 (200)	11.3 (377)	4.7 (160)
Fuel cost	\$/gge	3	TBD	TBD

Note: Targets must be met simultaneously. Results are not accurate to the number of significant figures shown.

[1] Volume results do not include void spaces between components (i.e., no packing factor was applied).

- Note that these systems are based on “current technology” and do not necessarily meet other DOE targets (e.g. refueling rate)
- ANL is evaluating mass and volume projections for systems that meet all other DOE targets not shown here

We are in the process of finalizing the alanate and sodium borohydride on-board results and conducting the off-board assessment.

- Finalize results for the on-board alanate and sodium borohydride systems, including:
  - Peer review and incorporate feedback
  - Run single- and multi-variable sensitivity analysis
  - Publish interim report on sodium alanate – Milestone
- Conduct off-board analyses for alanate and sodium borohydride systems and integrate into a Well-to-Wheels analysis
  - WTT and WTW energy use and GHG emissions
  - Vehicle integration and efficiency impacts
  - Hydrogen "refueling cost" and storage system "ownership cost"
  - Publish interim report on sodium borohydride – Milestone
- Continue to work with DOE, H2A, other analysis projects, developers, National Labs, and Tech Teams

Future Work FY07 New Cases

Specific technologies are chosen for assessment by DOE in light of results and progress within the Grand Challenge program.

Category	Initial Cases	Tech Status[1]	Storage State	H_2 Release	Refueling Type
Compressed and Liquid Hydrogen	5,000 & 10,000 psi	Pre-commercial	Gas	Pressure regulator	cH_2 gas
Reversible On-board: Metal Hydrides and Alanates	Sodium Alanate (UTRC)	Proof of Concept Prototype	Solid	Endothermic desorption	cH_2 gas and HTF loop
Regenerable Off-board: Chemical Hydrides	Sodium Borohydride (MCell)	Early Prototype	Aqueous solution	Exothermic hydrolysis	Aqueous solution in/out
High Surface Area Sorbents: Carbon	TBD	R&D	Solid (low T?)	Endothermic desorption	cH_2 gas (low T?)

[1] For discussion purposes only. Developer claims may vary.

Next we will complete the assessment of a second chemical hydride storage technology and begin the assessment of a technology TBD.

Acknowledgement

Thank You

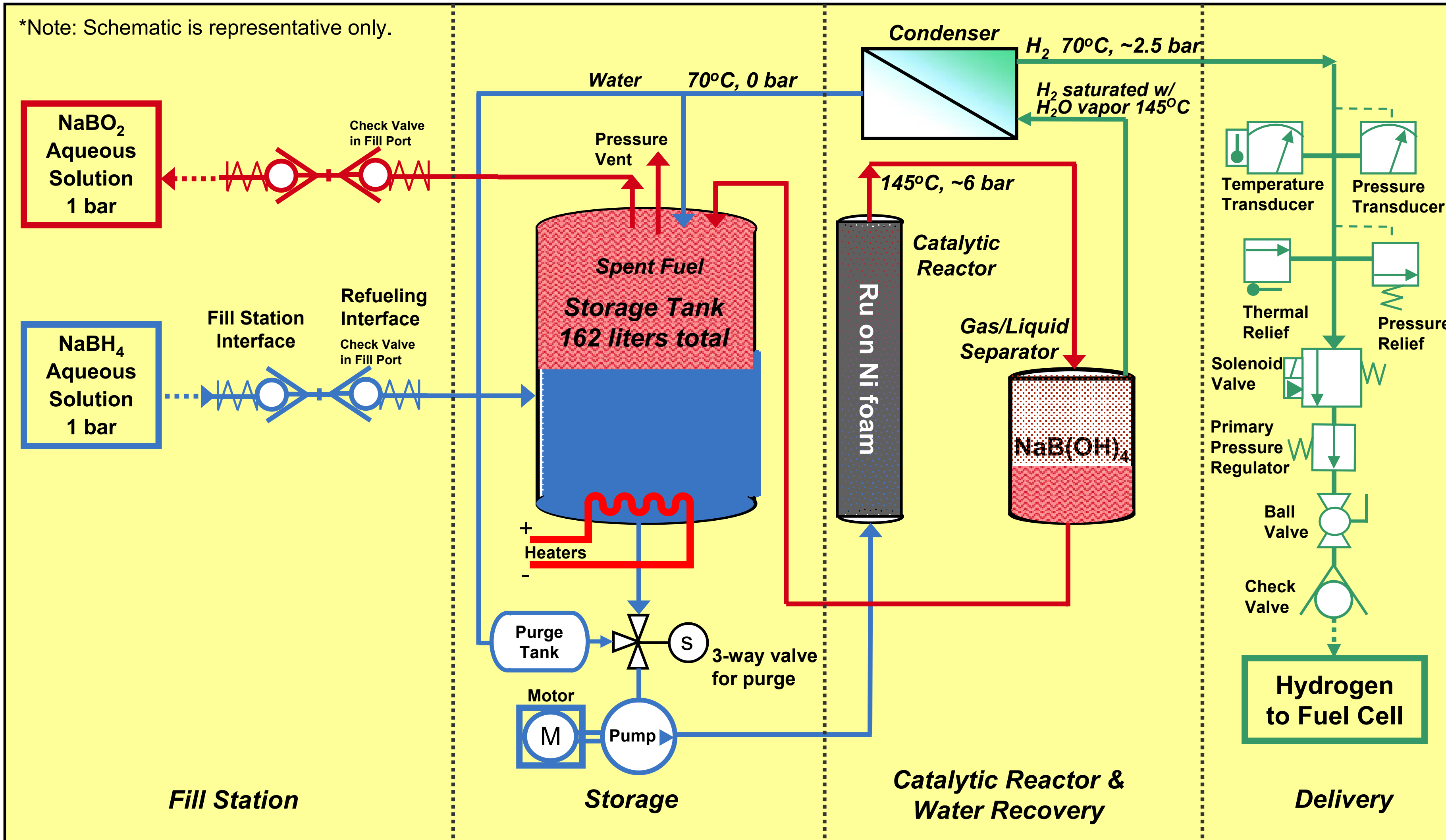
Questions?

Backup Slides Response to Reviewers Comments

- "Need more frequent update and coordination with the Tech Team" and "Need to constantly work towards keeping all of the PIs of the other DOE projects 'in the loop' on their work"
  - Presented at 7 meetings with Tech Teams and 12 meetings with developers (4 and 9 since May 2005)
  - Presented to public at DOE Merit Review, Fuel Cell Seminar, and NHA
  - Participated in numerous other meetings/conference calls with DOE, ANL and developers
- "The values used in analysis vary from the actual values achieved in storage projects" and "The UTRC results seem to show even significantly worse performance characteristics than proposed from this model"
  - Some variance is expected due to the fact that we are using a consistent set of design parameters (e.g. 5.6 kg H_2) and assumptions (e.g. designs for high-volume manufacturing) while developers are not (e.g. different sizes, one-off "prototype systems")
  - We compare our results to developers' measured and projected values as they become available
  - To date, only minor changes to our assumptions have been made based on these comparisons
- "The urgency for these analyses is acute" and "Faster turn around" **versus** "It is too early in the [Grand Challenge] program to expect any directionally correct results"
  - We are in constant dialogue with DOE, Tech Teams and developers so we can prioritize activities
  - Project is operating according to the assigned annual budget
- "The assumptions used in developing the analysis were conservative" **versus** "Lots of the numbers used are very optimistic based on the actual progress of the UTRC project"
  - The project team is attempting to strike a balance between evaluating today's sub-optimal "prototype system" and a projected "future system" that may have overly optimistic performance/cost assumptions
  - We independently develop or verify model inputs and review them with developers and stakeholders
  - The remaining uncertainty is addressed in the sensitivity analyses

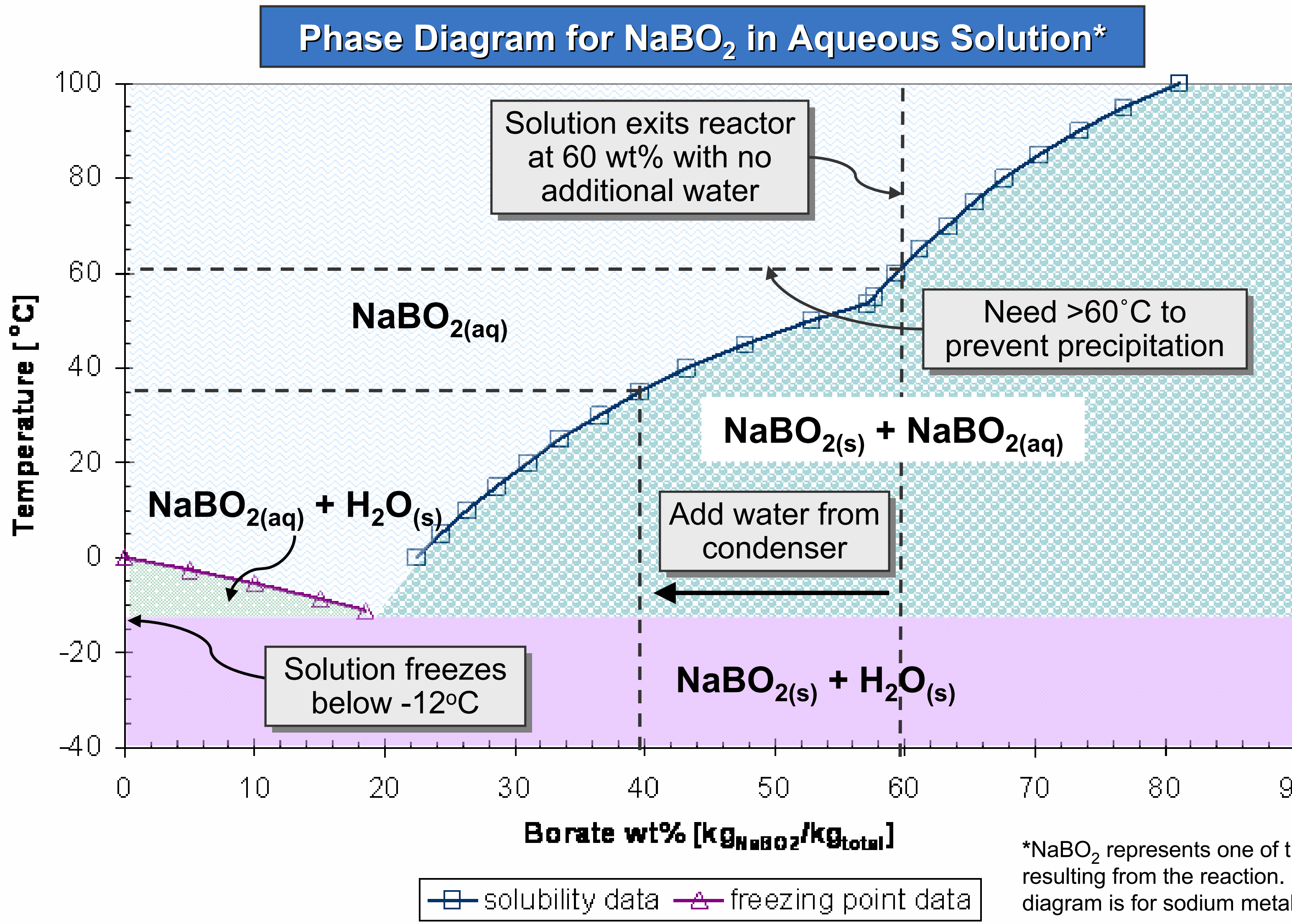
- Fuel Cell Seminar
  - Lasher, et al; *Comparison of On-Board Hydrogen Storage Options*
  - November 2005, Palm Springs CA
- FreedomCAR & Fuel Tech Team Meetings
  - July 2005, Columbia MD (Delivery)
  - September 2005, Washington DC/Detroit MI (Storage)
  - January 2006, Washington DC (Analysis Workshop)
  - April 2006, Detroit MI (Storage)
- COE System Analysis Meetings
  - September 2005, Washington DC (Metal Hydride)
  - October 2005, Argonne IL (Chemical)
  - November 2005, Palm Springs CA (All)

The storage tank is the largest and heaviest component, while water management is the most critical process in a NaBH$_4$ storage system.



*Sensors, safeties and controls based on the requirements defined in the draft European regulation for "Hydrogen Vehicles: On-board Storage Systems" and US Patents 6,041,762; 6,709,497.
**Additional safety and start-up components may be required.

Water and thermal management are required to avoid solution precipitation and freezing adding to system complexity.



*$NaBO_2$ represents one of the borate forms resulting from the reaction. Here the phase diagram is for sodium metaborate 4 mol

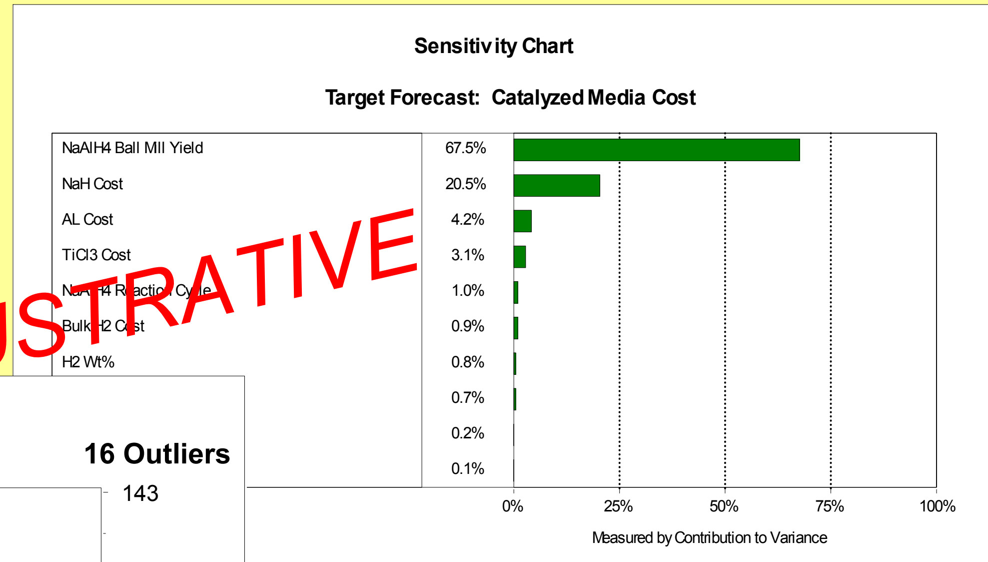
We made a number of system-level design assumptions based primarily on literature review and discussions with developers and stakeholders.

System Element	Design Parameter	Value	Basis
Reactor	Heat of Decomposition	-37.2 kJ/kg H_2	Based on reaction thermodynamics (300 kJ/mol $NaBH_4$)
	Catalyst	Ru on Ni substrate	MCell: Zhang, et al (NHA '04) and conversation w/ Wu and Mohring
	Catalyst Concentration	1 wt% of substrate	
	Conversion Efficiency	92%	MCell: Zhang, et al (NHA '04). Reactor sized to deliver up to 40% peak demand flow (1.6 g H_2/s) at 92% conversion. Reactor will also deliver 100% peak demand flow, but at lower conversion efficiency.
	Reactor Throughput (SLPM H_2 / liter reactor)	120	
	Peak Operating Temp	145 °C	MCell Natrium vehicle
	Max. Pressure	6 bar (88 psig)	MCell Natrium vehicle
Gas-Liquid Separator	Settling Velocity	~0.1 m/s	Chem-Pet Process Technology Ltd (Monnery '00) and various manufacturers' product literature
	Aspect Ratio, L/D	3.3 - 5	
Condenser	Max. Heat Duty	32 kW	Calculated duty to condense H_2O from H_2 stream at full power
	Exit Temp / Humidity	70°C / 100% RH	Assumed fuel cell operating conditions
	Max. Ambient Temp	50 °C	FreedomCAR Targets (includes solar load)
	Fan Power	750 W	TIAX heat exchanger design calculation

Multi-variable sensitivity analysis is used to estimate the dependence and sensitivity of cost on/to the critical cost drivers.

Multi-Variable Sensitivity Analysis: Example – Sodium Alanate Media Cost

Media Cost	$/kWh
Mean	5.64
Std. Dev.	0.75
Base Case	4.85



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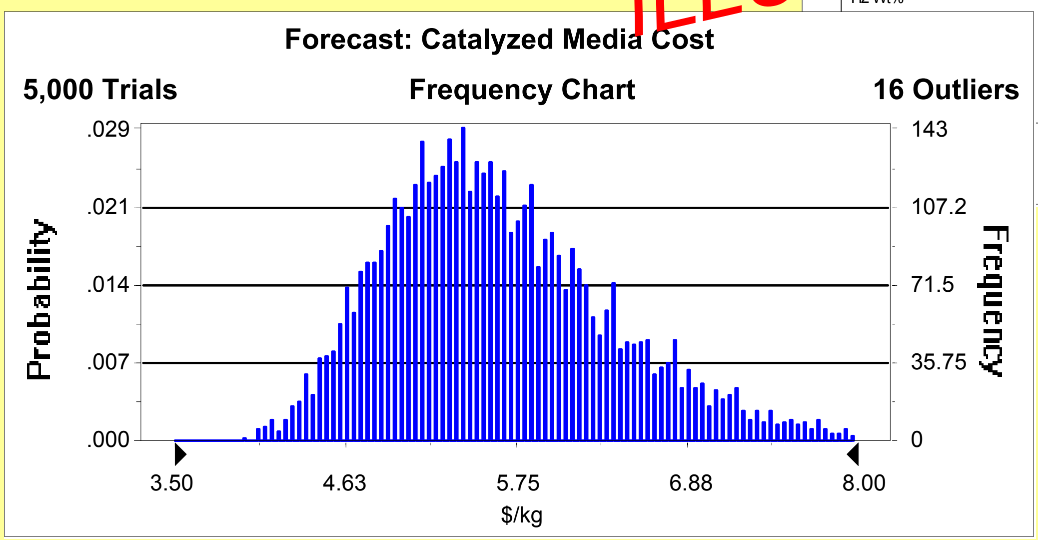

Well-to-Tank energy use and GHG emissions will be calculated using the appropriate fuel cycle efficiencies and GHG factors.