Analyses of Hydrogen Storage Materials and On-Board Systems

Project ID # ST19

DOE Merit Review
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Reference: D0268

This presentation does not contain any proprietary or confidential information

Timeline

- Start date: June 2004
- End date: Sept 2009
- 14% 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
- FY04 = $112k
- FY05 = $200k

Partners

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

Objectives

- Overall: Help guide DOE and developers toward promising R&D and commercialization pathways by evaluating the various on-board hydrogen storage technologies on a consistent basis
- Past Year: Develop system-level designs and estimate the cost, weight, and volume for a base case metal hydride/alanate hydrogen storage system
  - Selected sodium alanate as the base case
  - Developed results and compared to DOE targets and results for compressed hydrogen storage

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

Performance/ Tech Assessment

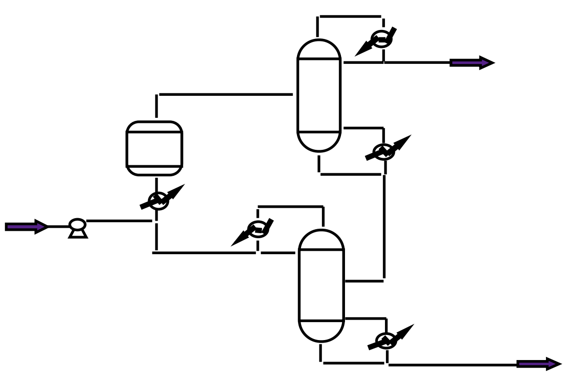
- Literature Search
- Outline Assumptions
- System Design and Configurations
- Process Models

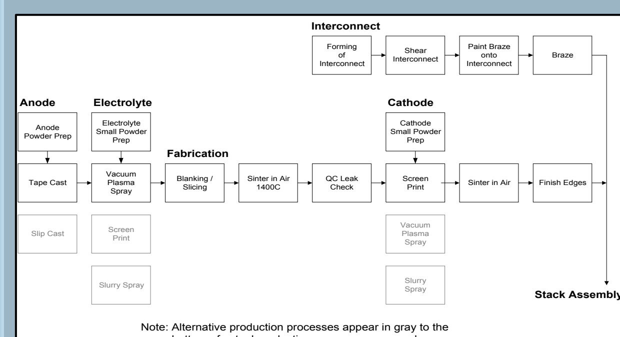
Cost Modeling

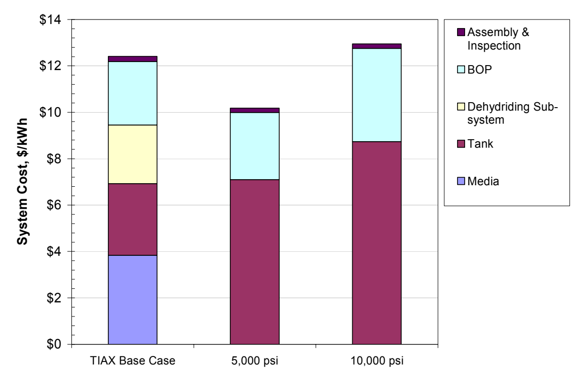
- Document BOM
- Determine Material Costs
- Identify Processes and Mnf. Equipment
- Sensitivity Analyses

Overall Model Refinement

- Developer and Industry Feedback
- Revise Assumptions and Model Inputs







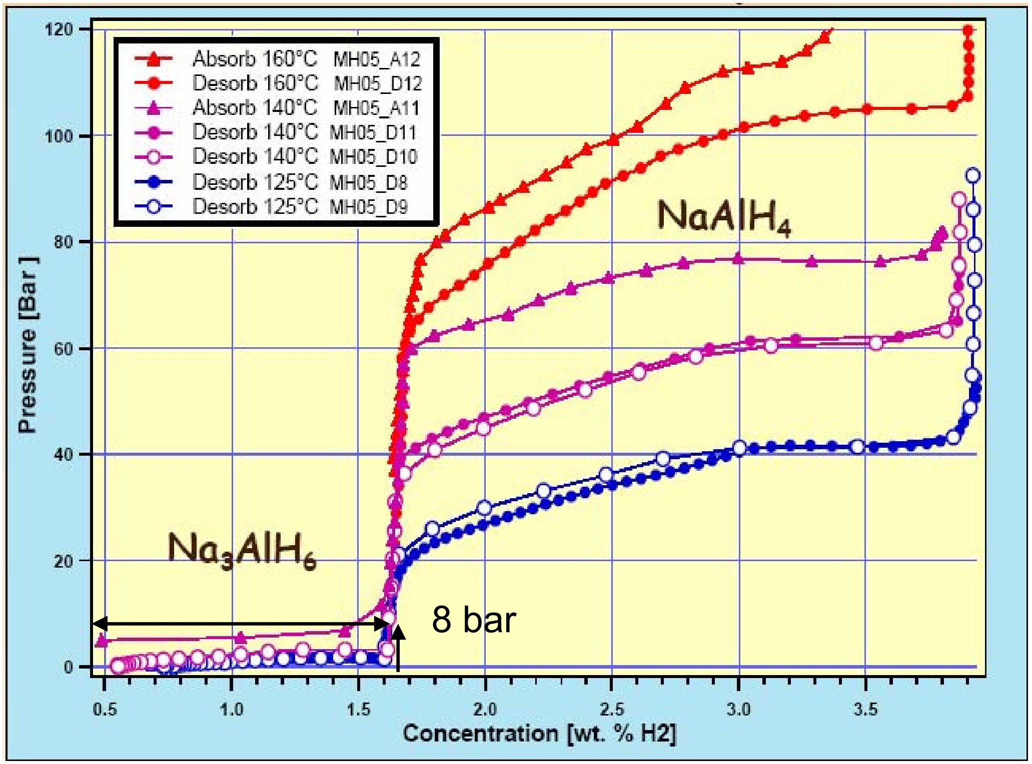
BOM = Bill of Materials

We made design assumptions for the $NaAlH_4$ system based on literature review, developer feedback and TIAX experience.

	Design Parameter	Value	Basis
Media	H_2 Storage Capacity	5.6 kg	ANL drive-cycle modeling
	$NaAlH_4$ H_2 Capacity	4 wt%	UTRC (Anton, Merit Review, May 04)
	Catalyst	$TiCl_3$	Bogdanovic & Schwickardi, JAC 97
	Catalyst Concentration	4 mol%	Bogdanovic & Sandrock, MRS 02
	Powder Packing Density	0.6	UTRC (Anton, Merit Review, May 04)
Thermal	Heat of Decomposition	41 kJ/mol H_2	Reaction thermodynamics
	Min. Temperature	100 ^oC	SNL (Wang, Merit Review, May 04)
	Max. Temperature	186 ^oC	SNL (Gross, JAC 02)
	Media Conductivity	< 1 W/m K	SNL (Wang, Merit Review, May 04)
	Media (hydrided) Specific Heat	1,418 J/kg K	SNL (Dedrick, JAC 04 - draft)
	Al Foam Conductivity	~52 W/m K	Metal Foams ~ k_{eff}=0.28$k_{Al@473K}$
	Al Specific Heat	~912 J/kg K	Aluminum alloy 2024 @473K
Mechanical	Max. Pressure	100 bar (1470 psi)	UTRC (Anton, Merit Review, May 04)
	Pressure Safety Factor	2.25	Industry standard
	Liner Thickness	2 mm (14 ga)	Estimate required for integrity

We assume $NaAlH_4$ decomposes in a reversible two step reaction to achieve 4 wt% H_2 under practical conditions.

- Theoretical = 5.6 wt%
- "Demonstrated" ~ 4 wt% (absorption/desorption)
  - P ~ 100 / 2 bar
  - T ~ 100 / 120 ˚C
- $TiCl_3$ + $NaAlH_4$ = 3.2 wt%
  - 4 mol% Ti-precursor added to catalyze reaction
  - Ti + $NaAlH_4$ = 3.8 wt%
- High pressure output (e.g. 8 atm) would limit to 1st Step

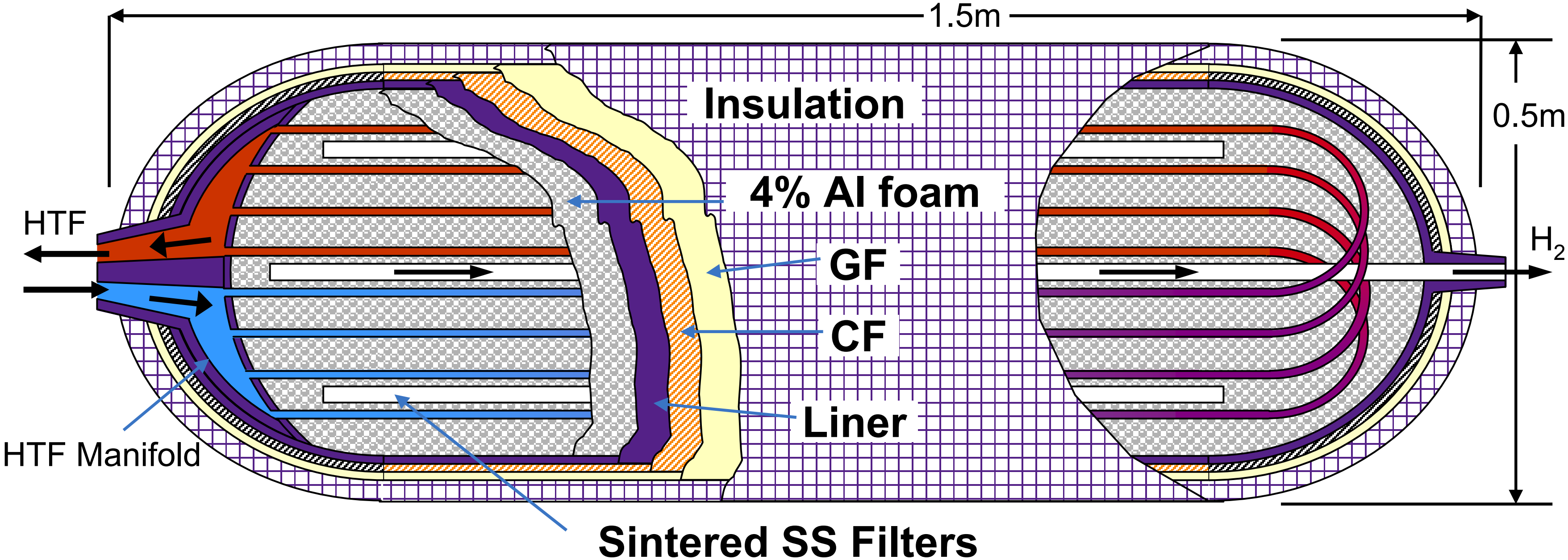


Reference: Gross, K. (SNL) presentation at DOE Hydrogen and Fuel Cells Annual Merit Review, May 2003

1st Step:	$NaAlH_4 \leftrightarrows 1/3\ Na_3AlH_6 + 2/3\ Al + H_2(g)$	H_2 wt%=3.7
2nd Step:	$Na_3AlH_6 \leftrightarrows 3\ NaH + Al + 3/2\ H_2(g)$	H_2 wt%=1.9

We developed a conceptual design for a tank to accommodate rapid heat exchange and high adsorption pressure conditions (100 bar).

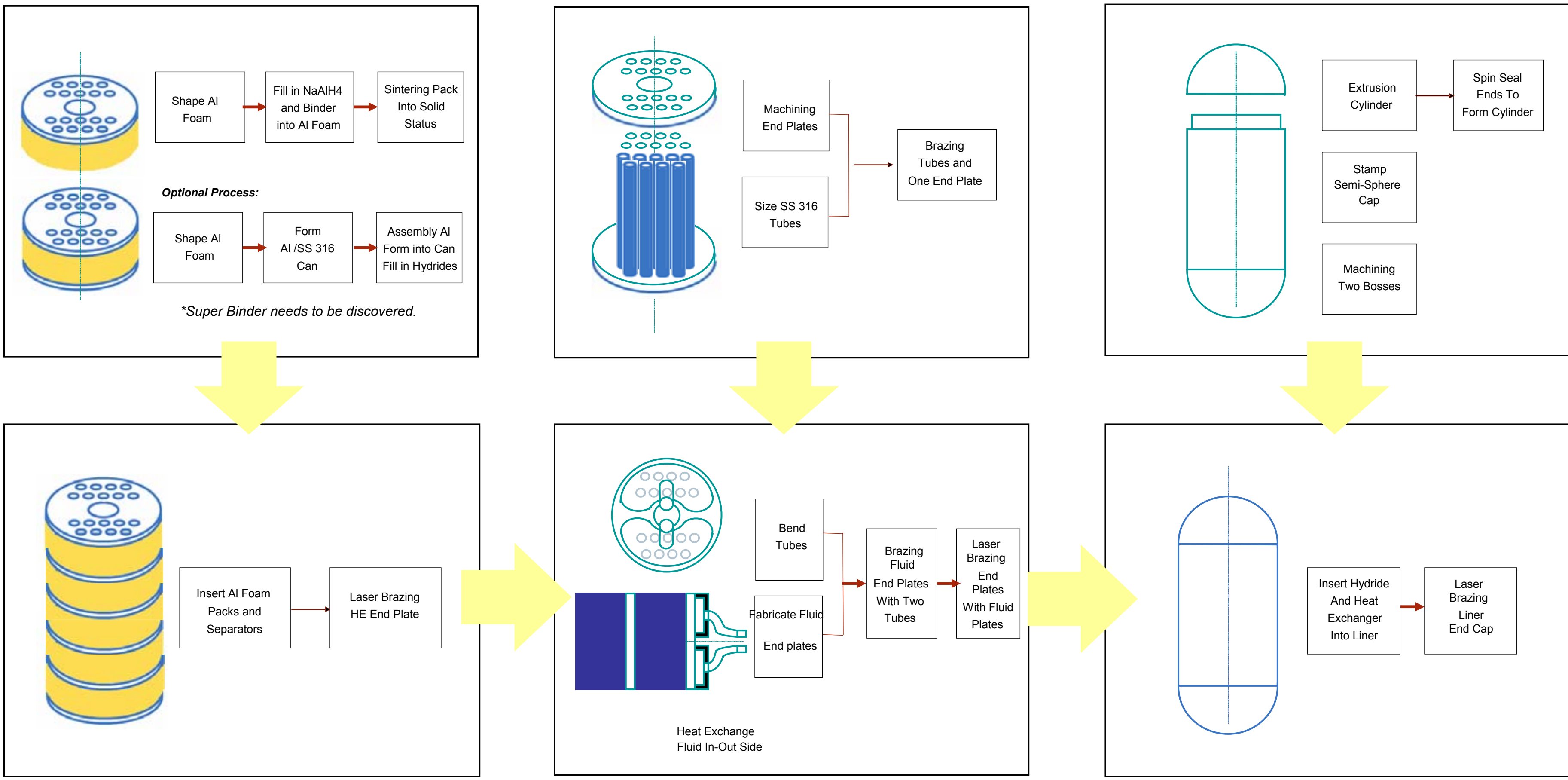
TIAX Base Case Design (5.6 kg H_2): Carbon Fiber Composite Tank



Metal Foam

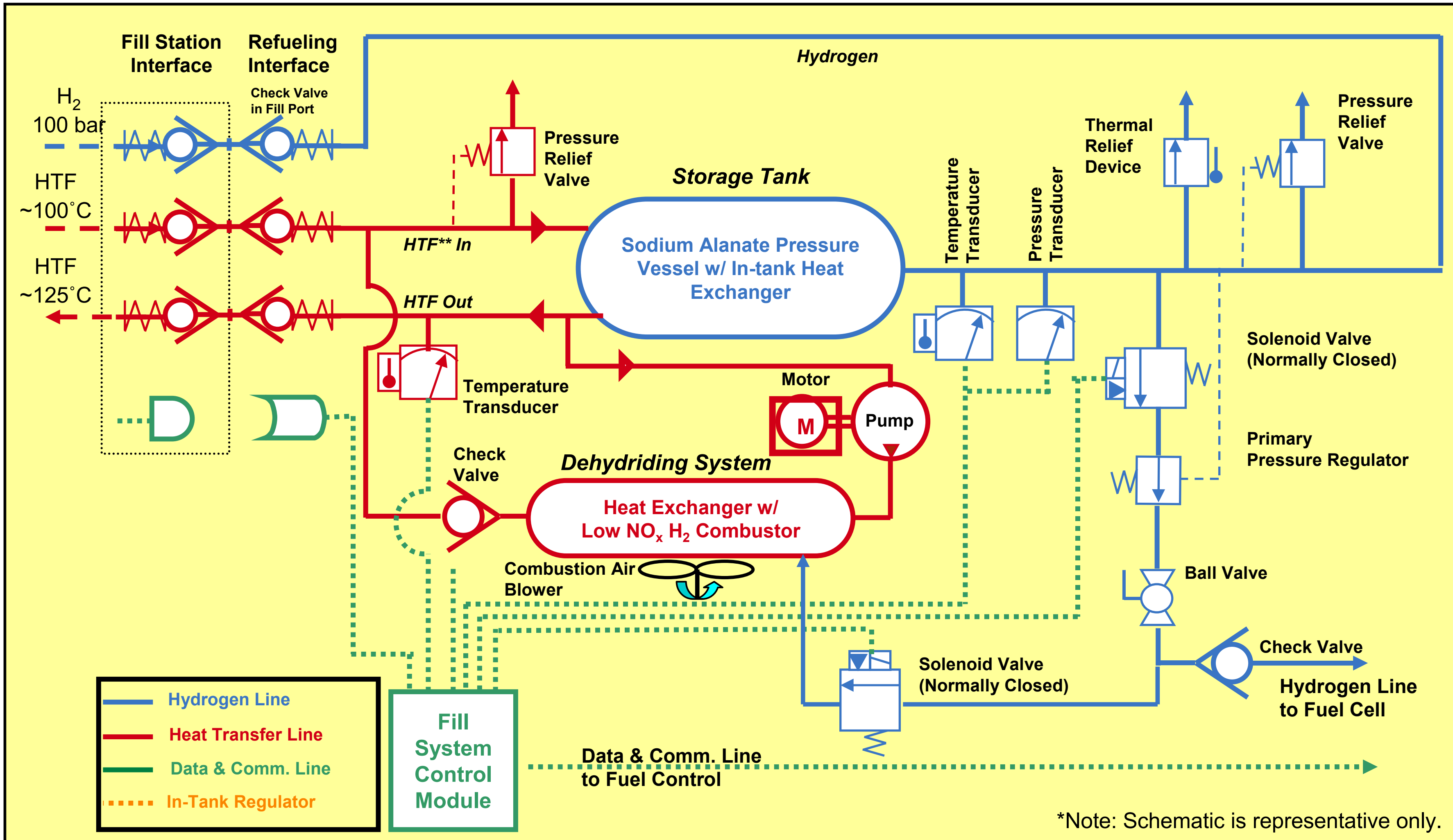
Legend	
Al = Aluminum	HTF = Heat Transfer Fluid
GF = Glass Fiber	HX = Heat Exchanger
CF = Carbon Fiber	SS = Stainless Steel

We assumed a tank manufacturing process that loads the alanate in several automated steps under an inert atmosphere.

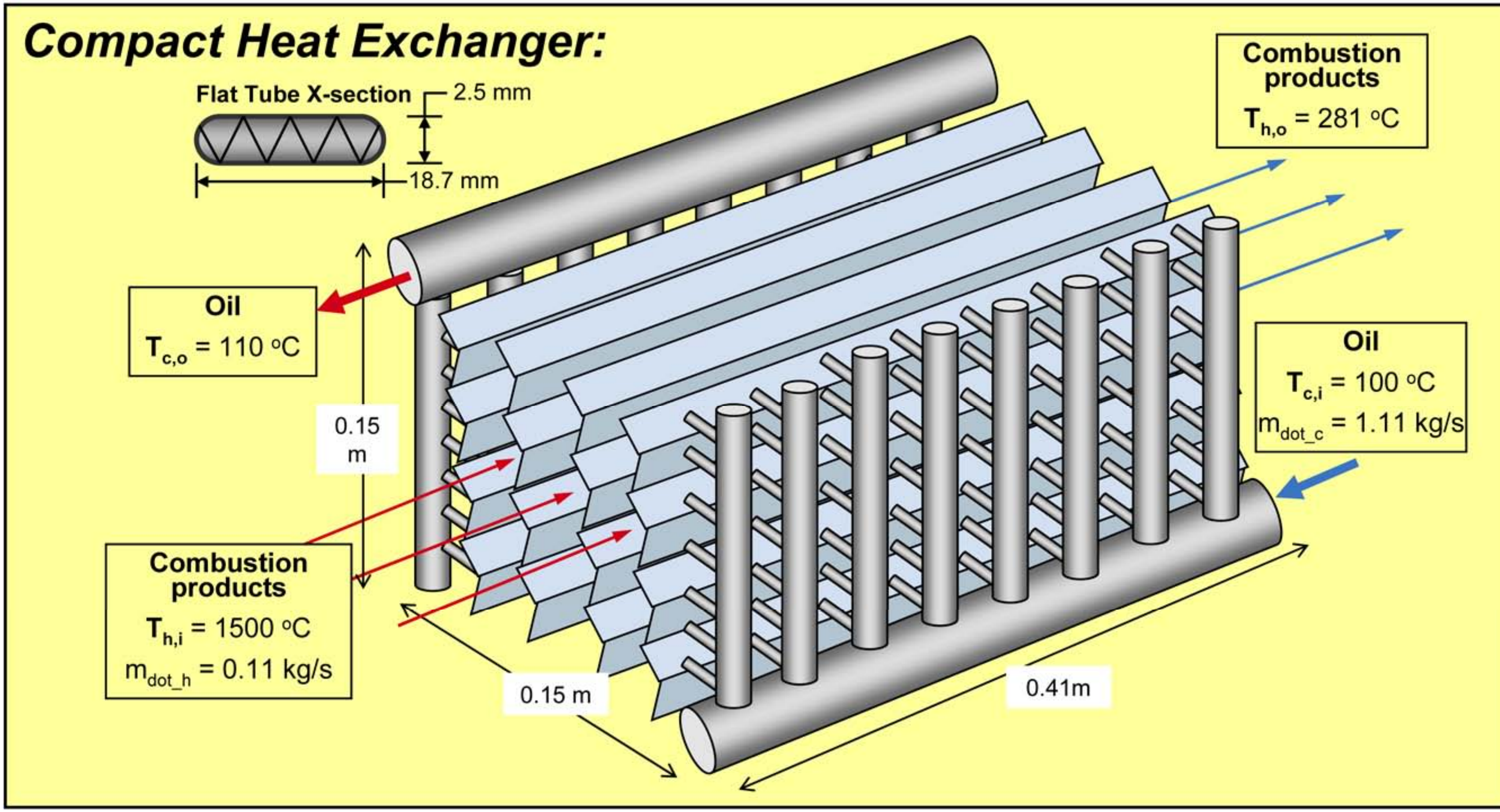


Alternative processes, such as loading the alanate in molten form after CF curing, may be necessary for high volume manufacture.

The complete system requires significant balance of plant (BOP) components for overall thermal management and flow control.



We sized a compact, fin and tube design for the heat transfer fluid (HTF) heat exchanger.

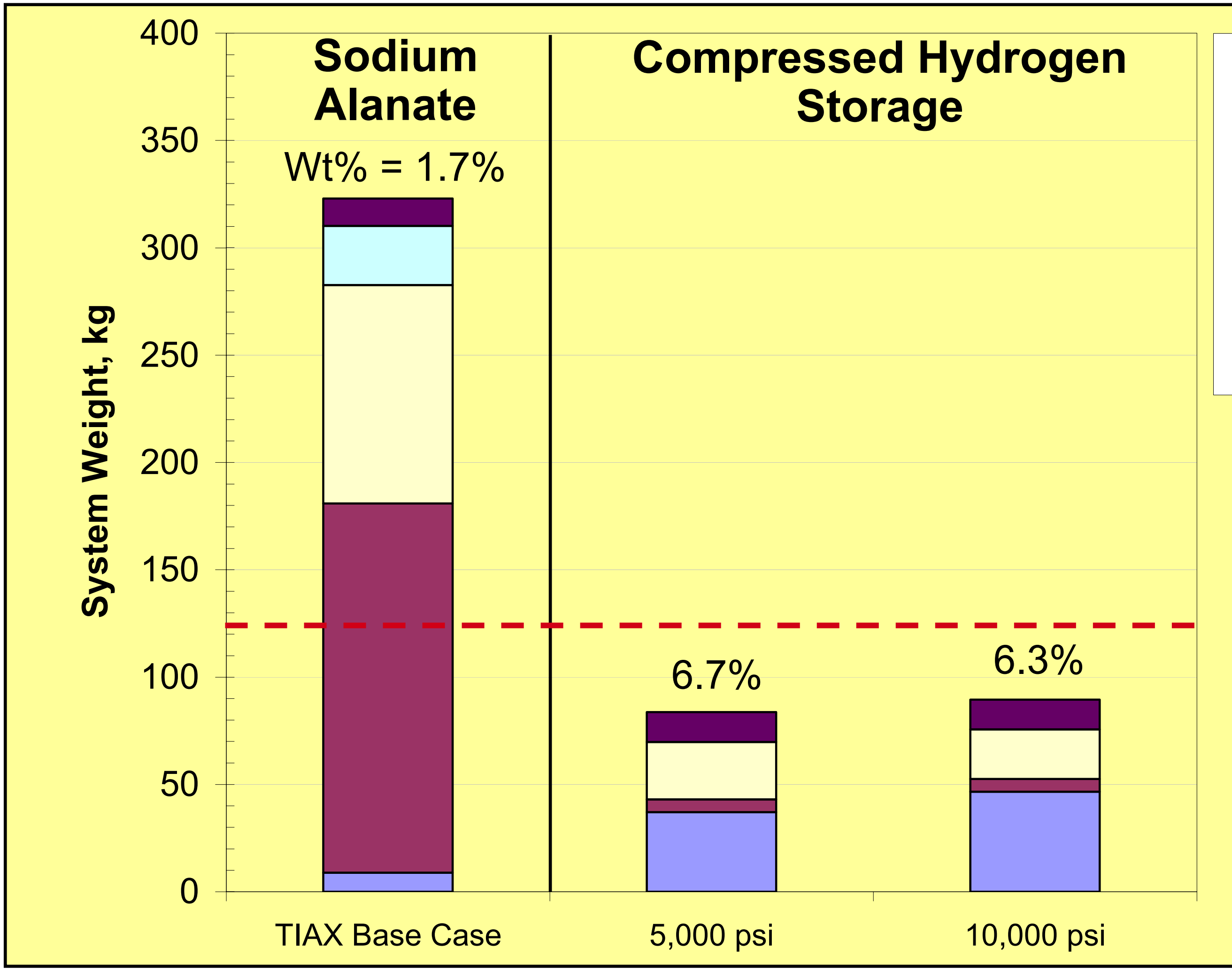


Thermal integration with the stack was not considered at this time.

We have identified a number of system-level issues that must be addressed by the on-going R&D.

Issues	Comments
Start-up	• 33 MJ (5% of 5.6 kg H_2) required to heat media from 0°C • Is secondary H_2 storage (or battery/electric heater) needed for start-up?
Material Life	• Limited cycling data • Powder and catalyst can segregate and lose effectiveness
Safety	• Powder is highly explosive, reacts with water or air • Is an inert atmosphere needed for vehicle refueling and tank manufacturing?
Thermal Integration	• 24% H_2 required for dehydriding heat • Is waste heat from power unit sufficient and coincident?
Refueling	• Two-fluid dispensing (H_2 gas and HTF) is required • Long refueling times (minutes or hours?)

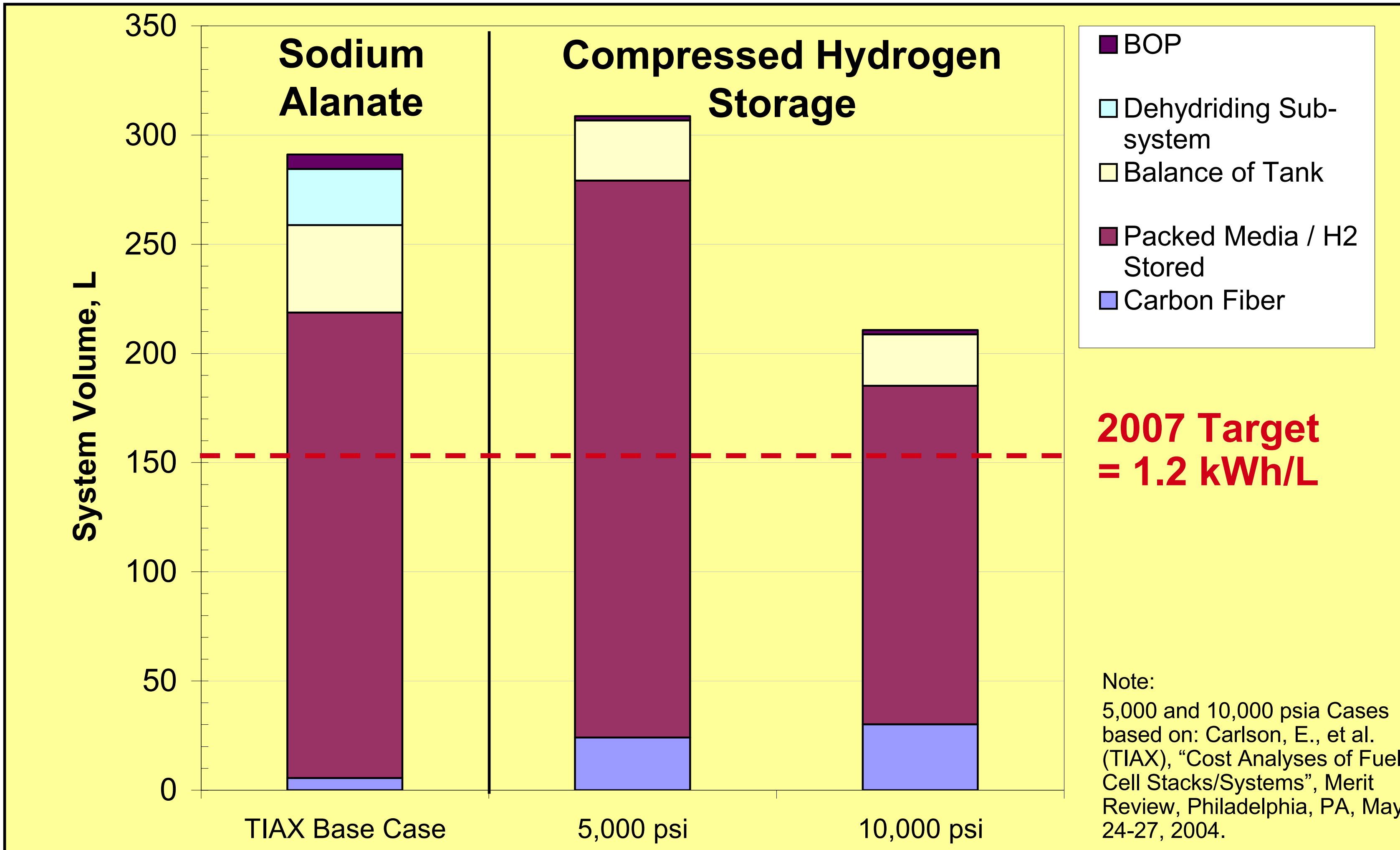
Sodium alanate will not meet the DOE weight target. Materials with greater than 7 wt% may be required to meet even the '05 target.



Note:

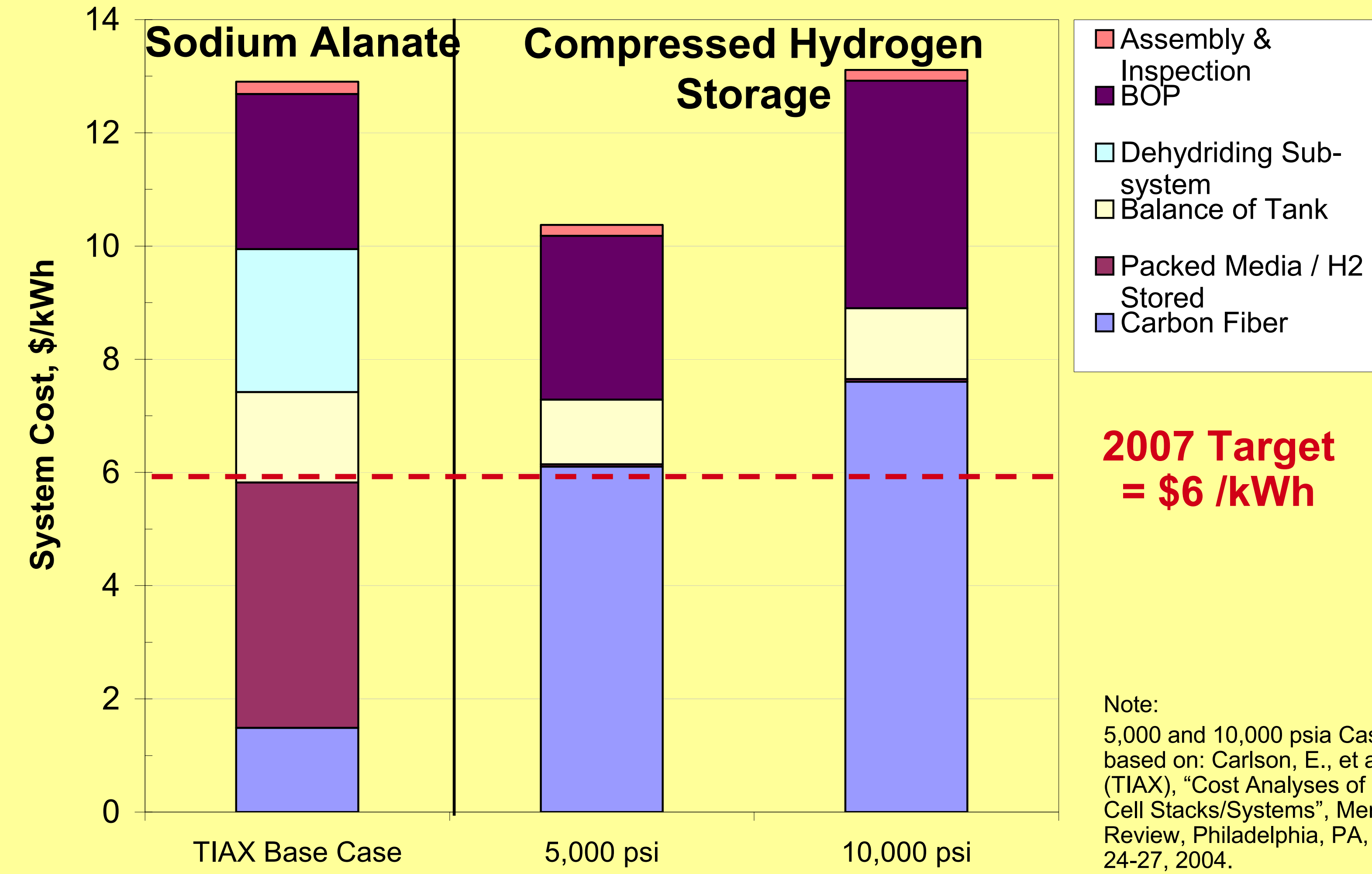
5,000 and 10,000 psia Cases based on: Carlson, E., et al. (TIAX), "Cost Analyses of Fuel Cell Stacks/Systems", Merit Review, Philadelphia, PA, May 24-27, 2004.

The sodium alanate system will likely be about 40% larger than the 10,000 psi compressed hydrogen storage system.



Note: Volume results do not include void spaces between components (i.e., 100% packing factor was applied).

Our assessment indicates the manufactured cost of a sodium alanate system will be on-par with 10,000 psi compressed gas.



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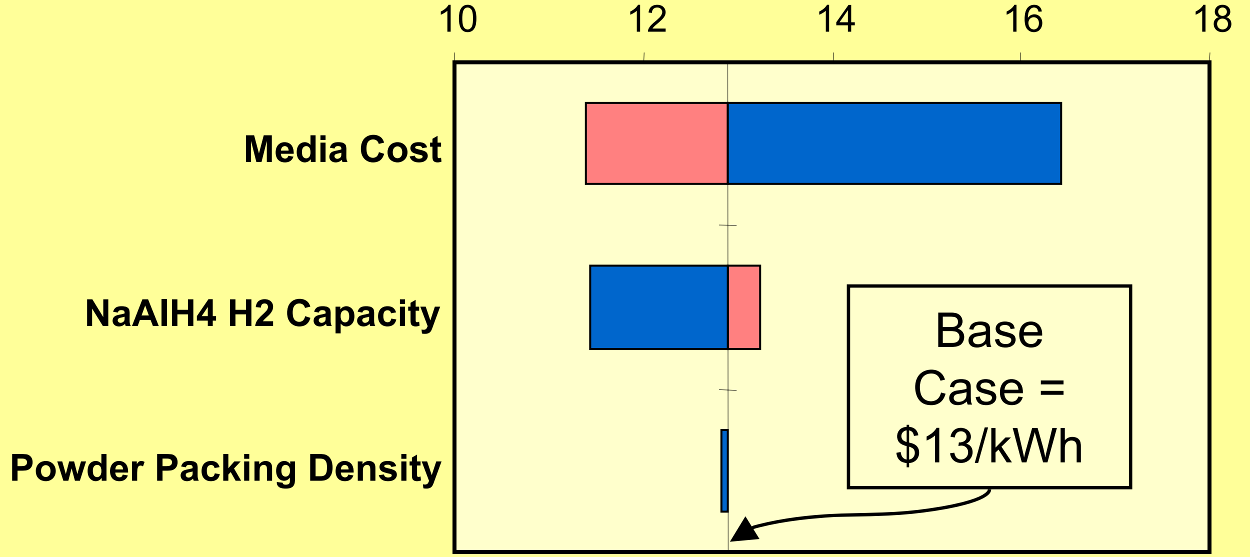
Assuming a very optimistic media cost of $3/kg reduces the overall cost of the system by less than 15%.

Sensitivity Analysis - Factory Cost ($/kWh)



Factors	TIAX Base Case		
	Baseline	Min	Max
Catalyzed Media Cost ($/kg)	5.2	3	10
$NaAlH_4$ H_2 Capacity	4%	3.7%	5.6%
Powder Packing Density	0.6	0.6	0.9

Conclusions

- Media hydrogen capacity
  - Some alanates could have higher reversible wt%
  - But more challenging thermal requirements
  - May need >13 wt% to achieve 9 wt% target
- Other material issues
  - Kinetics are slow—refueling and transient response
  - Life is unknown—cycling and poisoning
- Tank and BOP
  - ~60% of system cost and ~50% of system weight
  - Containment and contamination
- System integration
  - Thermal integration with power unit is critical
  - 1.24X larger if H_2 needed for dehydriding reaction is included

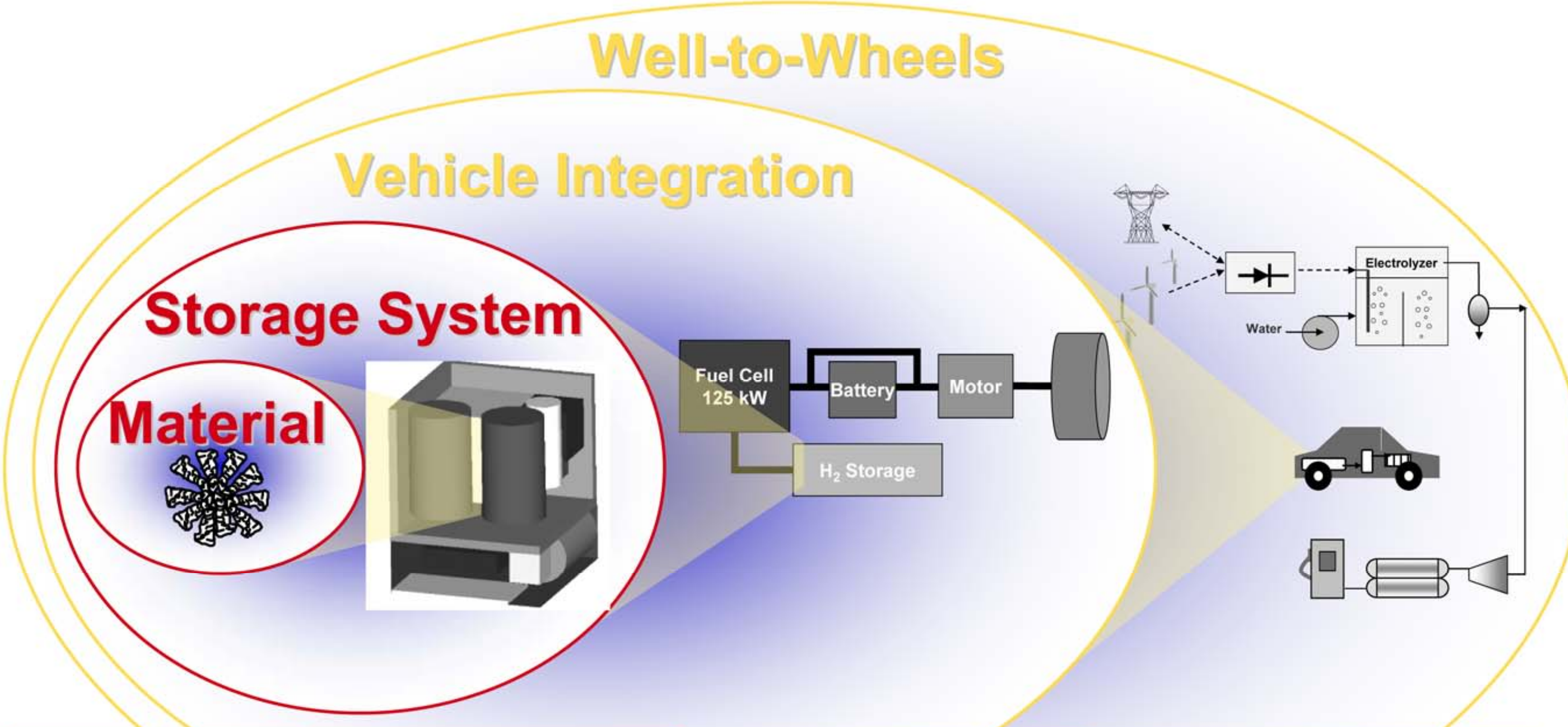
We are in the process of evaluating the base case for chemical hydrides and will begin the assessment of high surface area sorbents in 2006.

Storage Technology	Status	Base Case	Tech Status	Storage State	H_2 Release	Refuel-ing
Compressed and Liquid Hydrogen	Done 2003*	5,000 psi	Mature	Gas	Pressure regulator	H_2 gas
Reversible On-board: Alanates	Done 2005	Sodium Alanate	Early proto-type	Solid	Endo-thermic desorption	H_2 gas and HTF loop
Regenerable Off-board: Chemical	WIP 2005	Sodium Boro-hydride	Proto-type	Aqueous solution	Exo-thermic hydrolysis	Aqueous solution in/out
High Surface Area Sorbents: Carbon	2006	TBD	R&D	Solid (low T?)	Endo-thermic desorption	H_2 gas (low T?)

[1] HTF = Heat Transfer Fluid

* Compressed hydrogen was evaluated under a separate DOE contract.

In future work, we will evaluate overall WTW performance and lifecycle cost for all the hydrogen storage options.



- Material wt %
- P, T requirement
- Thermo, kinetics

- BOP requirements
- System size, cost
- System issues

- Power unit and thermal integration
- Vehicle cost, weight
- Fuel economy

- Fuel chain requirement
- Ownership cost
- WTW energy, GHG

Publications and Presentations

- Presentations under the title: "Analyses of Hydrogen Storage Materials and On-Board Systems"; Lasher et al
  - Hydrogen Storage Tech Team Meeting; April 21, 2005; Detroit MI
  - Storage System Analysis Meeting; March 29, 2005; Washington DC
  - Hydrogen Storage Tech Team Meeting; August 19, 2004; Detroit MI
- Presentations under the title: "Comparison of Hydrogen Storage Options"; Lasher et al
  - NHA Annual Hydrogen Conference; March 30, 2005; Washington DC

Hydrogen Safety

- The most significant hydrogen hazard associated with this project is:
  - None
  - This is an analysis project with no on-going or proposed hands-on laboratory or hardware development work
- Our approach to deal with this hazard is:
  - None required