Hydrogen Storage Engineering
CENTER OF EXCELLENCE

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SAVANNAH RIVER NATIONAL LABORATORY

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Project ID#ST004

Overview

Timeline

- Start: February 1, 2009
- End: July 31, 2014
- 40% Complete (as of 3/31/11)

Budget

- Total Center Funding:
  - DOE Share: $ 40,715,000
  - Contractor Share: $ 3,901,000
  - FY '10 Funding: $ 8,344,000
  - FY '11 Funding: $ 6,775,000
- Prog. Mgmt. Funding
  - FY '10: $ 570,000
  - FY '11: $ 600,000

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
K. System Life-Cycle Assessment
O. Hydrogen Boil-Off
P. Understanding Physi/Chemi-sorption
S. By-Product/Spent Material Removal

Partners

SRNL Savannah River National Laboratory
Pacific Northwest National Laboratory
Los Alamos National Laboratory
JPL Jet Propulsion Laboratory California Institute of Technology
NREL National Renewable Energy Laboratory
California Institute of Technology
Michigan
OSU Oregon State University
HRI UQTR
Ford
GM
United Technologies Research Center
BASF The Chemical Company
Lincoln Composites A Member of Hexagon Composites Group

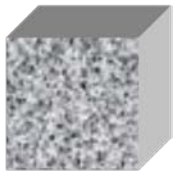
HSECoE

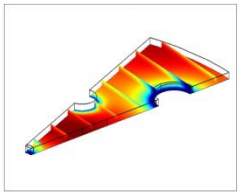
Center Goals

- **Quantify the requirements** for condensed phase hydrogen storage systems for light duty vehicle applications.
- **Coordinate with all other DOE hydrogen storage programs** to compile their data and systems requirements.
- **Identify the current state-of-the-art** for metal hydride, chemical hydride and adsorbent hydrogen storage systems.
- **Identify the technical barriers** to be overcome in achieving the 2015 On-Board Hydrogen Storage System Technical Targets.
- **Identify solutions** to overcoming these barriers.
- **Demonstrate the individual technologies** required to achieve the 2015 On-Board Hydrogen Storage System Technical Targets.
- **Demonstrate subscale prototype systems** for each of the storage system types
- **Disseminate new design tools, methodologies, and component requirements** needed to develop condensed phase hydrogen storage systems for light duty vehicle applications.

Why Perform Materials Development and System Engineering in Parallel?

continuous feedback





Materials → Thermal Management → H_2 Storage BoP → Fuel Cell → Vehicle → Wheels

Engineered Materials Properties

Heat Transfer Designs

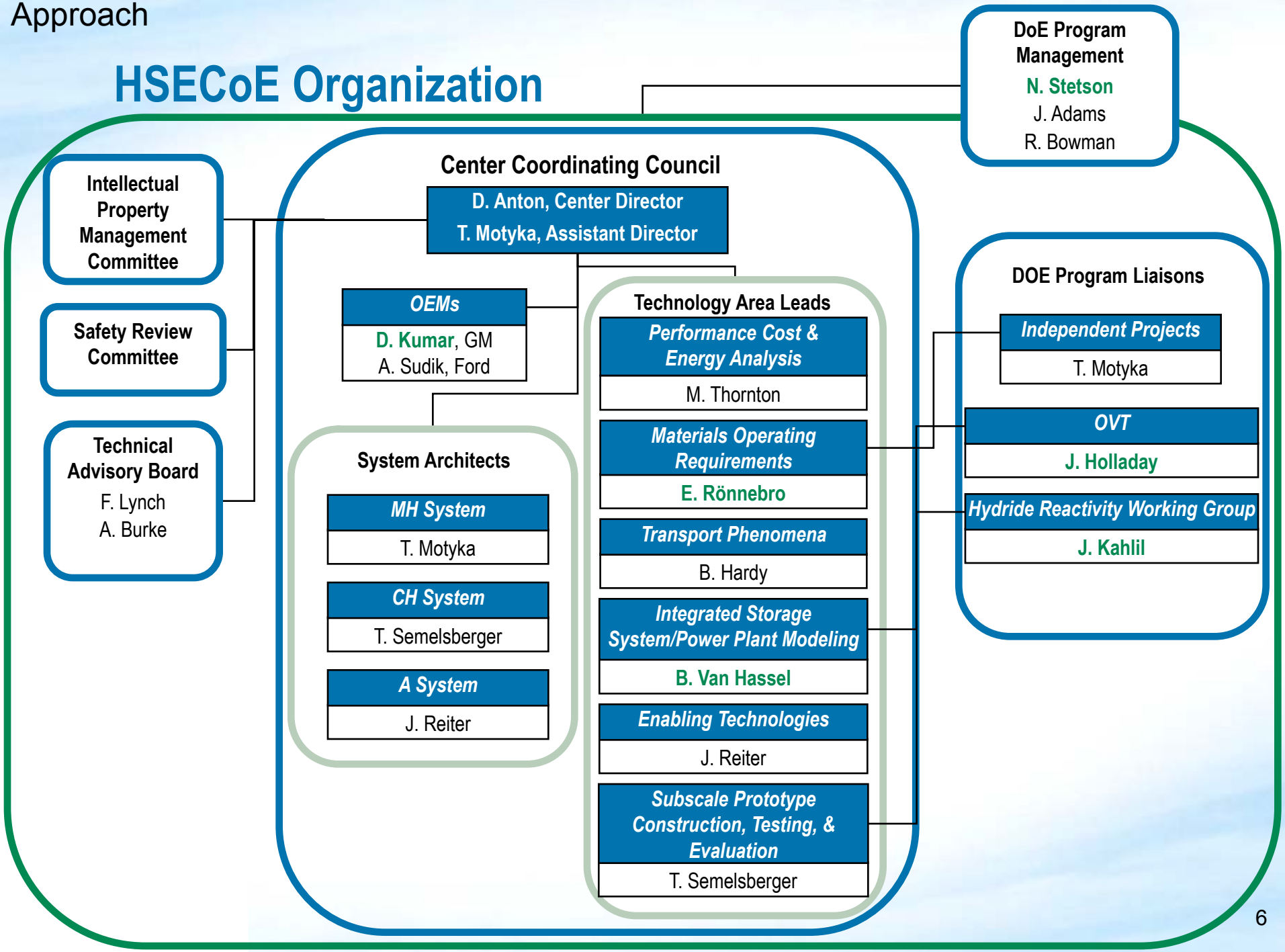
BoP Component Requirements

What is Really Needed of the Hydrogen Storage Media & System

Program Outline

- **Phase 1: System Requirements and Model Development**
  - Identify hydrogen storage system requirements, develop energy and thermal models, build BoP component catalogue, gather required media data and identify and fill voids in knowledge bank.
- **Phase 2: Novel Concepts: Model, Design & Evaluation**
  - Using developed models with an understanding of system technical barriers, identify and verify novel solutions to barriers culminating in selection of subscale prototype systems to move forward with demonstration
- **Phase 3: Subscale Prototype Construction & Evaluation**
  - Evaluate subscale prototypes to determine progress towards meeting 2015 technical targets and limits on current technologies.

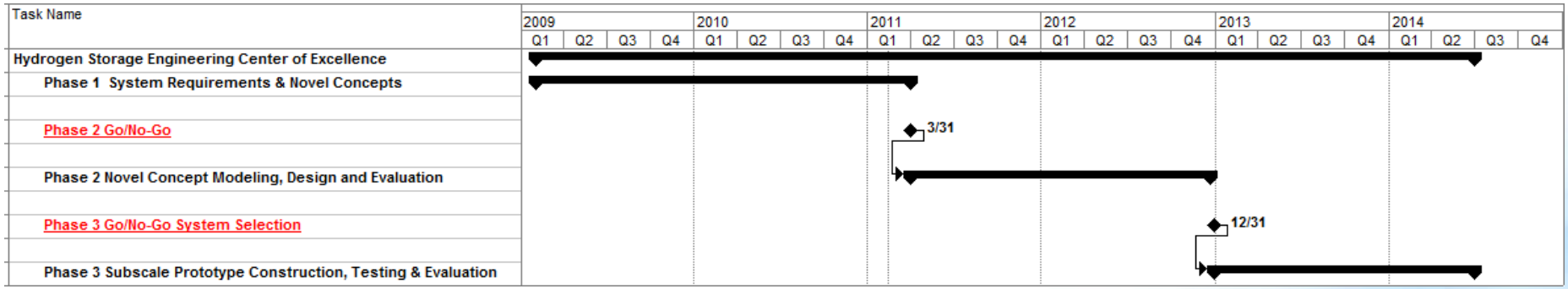
HSECoE Organization



Milestone

Important Dates

- Duration: 5.5 years
  - Phase 1 Start: Feb. 1, 2009
  - Phase 1-2 Transition: March 31, 2011
  - Phase 2 Start: April 1, 2011
  - Phase 3 Go/No-Go Determination: Dec 31, 2012
  - Phase 3 Start: July 1, 2013
  - Completion Date: June 30, 2014



HSECoE

Original HSECoE Go/No-Go Decision Metrics

Phase I / Phase II Go/No-Go Decision Q3 Y2:	Provide a **system model** for each material sub-class (metal hydride, adsorption, chemical hydride) which shows: • **4** of the DOE 2010 numerical system storage targets are fully met • The status of the remaining numerical targets must be at least **40%** of the target or higher
Phase II / Phase III Go/No-Go Decision Q2 Y4:	Provide at least one full scale system design concept (5kg H_2 stored) where: • **6** of the DOE 2015 numerical targets are fully met • The status of the remaining numerical targets must be at least **50%** of the target or higher

These Go/No-Go decisions require the HSECoE to consider and approach each of the DOE goals individually, and not concentrate only on one or two.

Revised HSECoE Go/No-Go Decision Metrics

Phase I / Phase II Go/No-Go Decision Q3 Y2:	Provide a **system model** for each material sub-class (metal hydride, adsorption, chemical hydride) which shows: • **4** of the DOE 2010 numerical system storage targets are fully met • The status of the remaining numerical targets must be at least **40%** of the target or higher

This approach requires consideration of all targets, but will be dominated by current materials properties which we know to be inadequate. Thus setting up the HSECoE for failure.

What really needs to be accomplished is to determine the engineering technical barriers, both in systems and in media, quantify their impact on target achievement and demonstrate the most capable hydrogen storage systems with the materials and technology available.

Revised HSECoE Go/No-Go Decision Metrics

	Provide a **system model** for each material sub-class (metal
	• The status of the remaining numerical targets must be at least **40%** of the target or higher

We will track to these targets, but with allowance given for current media limitations.

This approach requires consideration of all targets, but will be dominated by current materials properties which we know to be inadequate. Thus setting up the HSECoE for failure.

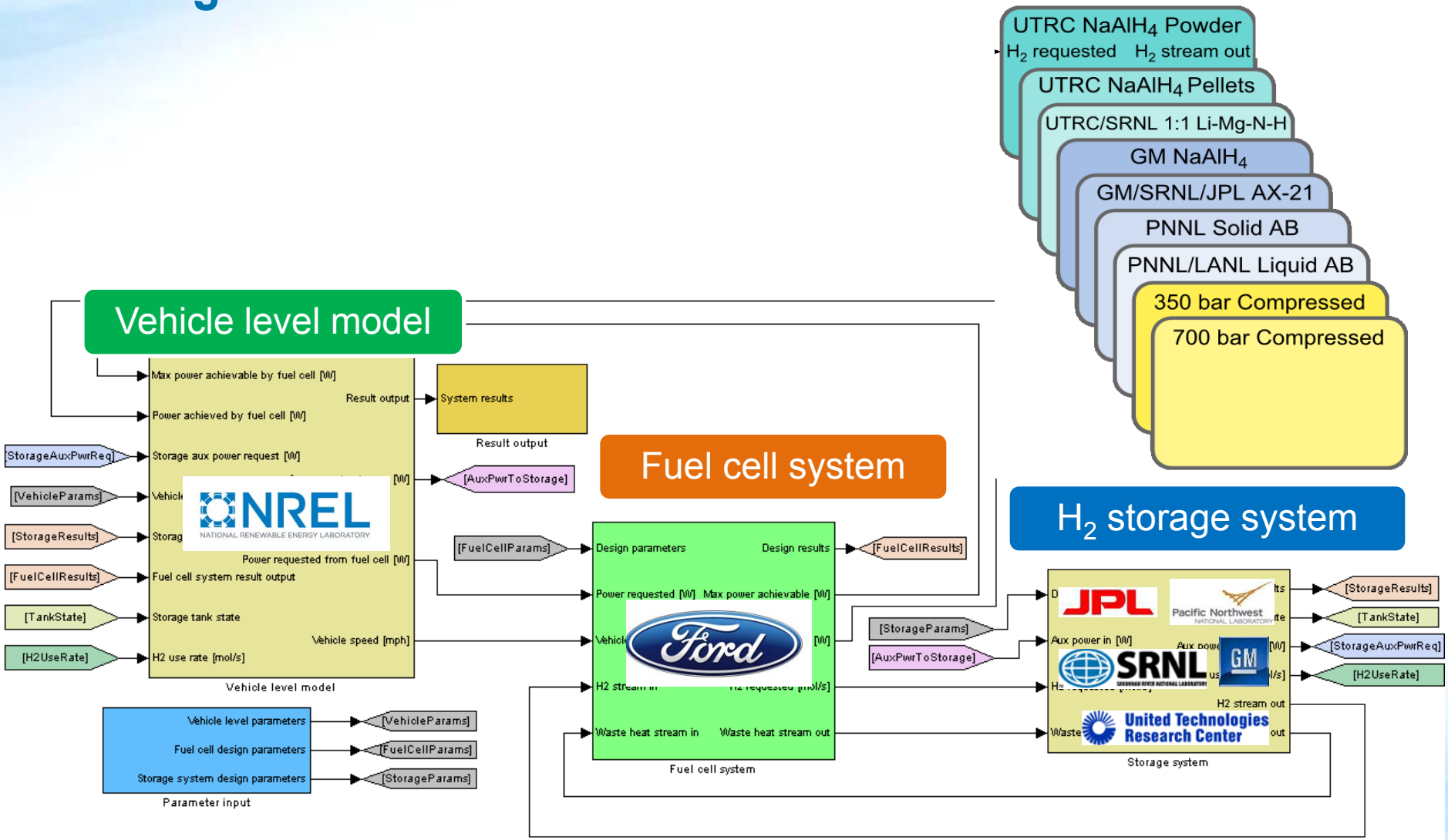
What really needs to be accomplished is to determine the engineering technical barriers, both in systems and in media, quantify their impact on target achievement and demonstrate the most capable hydrogen storage systems with the materials and technology available.

Revised HSECoE Go/No-Go Decision Metrics

Phase I / Phase II Go/No-Go Decision Q3 Y2:	Provide a system model for each material sub-class (metal hydride, adsorption, chemical hydride) which shows: • **Status towards** all of the DOE 2010 numerical system storage targets • Propose **viable technical approaches** which would allow meeting of DoE 2010 Technical Targets assuming reasonable storage media properties
Phase II / Phase III Go/No-Go Decision Q2 Y4:	Provide **full scale system design concepts** (5.6 kg H_2 stored) based on experimentally verified models which would allow **meeting of DoE 2015 Technical Targets** assuming reasonable storage media properties

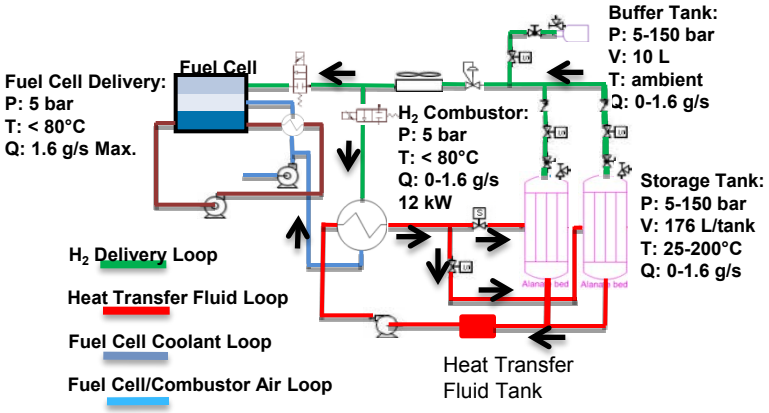
These Go/No-Go decisions require the HSECoE to consider and approach each of the DOE goals individually, with allowance given for current media limitations.

Integrated Model Framework

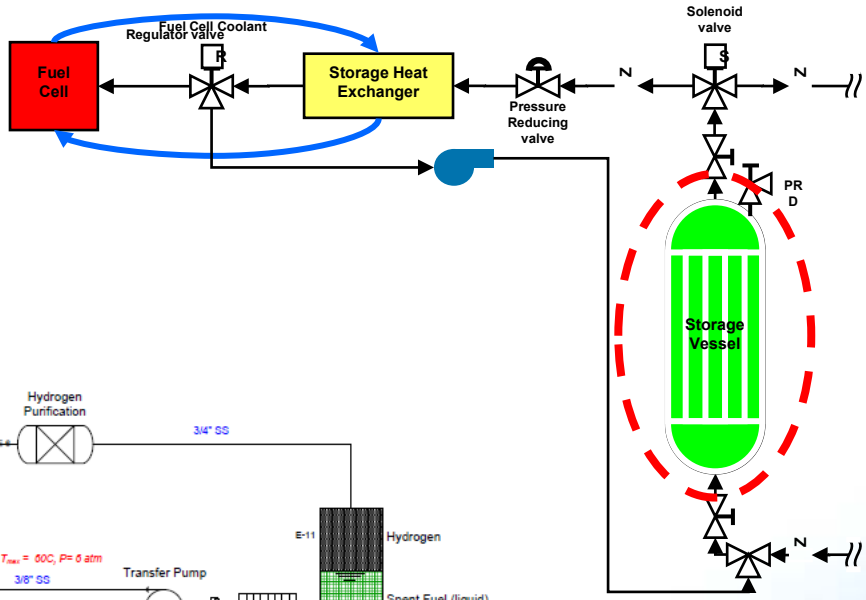


Storage System and BoP Design Concepts

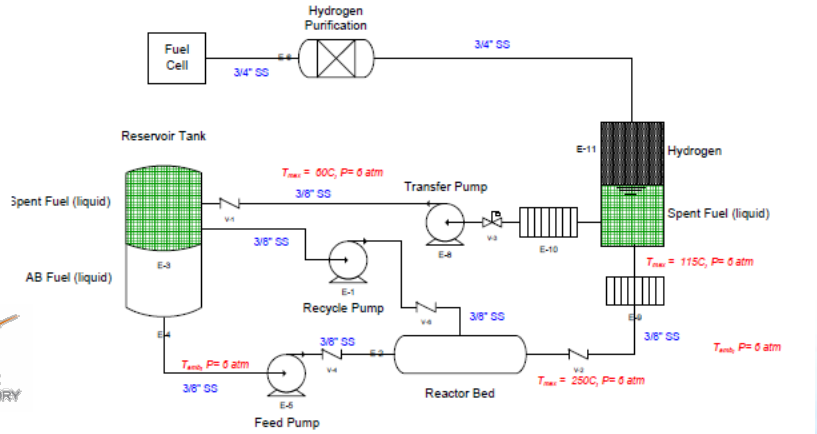
$NaAlH_4$ Metal Hydride Dual Tank System



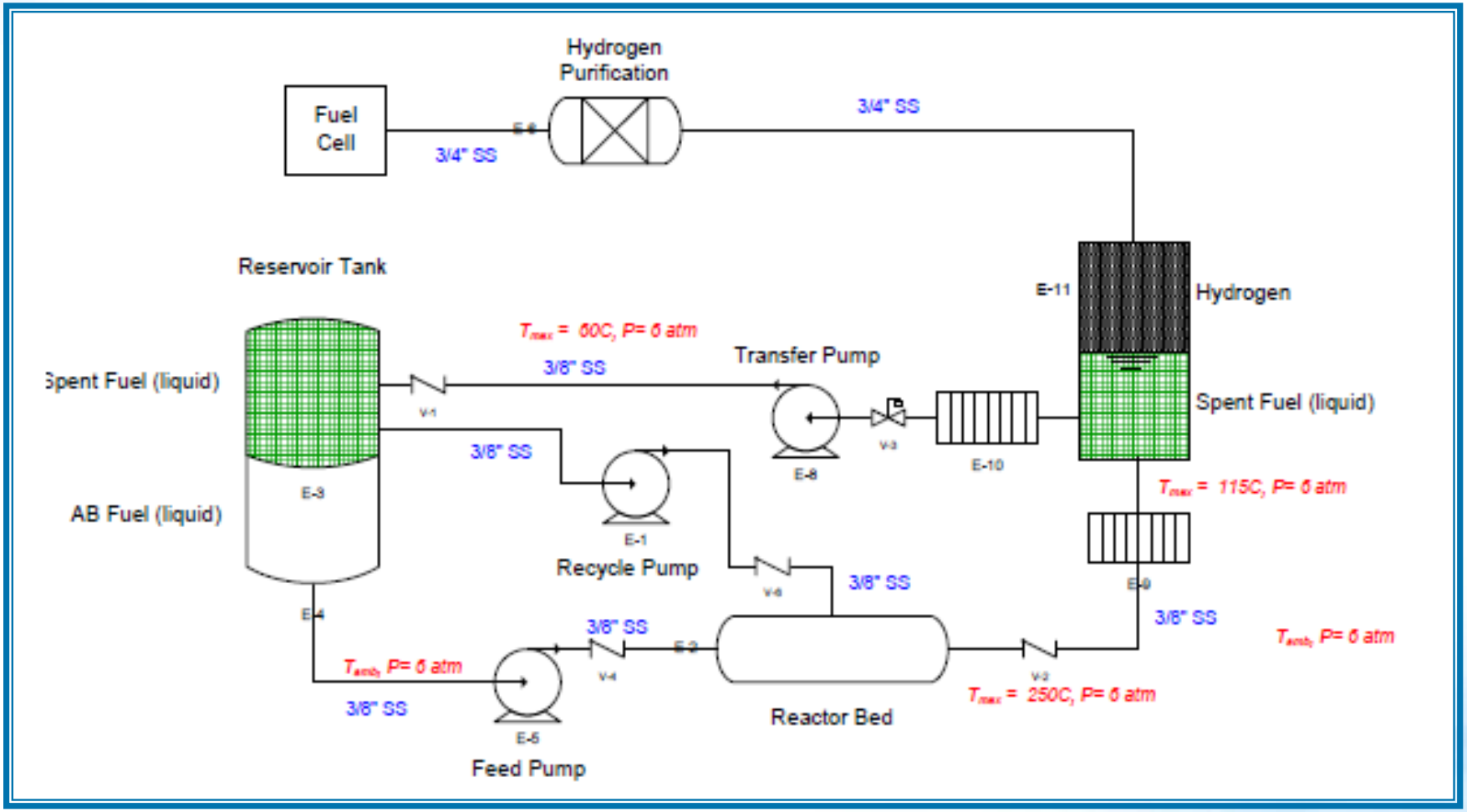
AX-21 Adsorbent Flow Through Cooling System



Fluid AB Chemical Hydride Flow Through Reactor System



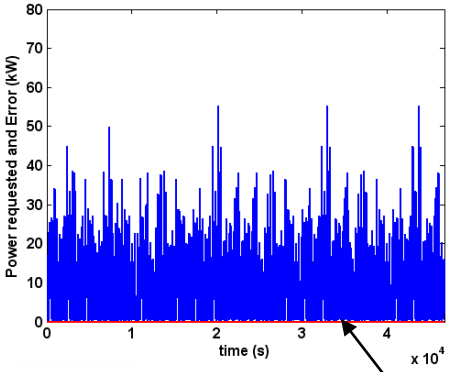
Details of Fluid AB Reactor Design

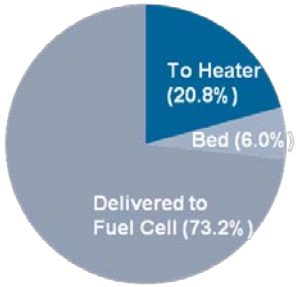


Drive Cycles and $NaAlH_4$ Dual Bed Drive Cycle Analysis

Drive Cycle	Test Schedule	Cycle	Description	Target	Temp. (°C)
1	**Ambient Drive Cycle** - Repeat the EPA FE cycles from full to empty and adjust for 5 cycle post-2008	UDDS	Low speeds in stop-and-go urban traffic	System Size	24
		HWFET	Free-flow traffic at highway speeds		24
2	**Aggressive Drive Cycle** - Repeat from full to empty	US06	Higher speeds; harder acceleration & braking	Min. Flow Rate & Transient Response	24
3	**Cold Drive Cycle** - Repeat from full to empty	FTP-75 (cold)	FTP-75 at colder ambient temperature	Start time to Full Flow Rate (-20°C)	-20
4	**Hot Drive Cycle** - Repeat from full to empty	SC03	AC use under hot ambient conditions	Start time to Full Flow Rate (20°C)	35
5	**Dormancy Test**	n/a	Static test of the storage system-31 days	Dormancy	35

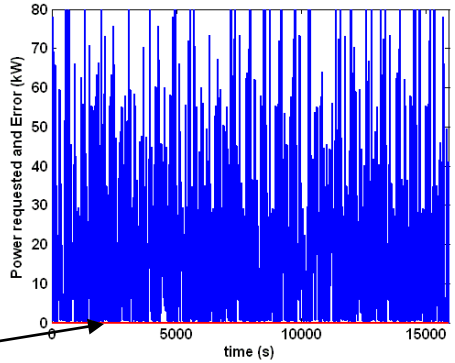
Ambient Drive Cycle

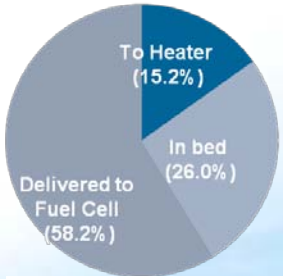




Hydrogen Utilization: Drive Cycle 1

Aggressive Drive Cycle





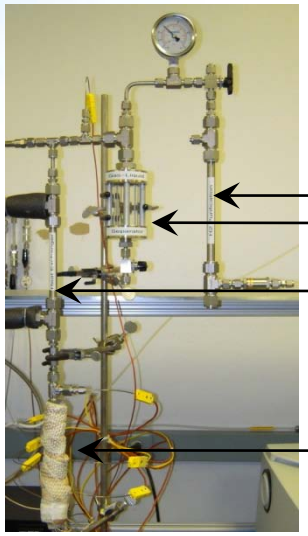
Hydrogen Utilization: Drive Cycle 2

Difference between demand and supply is shown in RED

Validation Experiments Planned/Underway

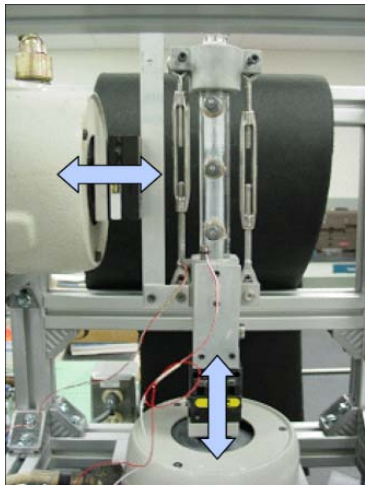
Fluid AB Flow Through Reactor

Los Alamos NATIONAL LABORATORY EST. 1943



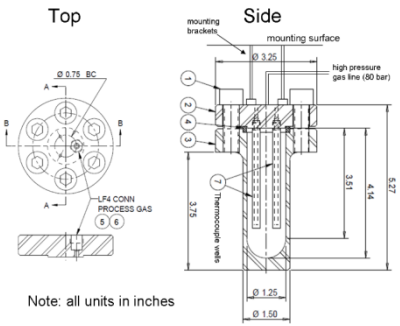
Cryogenic Adsorbent Component Test System

HRI UOTA



AX-21 Vibration Compaction

United Technologies Research Center



Neutron Imaging Of Adsorbent Component

Ford

MICHIGAN

Solid AB Mass Flow System

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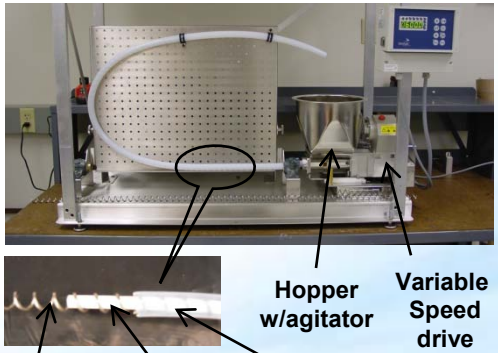
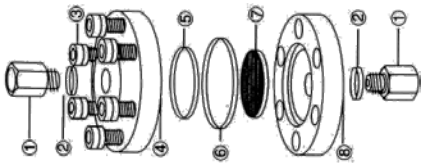


H2 Gas Stream Particulate Measurement



United Technologies Research Center

Permeability Measurement

Ford

HSECoE

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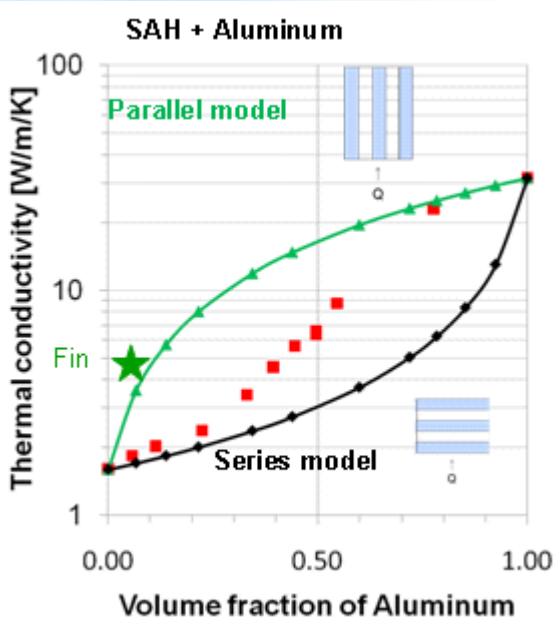
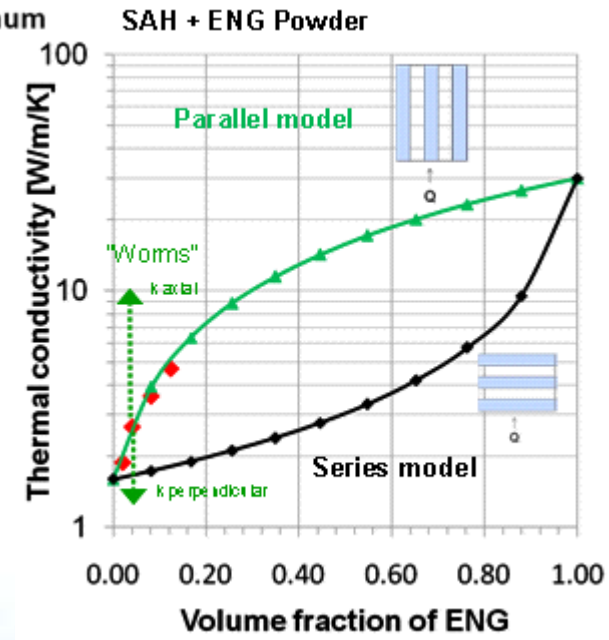
Pelletization/Thermal Conductivity Enhancement





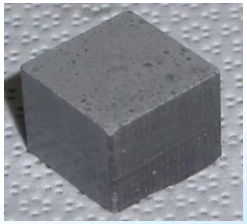
Transferability to Li-Mg-N-H system

as-milled

discharged

- **Requires thermal conductivity enhancement**

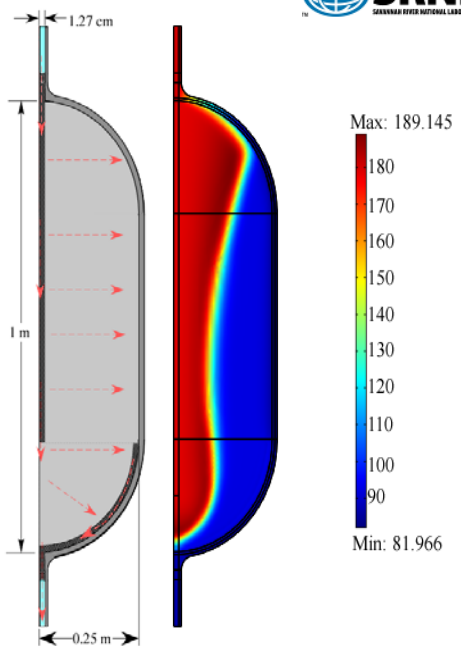
as-milled + 5 wt. % ENG



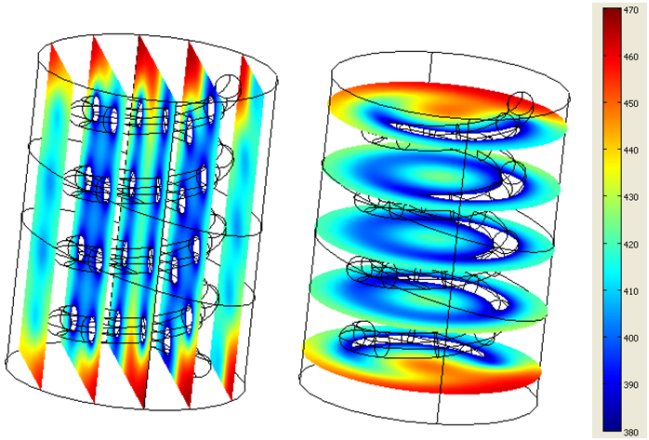
Transport Phenomena

Thermal Models

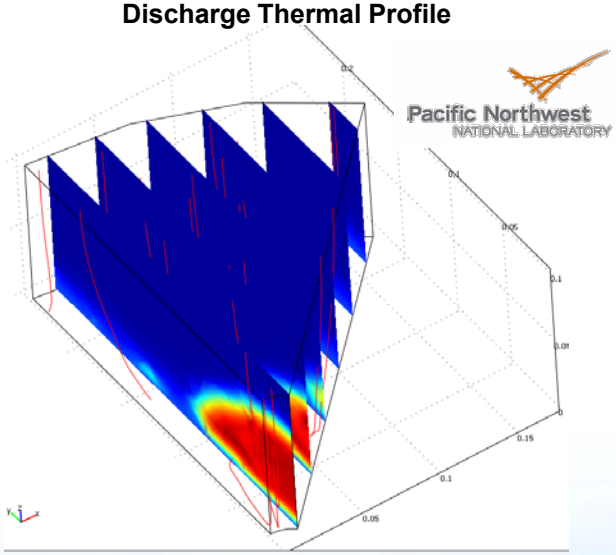
Adsorbent System
Discharge Thermal Profile



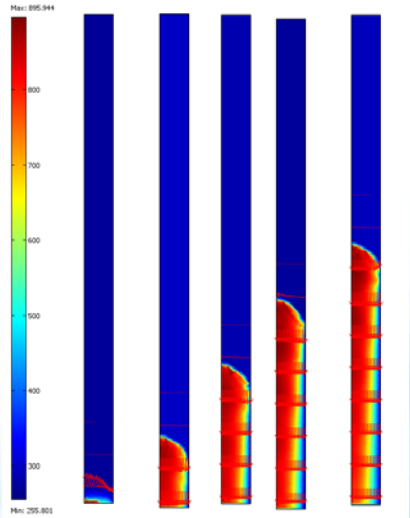
Metal Hydride System
Discharge Thermal Profile



Chemical Hydride Flow through Reactor
Discharge Thermal Profile



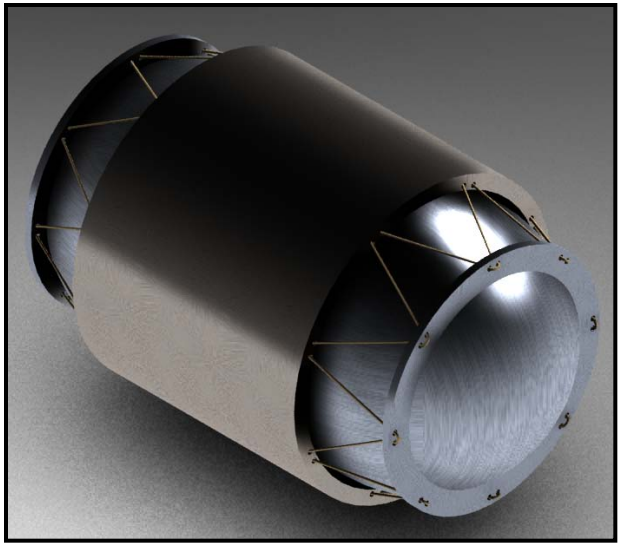
Fixed Bed Chemical Hydride Sys
Discharge Thermal Profile



Storage Component Concepts

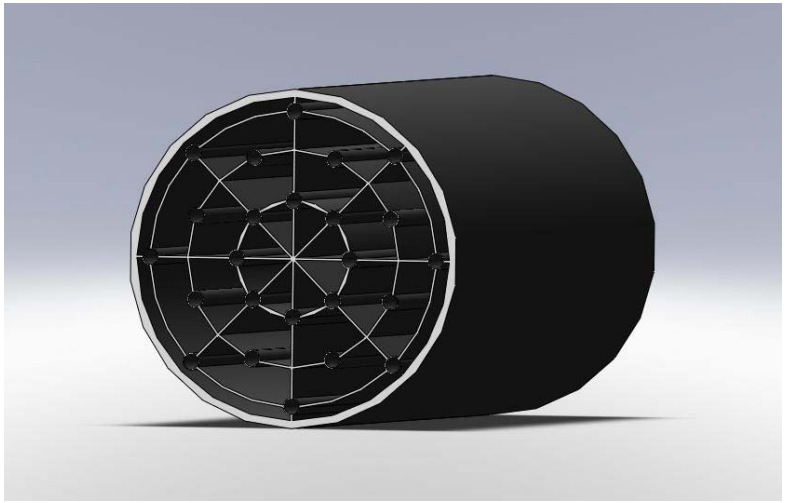
Adsorbent Vacuum Insulated Cryogenic Tank

JPL Jet Propulsion Laboratory California Institute of Technology



$NaAlH_4$ Metal Hydride Tank

GM



Fluid AB, Fixed Bed Chemical Hydride Tank

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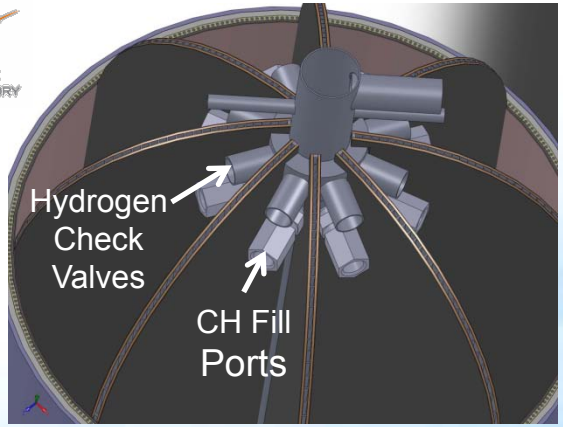
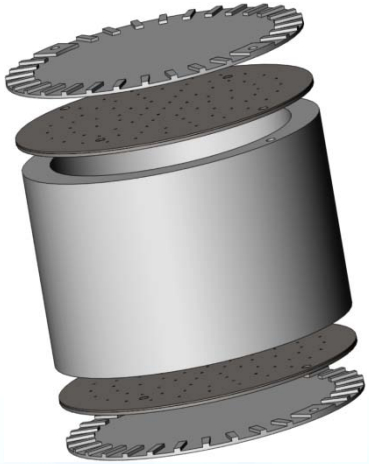


Modular Adsorbent Cryogenic System

OSU Oregon State UNIVERSITY



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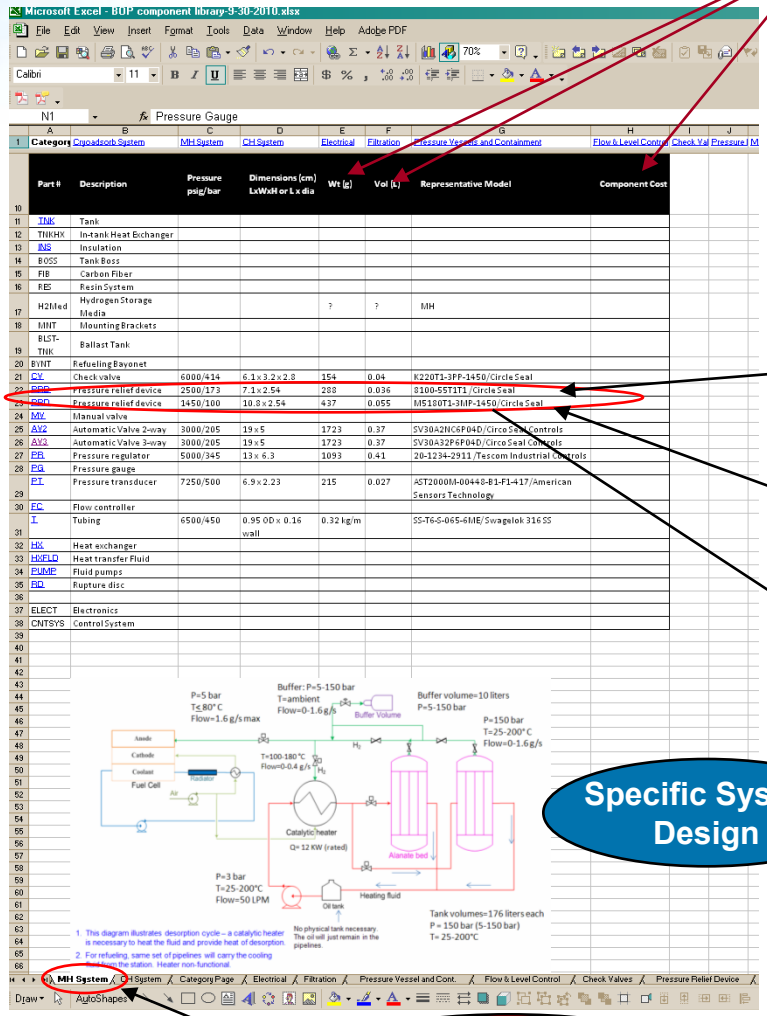
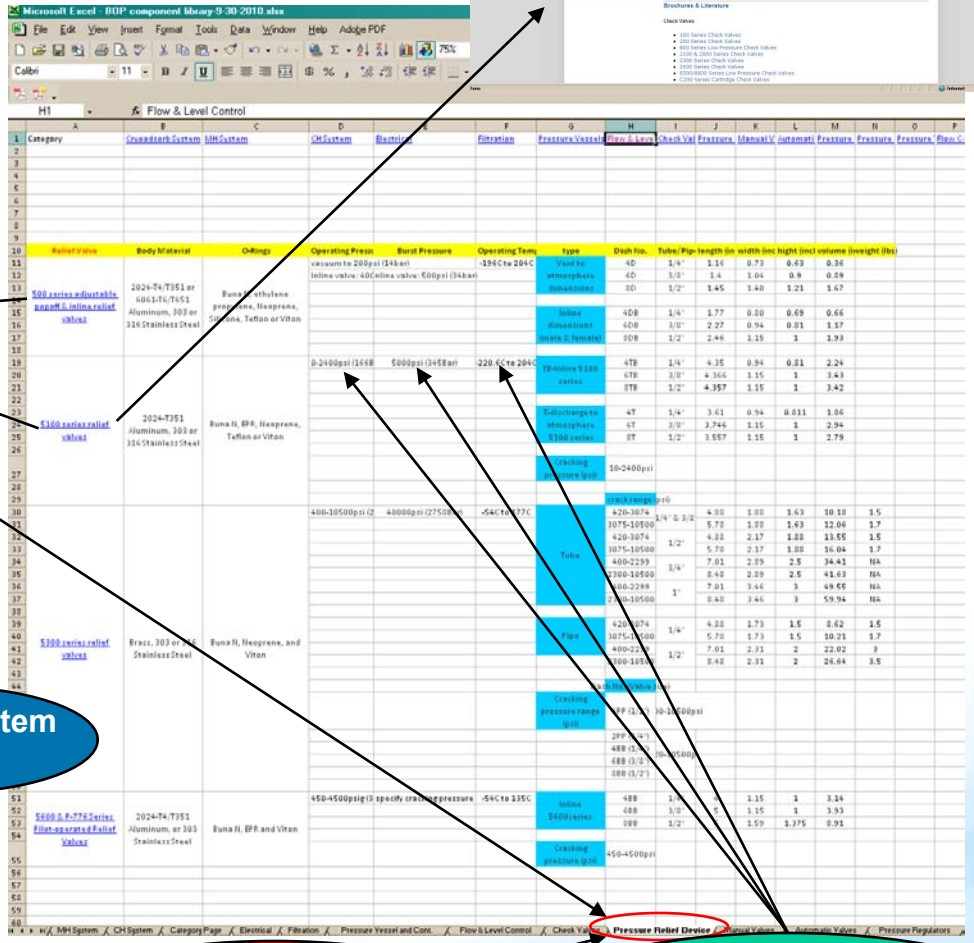
Enabling Technologies

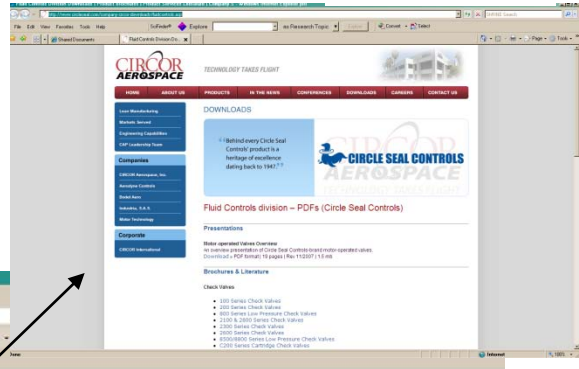
BoP Catalogue on SharePoint

Volume
Weigh
Cost



Specific System Design





Metal Hydride System

Pressure Relief Device

Operating Pressure
Burst Pressure
Operating Temperature

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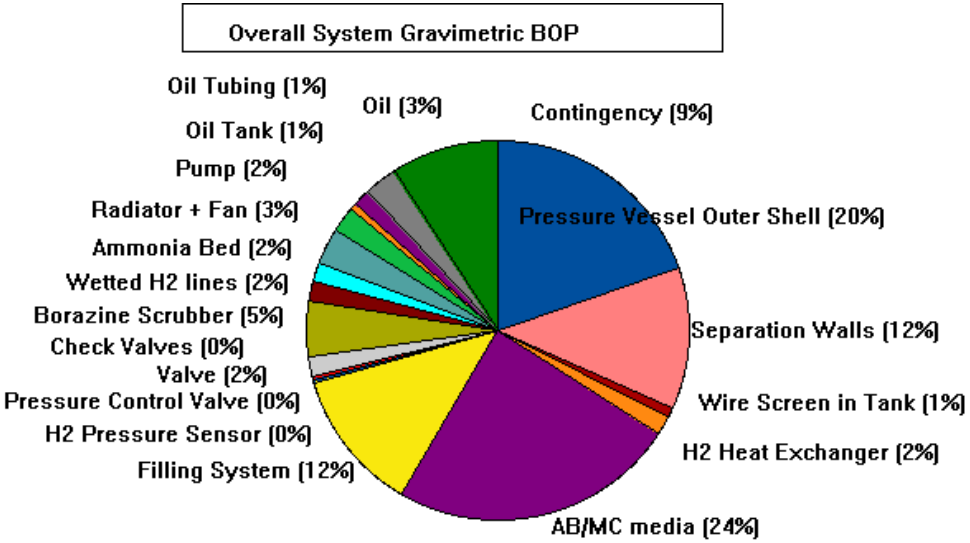
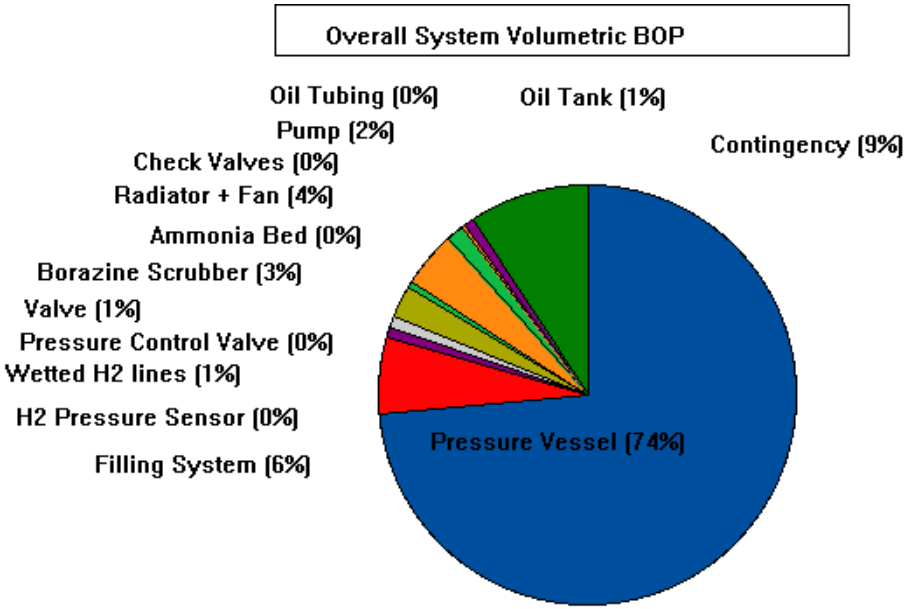
BoP Summary:
Total System Comparison (Fixed Bed Chemical Hydride System)

	Calculated	System	2010 Goal	2015 Goal		Fraction of 2010 Goal
Gravimetric Density	155.4	**.036**	.045	**.055**	Kg/Kg	80%
Volumetric Density	236	**.0237**	.028	**.040**	Kg/L	85%
Parasitic Power	168		W continuous			
	1068		W maximum			



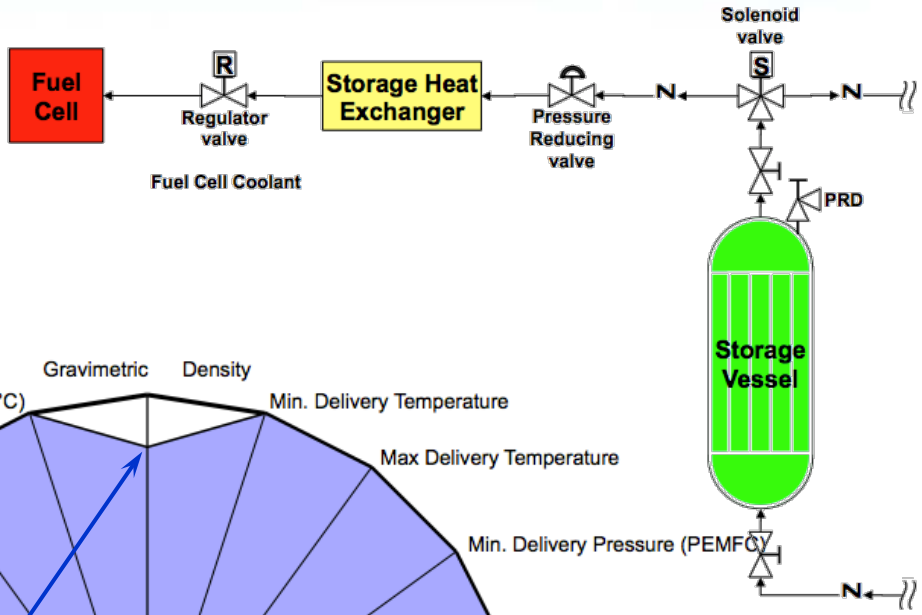
The vessel volume will be based on the AB/MC bulk density



HSECoE

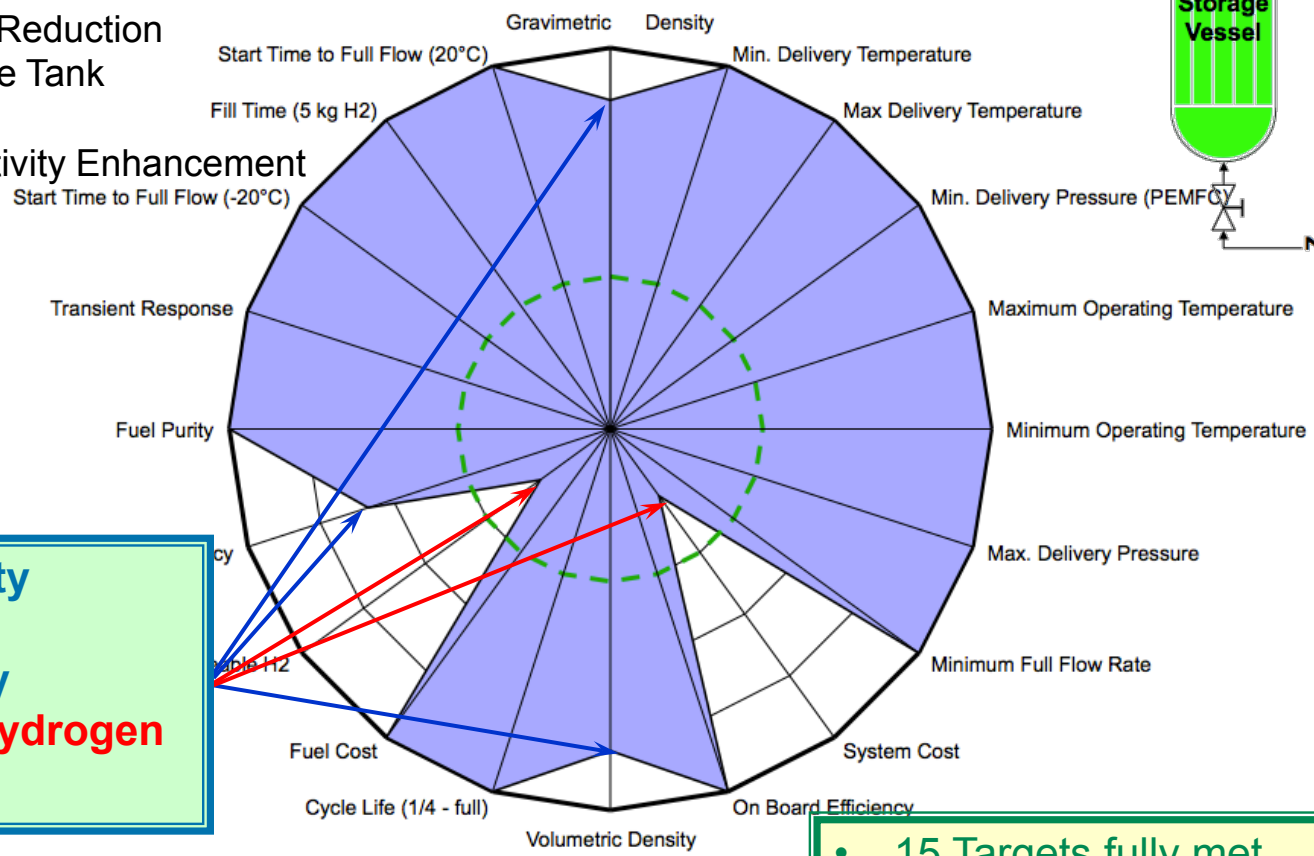
Adsorbent System Status

AX-21 Cryo-Adsorbent: 2010 Targets



Priority Technical Thrusts

- Flow through Cooling
- Advanced Vacuum Jacket Multi-Layer Insulation
- System Optimization
- BoP Component Cost Reduction
- Type 4 Cryo-Composite Tank
- Compressed Media
- ENG Thermal Conductivity Enhancement

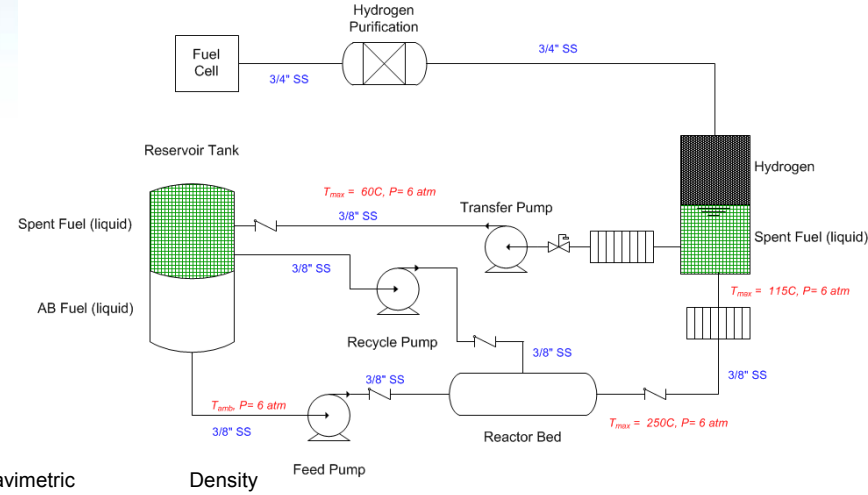


1. **Gravimetric Density**
2. **System Cost**
3. **Volumetric Density**
4. **Loss of Useable Hydrogen**
5. **WTPP Efficiency**

- 15 Targets fully met
- 3 Targets above 40%
- 2 targets below 40%

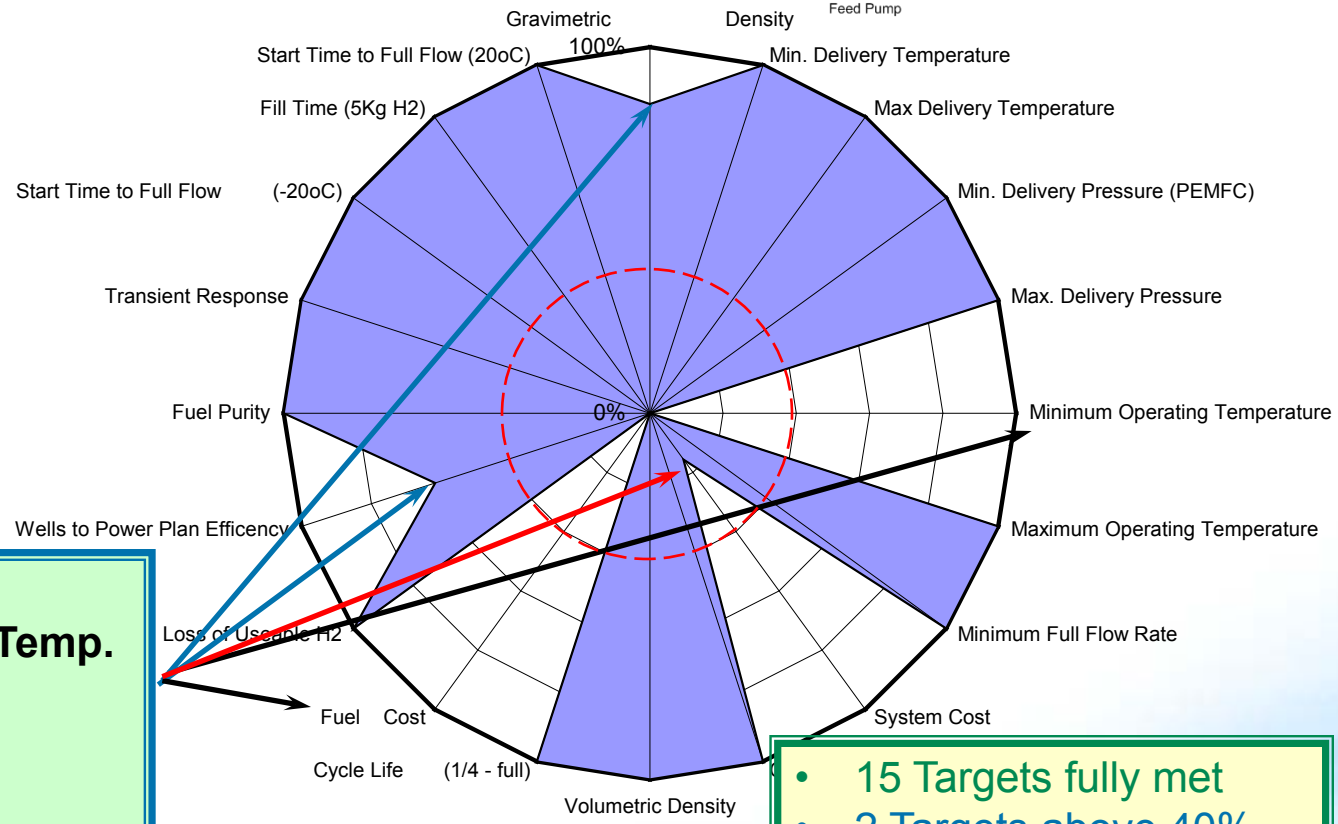
Chemical Hydride System Status

Fluid-Phase Ammonia-Borane: 2010 Targets



Priority Technical Thrusts

- System Optimization
- BoP Component Cost Reduction
- Liquid AB Low Temperature Properties
- Slurry AB Properties
- Impurity Mitigation



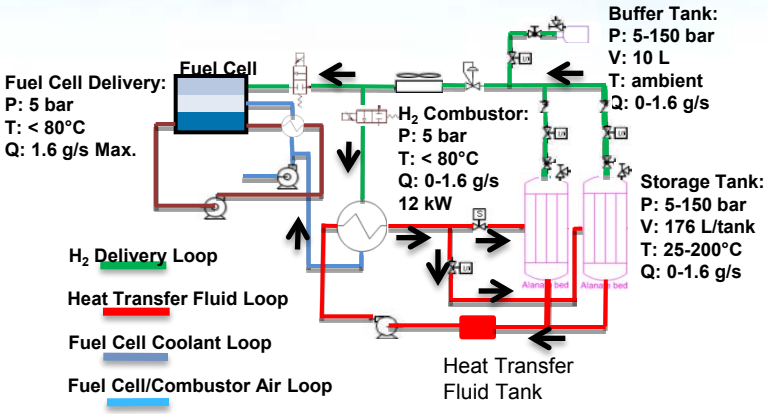
1. **Gravimetric Density**
2. **Minimum Operating Temp.**
3. **System Cost**
4. **Fuel Cost**
5. **WTPP Efficiency**

- 15 Targets fully met
- 2 Targets above 40%
- 1 Targets below 40%
- 2 Target undetermined

HSECoE

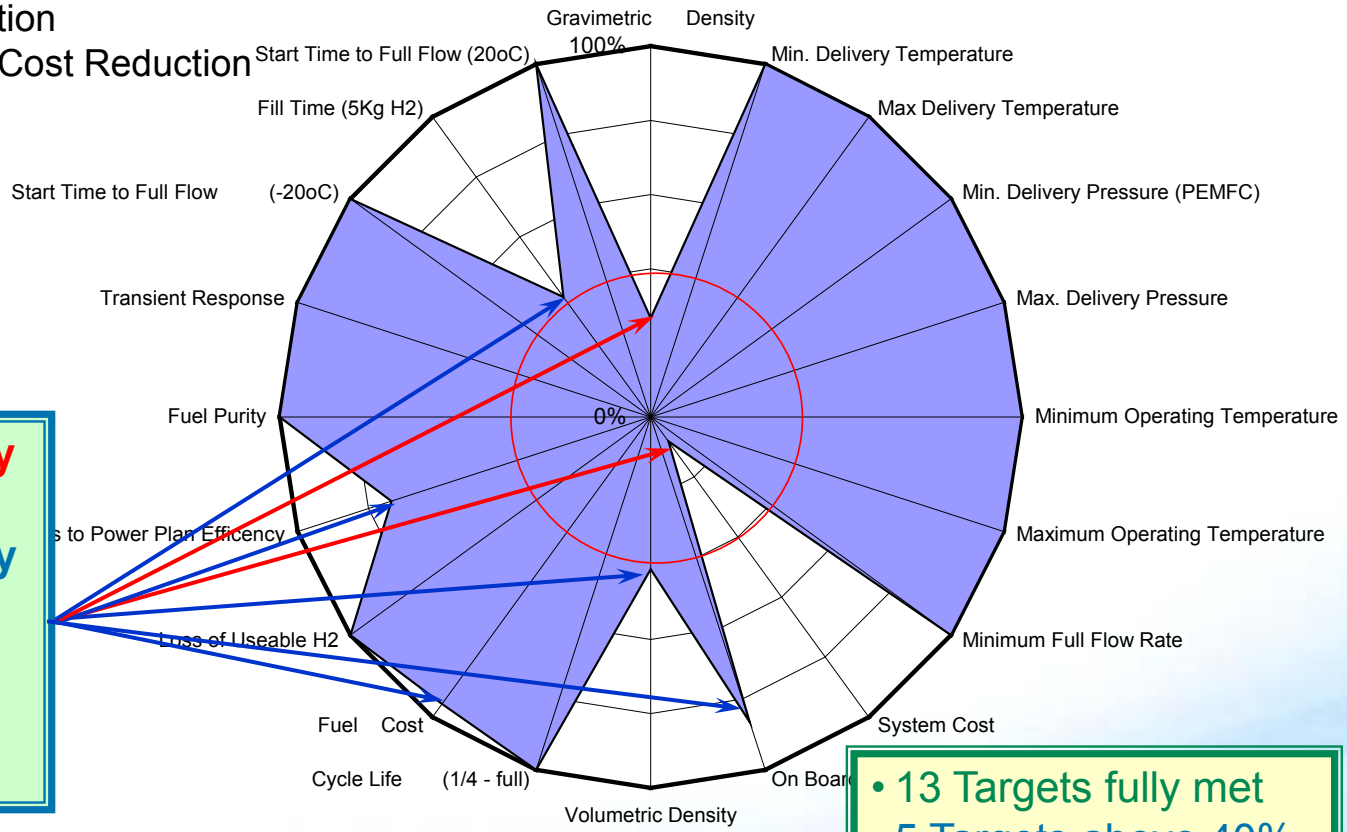
Metal Hydride System Status

$NaAlH_4$: 2010 Targets



Priority Technical Thrusts

- Type 4 Composite Tank
- Compressed Media
- ENG Thermal Conductivity Enhancement
- Advanced Catalytic Combustor
- System Optimization
- BoP Component Cost Reduction



1. **Gravimetric Density**
2. **System Cost**
3. **On-board Efficiency**
4. **Volumetric Density**
5. **Fuel Cost**
6. **WTPP Efficiency**
7. **Fill Time**

- 13 Targets fully met
- 5 Targets above 40%
- 2 Targets below 40%

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Status Towards Technical Targets

Technical Target	Units	2010	2015	Ultimate	Metal Hydride	Chemical Hydride	Adsorbent
Permeation & Leakage	*scc/hr*	#	#	#	s	s	s
Toxicity		#	#	#	s	s	s
Safety		#	#	#	s	s	s
Gravimetric Density	*kgH $_2$/kgSystem*	0.045	0.055	0.075	**0.012**	**0.038**	**0.039**
Min. Delivery Temp.	*^{o}C*	-40	-40	-40	-40	-40	-40
Max. Delivery Temp.	*^{o}C*	85	85	85	85	85	85
Min. Delivery Pressure (PEM)	*bar*	5	5	3	5	5	5
Max. Delivery Pressure	*bar*	12	12	12	12	12	12
Min. Operating Temperature	*^{o}C*	-30	-40	-40	-30	-	-30
Max. Operating Temperature	*^{o}C*	50	60	60	50	50	50
Min. Full Flow Rate	*[gH $_2$/s]/kW*	0.02	0.02	0.02	0.02	0.02	0.02
System Cost*	*$/kWh net*	4	2	TBD	**49.0**	**25.6**	**18.5**
On-Board Efficency	*%*	90	90	90	**78**	97	95
Volumetric Density	*kgH $_2$/liter*	0.028	0.040	0.070	**0.012**	0.034	0.024
Cycle Life	*N*	1000	1500	1500	1000	1000	1000
Fuel Cost*	*$/gge*	3-7	2-6	2-3	7.3	-	4.89
Loss of Useable Hydrogen	*[gH $_2$/hr]/kgH $_2$*	0.1	0.05	0.05	0.1	0.1	**0.44**
WPP Efficency	*%*	60	60	60	**44.1**	**37.0**	**40.1**
Fuel Purity	*%*	99.97	99.97	99.97	99.97	99.97	99.99
Transient Response	*sec.*	0.75	0.75	0.75	0.75	0.49	0.75
Start Time to Full Flow (-20°C)	*sec.*	15	15	15	15	1	15
Fill Time	*min.*	4.2	3.3	2.5	**10.5**	**5.4**	**4.2**
Start Time to Full Flow (20°C)	*sec.*	5	5	5	5	1	5

** Previous Values* # non-quantified s - satisfactory

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Project Summary

Relevance: Bring **ALL** of the technologies being studied for hydrogen storage to demonstration

Approach: Model and demonstrate the necessary hardware required to build hydrogen storage systems, validate models and design and test prototype hydrogen storage systems.

Technical Accomplishments: (i) Technical targets prioritized, (ii) Drive cycles defined, (iii) Integrated Model Framework completed, (iv) System models completed for each media class, (v) Balance-of-Plant components identified (vi) Assessment of State-of-the-Art system performance complete for each system and (vi) Limiting technologies identified with plans to demonstrate solutions.

Collaborations:

Technical Back-Up Slides

Program Outline – Phase 1

- **Media characterization, data gathering and generation**
  - Materials limitations quantified and future research directions specified
- **BoP component identification and compilation**
  - Limiting and Missing BoP item identification
- **Thermal and mass flow model development**
  - Thermal and Mass flow system deficiencies identified
  - Ideal materials characteristics identification
- **System models developed and integrated**
  - Required BoP items identified
  - Approaches identified to overcome technical barriers
- **Vehicle model and drive cycle test matrix developed**
  - Determined system sizing and efficiencies
  - Common basis for comparison of systems against targets

Program Outline – Phase 2

- Materials modification, scale-up and testing to meet specific system designs
- Assemble new BoP components and evaluate under actual operating conditions
- Test and evaluation of specific thermal and mass flow designs to refine and validate models
- Refine and expand system performance and cost models as new materials & component data is acquired
- Identify System Concepts to move forward to Sub-Scale Prototype Development

Program Outline – Phase 3

- Scale-up materials processing to assure adequate materials are available for sub-scale prototype construction
- Acquire all necessary BoP items for sub-scale prototype construction
- Design final sub-scale prototype components to be of a size scalable to a full size prototype
- Design and build where necessary testing facilities for sub-scale prototype evaluations
- Fabricate sub-scale prototypes
- Identify testing parameters to adequately demonstrate sub-scale prototypes
- Evaluate sub-scale prototypes and validate Center models
- Decommission sub-scale prototypes

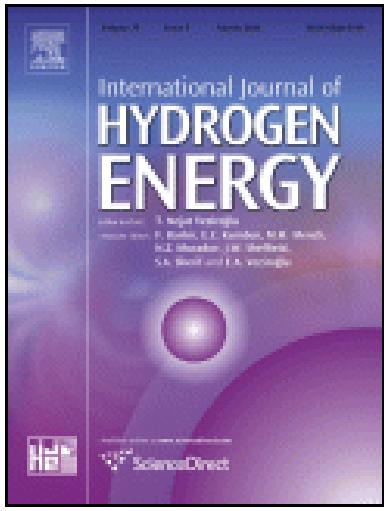
Summary of Major Decisions

- **Metal Hydrides**
  - LiMgN/TiCr(Mn)
  - Hybrid (Composite) Tank
  - Compressed Media
  - ENG Thermal Conductivity Enhancement
- **PCEA**
  - Drive Cycles Determined
  - Light Hybridization Approach
  - Unified Modeling Approach
  - Prioritized Targets
- **Adsorbents**
  - AX-21/MOF-5
  - Flow through Cooling
  - Hybrid (Composite) Tank
  - Compressed Media
  - ENG Thermal Conductivity Enhancement
  - Advanced Vacuum Jacket Insulation
- **Chemical Hydrides**
  - Fluid AB (slurry or liquid)
  - Flow Through or Fixed Bed Approach

AIChE Topical Conference Chaired

Hydrogen Storage System Engineering

2010 AIChE Annual Meeting
November 7th-12th, 2010
Salt Palace Convention Center
Salt Lake City, UT, USA



Co-Chairs:

D. Anton, S. Garrison, M. Dornheim & N. Kuriyama

- System Modeling:
  - *NREL, GM, UTRC, ANL, LNEG, Toyota*
- Heat and Mass Transfer Modeling:
  - *GKSS, SRNL, SNL*
- Applied Materials Development:
  - *LANL, U. British Columbia, PNNL, National Cheng Kung U., USC., Ford, U. Bath, SNL, Northwestern U., Banaras Hindu U., Hiroshima U., GKSS, SRNL, UTRC, CNRS, UN-Reno, AIST, Kansai U.*
- Infrastructure, Delivery & Demonstrations:
  - *LLNL, UQTR, ENNA, Higashifuji U., JMC, GKSS, Air Liquide, Kobe Steel*
- Risk Reduction:
  - *AIST, SNL, UTRC, SRNL,*

45 Submissions
9 Countries Represented:
- **Canada, China, France, Germany, India, Japan, Portugal, UK, USA**

Special Issue of IJHE to highlight
Storage System Engineering Proceedings