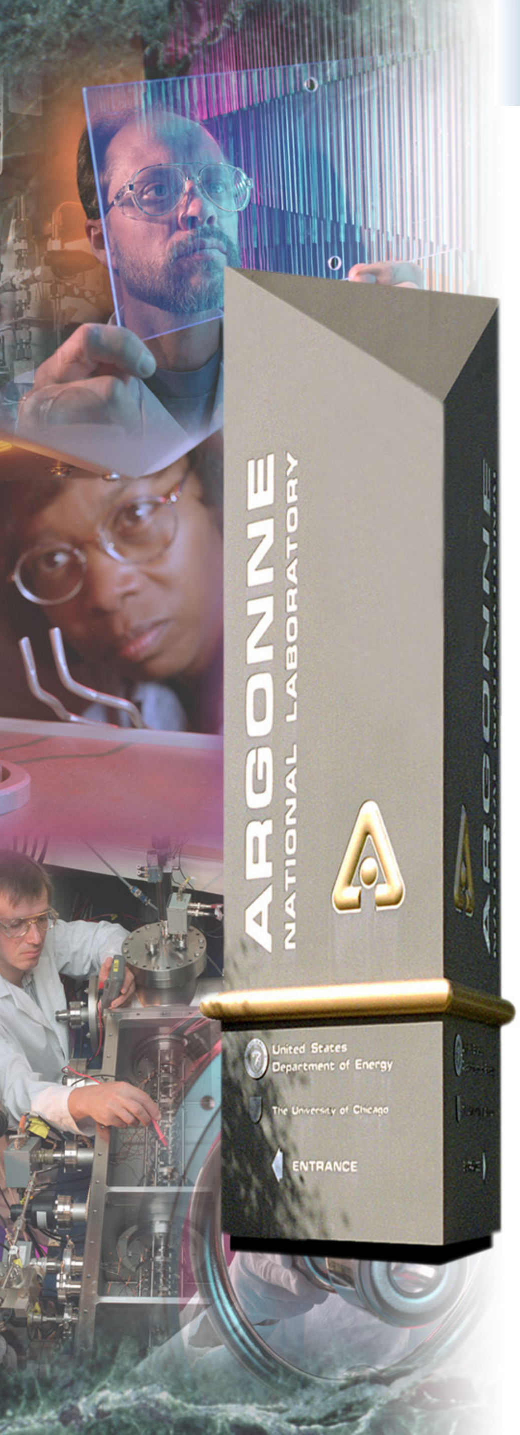

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System Level Analysis of Hydrogen Storage Options

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This presentation does not contain any proprietary or confidential information

Project ID: ST19

THE UNIVERSITY OF CHICAGO

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Overview

Timeline

- Project start date: Oct 2004
- Project end date: Sep 2009
- Percent complete: 33%

Budget

- FY05: $250 K
- FY06: $350 K

Barriers

- Addresses H_2 Storage Technical Barriers:
  - A: Cost
  - B: Weight and Volume
  - C: Efficiency
  - E: Refueling Time
  - M: Hydrogen Capacity and Reversibility
  - Q: Thermal Management
  - R: Regeneration Processes
  - T: Heat Removal

Interactions

- FreedomCAR and Fuel Partnership
- Storage Systems Analysis Working Group, MH COE, CH COE
- TIAX, LLNL, SNL, MCEL, APCI, H2A, University of Quebec

Objectives

- Perform independent systems analysis for DOE
  - Provide input for go/no-go decisions
- Model and analyze various developmental hydrogen storage systems
- Analyze hybrid systems that combine features of more than one concept
- Develop models that can be used to “reverse-engineer” particular technologies
  - Provide guidance to meet targets
- Identify interface issues and opportunities, and data needs for technology development

Approach

- Develop thermodynamic and kinetic models of processes in complex metal, carbon, and chemical hydrogen storage systems
- Calibrate, validate and evaluate models
- Work closely with the DOE Contractors, Centers of Excellence, Storage Tech Team, and Storage Systems Analysis Working Group
- Assess improvements needed in materials properties and system configurations to achieve H_2 storage targets

Technical Accomplishments

Metal Hydrides (Milestone: March 2006)

- Developed an Excel-based tool to help scientists evaluate how well their material, when used in a full-scale device, can meet DOE's storage targets

Carbon Storage (Milestone: December 2005)

- Determined under what conditions activated carbons at low T & high P can meet DOE's 2007 storage targets

Cryo-Compressed Hydrogen (Milestone: June 2006)

- Determined combinations of P & T to achieve 4.5 wt% gravimetric and 36 kg/m^3 volumetric capacity

Chemical Hydrogen (Milestone: September 2006)

- Evaluated regeneration energy consumption and fuel cycle efficiencies of candidate materials and processes

MHtool: Metal-Hydride Hydrogen Storage System Analysis Tool

To develop and make available to DOE contractors and Centers of Excellence a tool for use by the material developers to

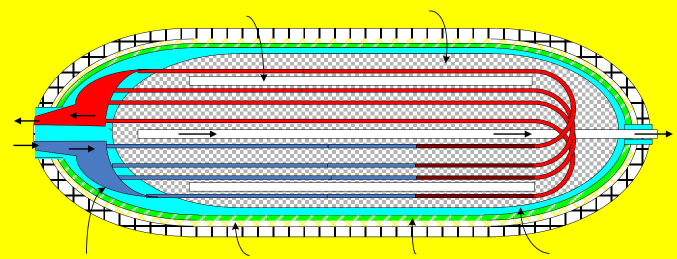
- Evaluate the performance of the material, when used in a full- scale device, vis-à-vis DOE's H_2 storage targets;
- Identify the specific deficiencies in material properties and their impact on performance of the storage system;
- Assess how much improvement is needed in the deficient material properties to meet the storage targets.

Modular Approach

Written on Microsoft Excel platform, modules run sequentially

- MCM characterizes storage material for composition and capacity
- SCM calculates the reversible storage capacity of medium, maximum DOD and SOC
- HTM determines the size of heat transfer system
- SM determines gravimetric and volumetric capacity of the system
- DM calculates the dynamic sorption behavior of the MH considering chemical kinetics and heat transfer

MHtool: Metal-Hydride Hydrogen Storage System Analysis Tool



1. MATERIAL CHARACTERIZATION MODULE
2. STORAGE CAPACITY MODULE
3. HEAT TRANSFER MODULE
4. SYSTEM MODULE
5. DYNAMIC MODULE

Example: Reversible Storage Capacity of Alanate Medium

Operating Conditions: 4% $TiCl_3$, 1.6 g/s min full flow rate of H_2, 100 bar supply P, 115°C discharge, 165°C charge

Effect of minimum delivery P on maximum DOD

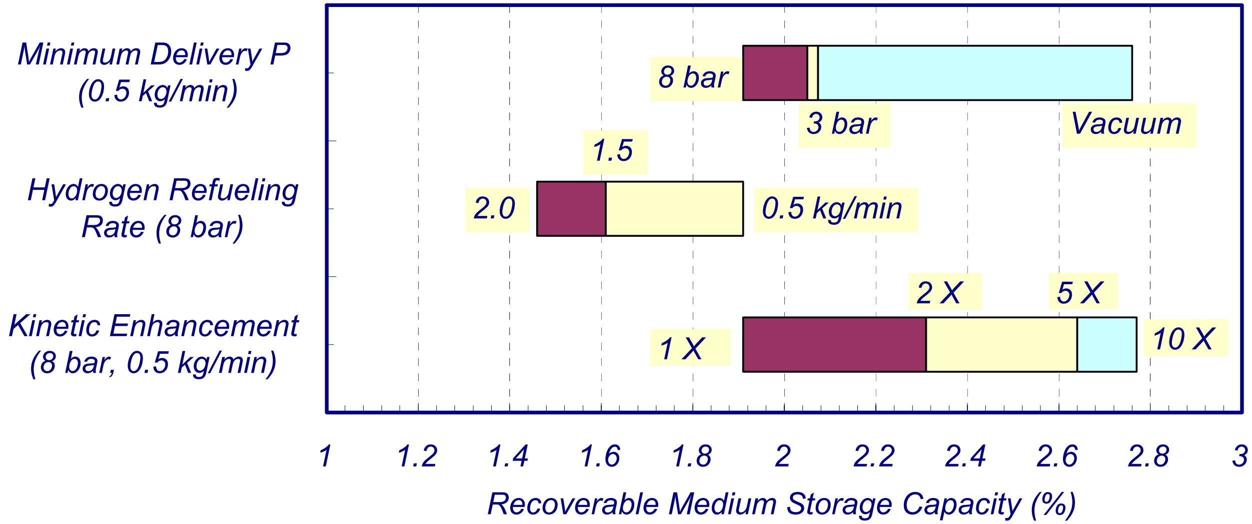
- $NaAlH_4$ dehydrogenation: 65% at 8 bar, 70% at 4 bar, 71% at 3 bar
- Na_3AlH_6 dehydrogenation: 0 at P<1.8 bar, 39% at 0.1 bar

Effect of refueling rate on maximum SOC

- 98% at 0.5 kg/min, 77% at 1.5 kg/min, 67% at 2 kg/min

Effect of discharge kinetics on maximum DOD

- 65% at 1X, 79% at 2X, 90% at 5X, 95% at 10X kinetics



Reference kinetics: Sandrock, Gross & Thomas, J Alloys Compounds, 2002

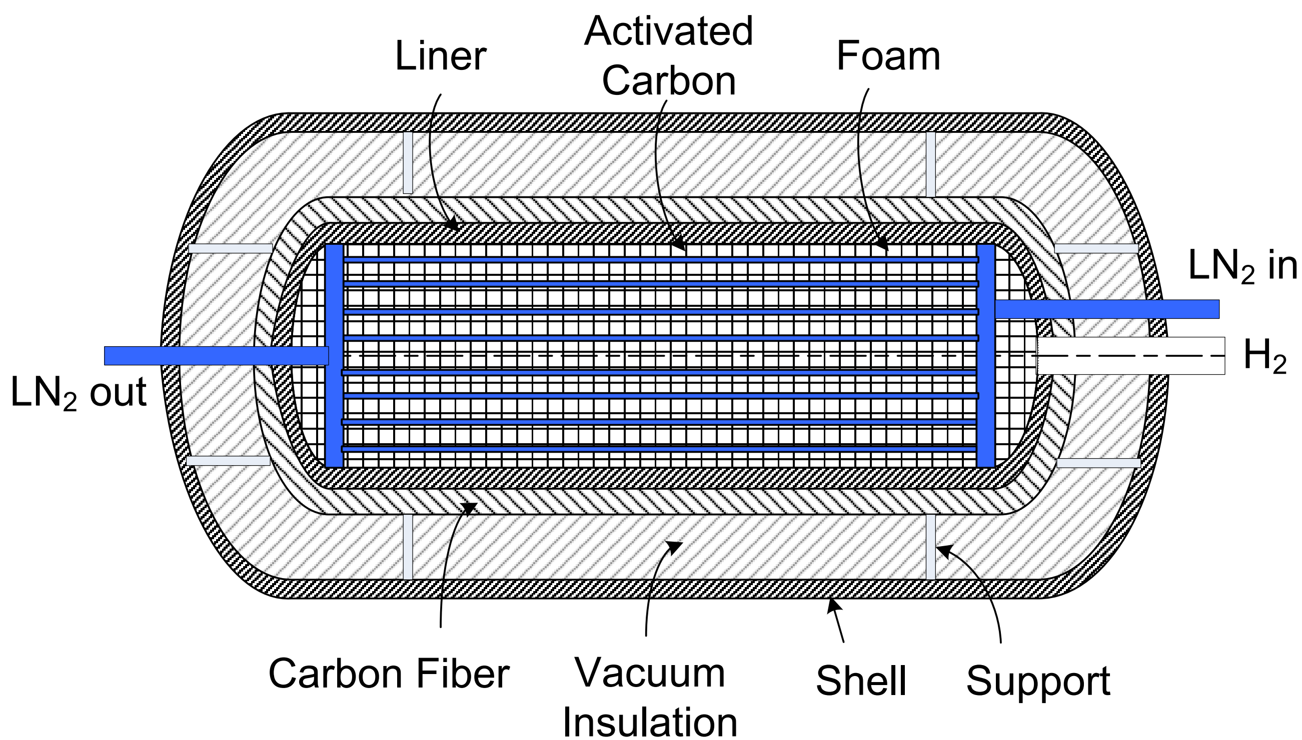
High-Pressure, Low-Temperature Storage of Hydrogen on Activated Carbon

- Determine the volumetric and gravimetric capacity of AC storage systems at low temperatures (77-150 K) and high pressures (P > 100 bar).
  - Compare amounts of H_2 adsorbed on AC and in void space.
  - Evaluate the heating and cooling requirements for the AC tank and how they may be accomplished.
  - Characterize dormancy and boil-off losses.
  - Estimate energy consumed in storing hydrogen.
- Determine the attributes of advanced AC/sorbents that can help meet 2007 targets of 4.5 wt% H_2 and 36 kg H_2/m^3 (1.2 kWh/L).

AC H_2 Storage System

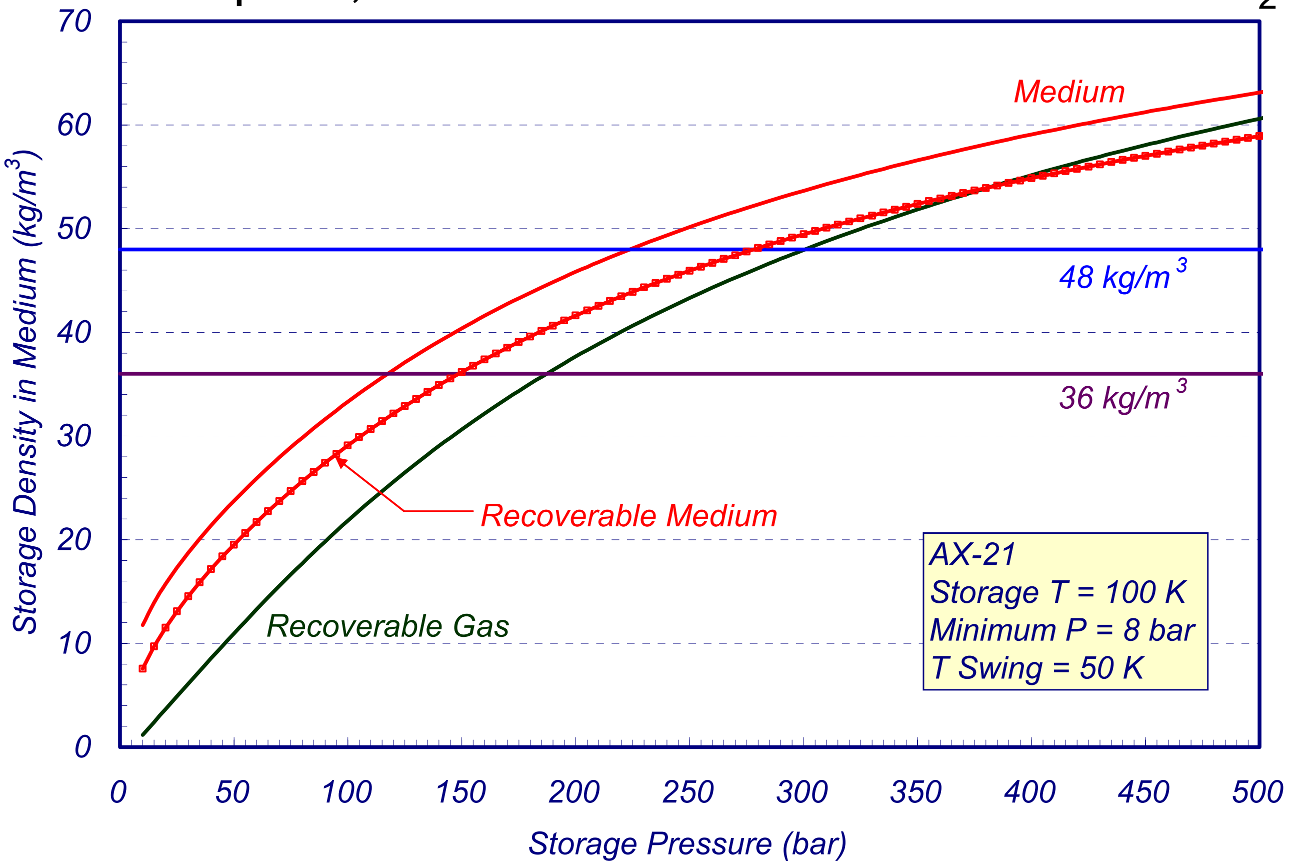
Thermally insulated, filament wound carbon fiber/epoxy PV

- Super AC powder medium
- Metal foam support
- In-tank HX and manifolds
- Al liner
- Carbon fiber
- Multi-layer vacuum insulation
- Al shell
- Miscellaneous



Recoverable H_2 Storage Density of AX-21 Medium at 100 K with Temperature Swing

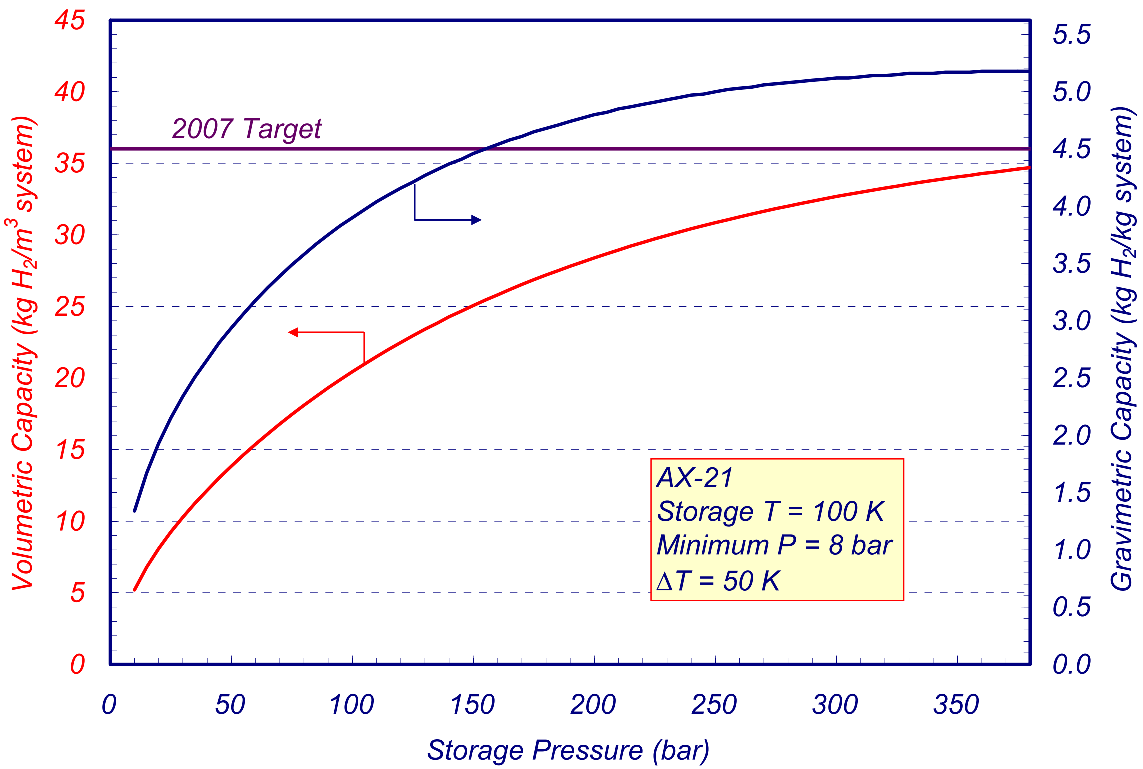
- With 50-K ΔT, the breakeven pressure is 380 bar.
- At 75% volumetric efficiency, 36 kg/m^3 target is reached at 280 bar.
- At breakeven point, AX-21 stores 16.5% of recoverable H_2 at 100 K.



Reference for adsorption isotherms: Bénard and Chahine, Int. J. Hydrogen Energy, 2001

Storage Capacity of AC System at 100 K

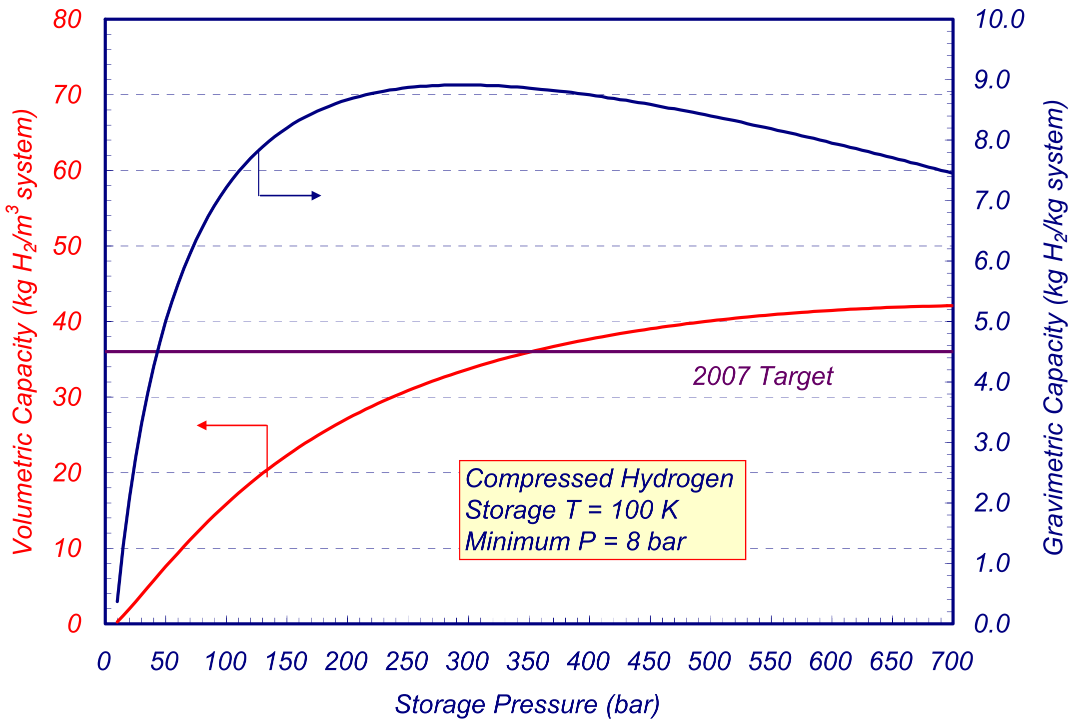
- At 100 K, the storage capacity of AC system is >4.5 wt% for P >150 bar and approaches 36 kg/m^3 at P = 380 bar.
  - Calculated volumetric capacity of AC medium is 60-62% at 150-380 bar.
- Need to increase sorption capacity of AX-21 by 61-82% and bulk density by ~100% to satisfy 2007 targets at 100 K and 100 bar.



Storage Capacity of Cryo-cH2 System at 100 K

Assumption: No on-board heat transfer system needed because the tank is charged with H_2 subcooled below 100 K.

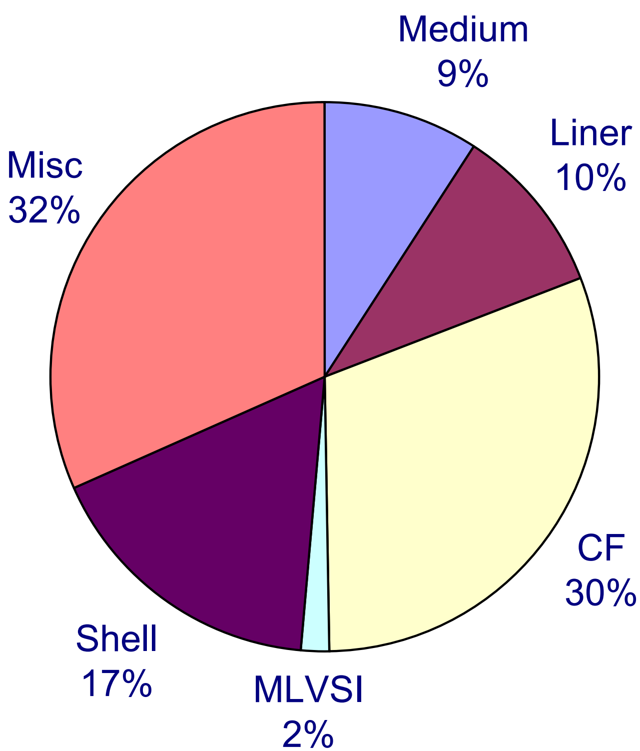
- May simultaneously meet the 2007 targets of 4.5 wt% and 36 kg/m^3 at P > 355 bar.
- May meet the 2010 target of 6 wt% but not the 45 kg/m^3 target.
- 8.9 wt% peak gravimetric capacity at 300 bar.



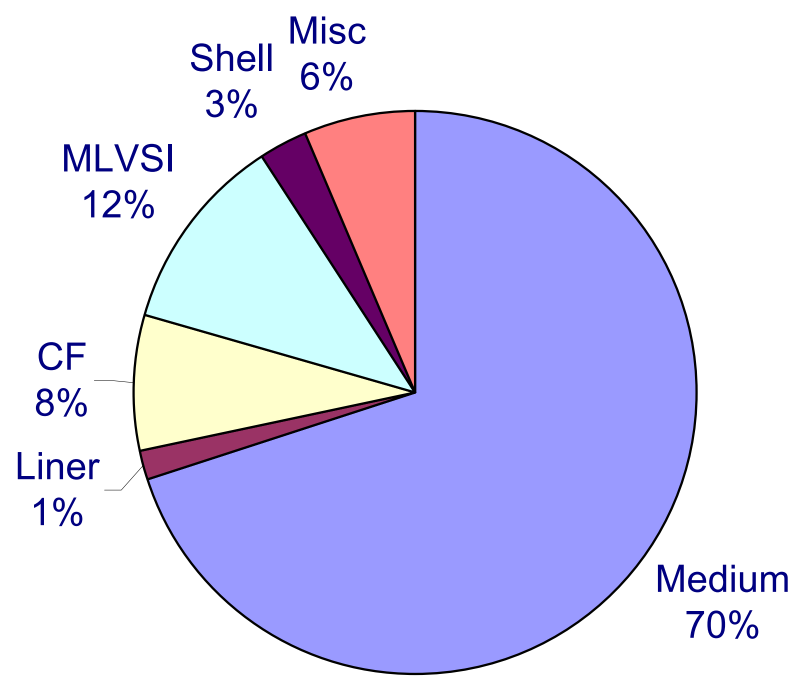
Weight and Volume Distribution Cryo-cH2 System: 100 K, 355 bar (Preliminary)

8.9 wt% gravimetric capacity

- CF accounts for 30% of the total weight



Weight Distribution



Volume Distribution

36 kg/m^3 volumetric capacity

- Gas medium accounts for 70% of the total volume

FCHtool: Fuel Cycle Efficiency of Different Hydrogen Storage Options

Defined efficiencies on the basis of primary energy consumed in producing, distributing and storing hydrogen

- Distinction between primary energy feedstocks (petroleum, coal, etc) and process fuels (gasoline, hydrogen, electricity, etc.)

Simple Microsoft Excel based tool with embedded Macros in Visual Basic Application language

- Arbitrary process steps to simulate any fuel cycle (H_2 pathway)
- GREET derived reference database for process fuel production, electricity generation, hydrogen production, hydrogen distribution, hydrogen storage, regeneration steps
- Outputs for primary energy consumption, efficiencies, and emissions of regulated pollutants and GHGs
- Consistency with H2A spreadsheet

Case Study

Considered centralized production of H_2 by SMR+PSA, 73% efficiency

Compressed H_2 at 350 or 700 bar

- 20 bar to 180 bar at production site, 5-stage compressor*
- 180 bar to 425 or 850 bar at refueling station, 2 or 3-stage compressor*
- Delivery by tube trailers for 1% & pipeline for 10% market share*

Liquid H_2 storage option

- Liquefaction plant at production site, >200,000 kg/d capacity*
- Delivery truck capacity: 400 kg (1% market), 4000 kg (10% market)*

MgH_2 slurry

- Included only electricity consumed by LTF-SOM process at 1150°C
- BU 2005 data: 3-V cell voltage (~1-V dissoc. potential with H_2), 100% current eff., 6.7 kWh/kg Mg (SafeH$_2$ quoted 10 kWh/kg)

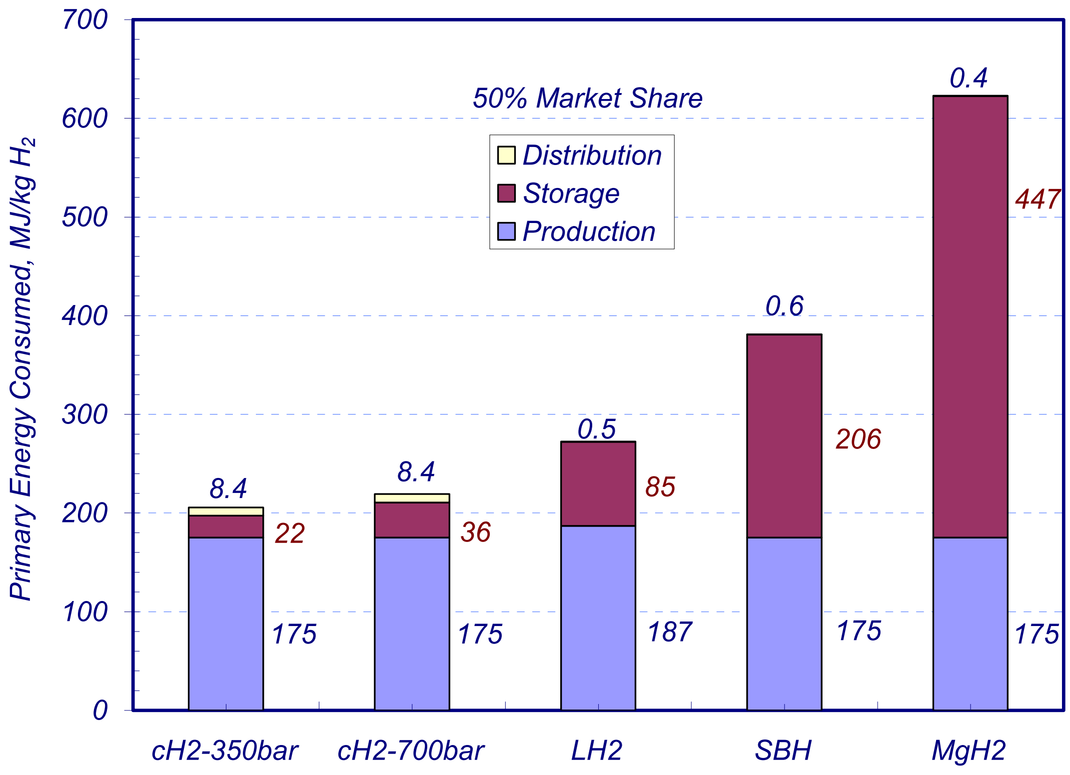
SBH system

- Included only electricity consumed by H-assisted NaOH electrolysis
- MCEL data: 1.2-V cell voltage (~1.07-V theoretical with H_2), 100% current eff., 1.6 kWh/kg Na (MCEL quoted 1.8 kWh/kg)

*Assumptions consistent with H2A

Primary Energy Consumed in Production, Storage and Distribution Steps (Preliminary)

- cH_2 option: Energy consumed in storage & delivery steps relatively small
- LH_2: Liquefaction requires 40% of energy consumed in production
- SBH: Energy consumed in storage & production steps about equal
- MgH_2: Regeneration requires >2.2 times energy consumed in production



Production
- SMR: H_2 at 20 bar

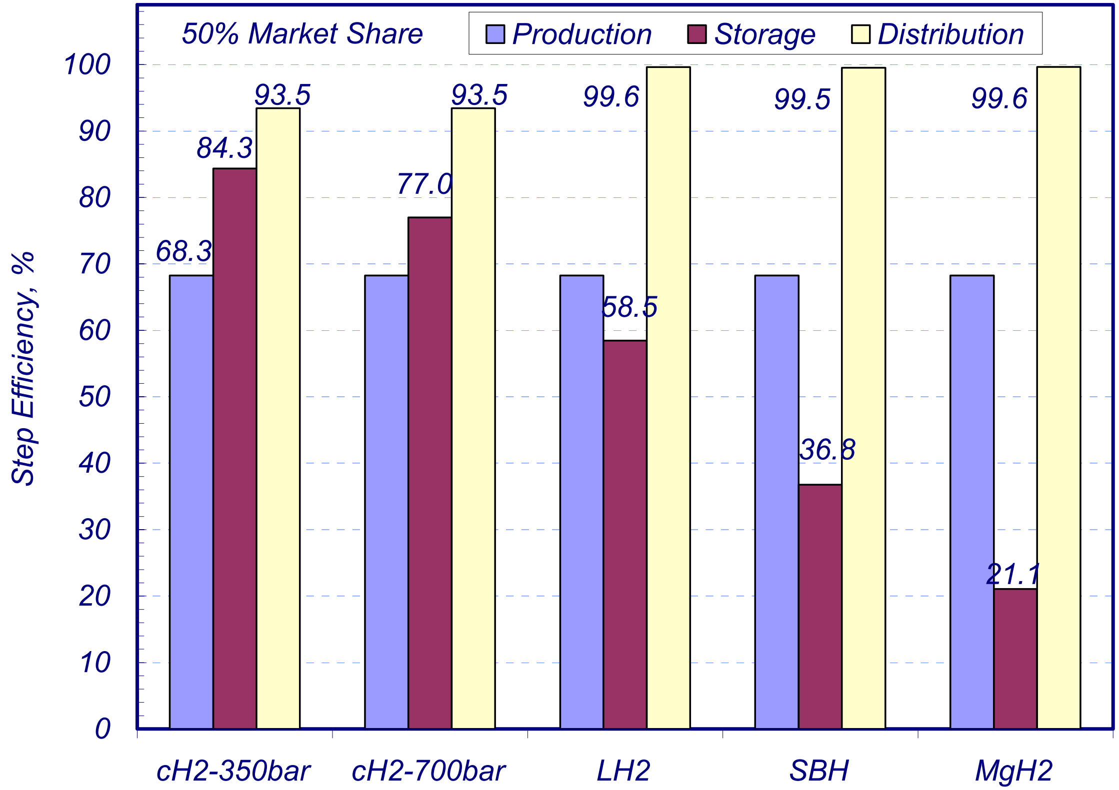
Distribution
- Pipeline transmission
- Trucking

Storage
- Compression
- Liquefaction
- CH regeneration

Preliminary Fuel Cycle Efficiencies

WTT efficiencies

- 58.1% for cH2 at 350 bar and 54.5% at 700 bar
- 43.9% for LH_2 option
- 31.3% for SBH and 19.2% for MgH_2 options



Future Work

Continue to work with DOE contractors and COE to model and analyze various developmental hydrogen storage systems.

Metal Hydrides

- PCT deconvolution module
- Module to derive kinetic constants from experimental data

Carbon Storage

- Extend work to carbon and other sorbents

Cryo-Compressed Hydrogen

- Independent analysis in support of DOE's go no-go decision

Chemical Hydrogen

- Evaluate regeneration energy consumption and fuel cycle efficiencies of candidate materials and processes
- Develop CHtool to help scientist evaluate how well their material can perform in a full scale on-board system to satisfy DOE's storage targets (kinetics, energetics, thermodynamics)

Summary and Additional Results

Metal Hydrides
- MHtool (Version 1.0) is being beta-tested prior to its release this FY.

Carbon Storage
- Commercially available AX-21 vs. cryo-cH2 at 100-150 K.
- >9.5 kWh/kg-H_2 energy consumed in N_2 liquefaction system*
- 10-90 days dormancy, boil-off rate < 2 g/h*
- To satisfy 2007 targets at 100 K and 100 bar, need to increase sorption capacity of AX-21 by 61-82% and bulk density by ~100%.

Cryo-Compressed Hydrogen
- At 100 K, cryo-cH_2 may meet 2007 targets at P>350 bar.
- Preliminary estimate of energy to fuel with cryo-cH_2: 5.6 kWh/kg H_2*.

Chemical Hydrogen
- Life cycle analysis needed to compare energy consumed in regenerating chemical hydrides.
- FCHtool (Version 2.0) is being beta-tested prior to its release this FY.

*Report being written to document the results

BACKUP MATERIAL

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Response to Reviewers' Comments

Maintain high degree of fidelity to DOE program goals

- Program plan closely aligned with DOE milestones and decision points.
- Monthly teleconference with DOE program manager
- Reviewed by Tech Team on semi-annual basis

Closer coordination with every project

- Formed Storage Systems Analysis Working Group
- Made presentations to teams from MH-COE and CH-COE
- Working closely with LLNL on cryogenic storage

Specific recommendations and additions or deletions to work scope

- Need to give more resources
- Need to give this project a higher priority
- Need to protect them from external pressures
- Need to develop parallel pathways for various storage alternatives

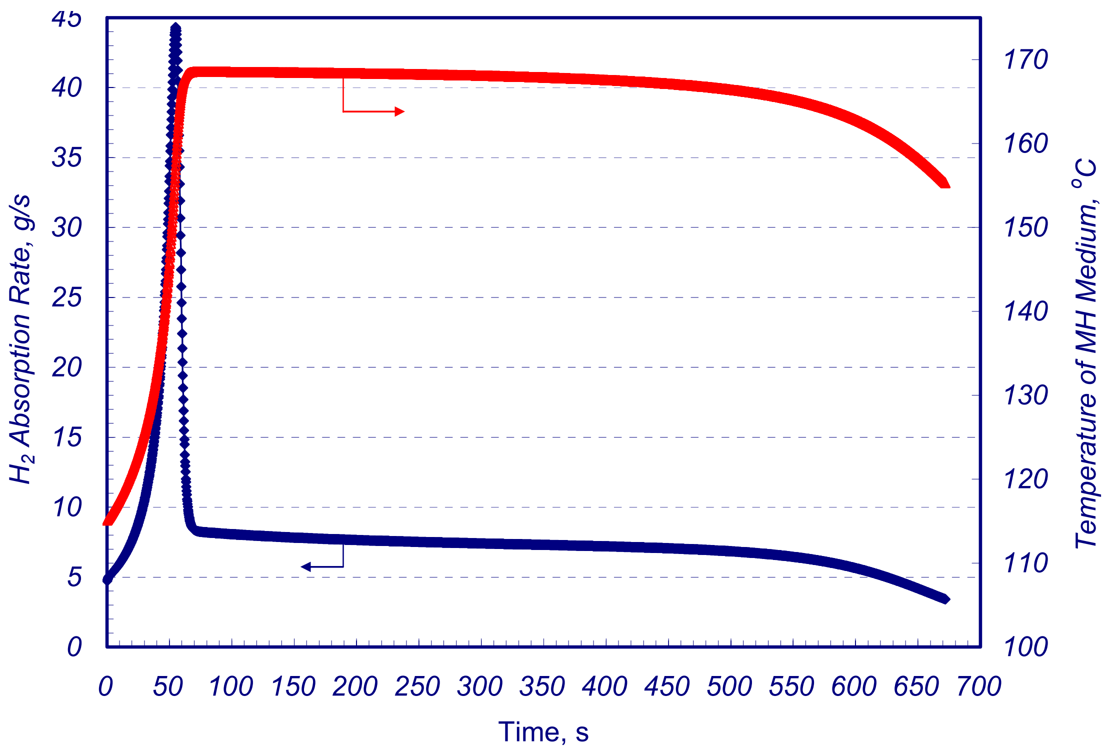
Publications and Presentations

1. R. K. Ahluwalia, “Sodium Alanate Hydrogen Storage System for Automotive Fuel Cells,” Submitted to International Journal of Hydrogen Energy, 2005.
2. R. K. Ahluwalia and J-K Peng, “MHtool: Metal-Hydride Hydrogen Storage System Analysis Tool,” DOE Metal Hydride Analysis Kick-Off Meeting, 29 September 2005, Washington, DC.
3. R. K. Ahluwalia, T. Q. Hua, M. Q. Wang, and R. Kumar, “System Analysis of Chemical Hydrogen Storage Options,” Chemical Hydrogen Storage Systems Analysis Meeting, 12 October 2005, Argonne, IL.
4. R. K. Ahluwalia, J-K Peng and T. Q. Hua, “System Level Considerations for Hydrogen Storage,” Storage Systems Analysis Working Group Meeting, 18 November 2005, Palm Springs, CA.
5. R. K. Ahluwalia, J-K Peng and T. Q. Hua, “On-Board Storage Systems Analysis,” DOE and FreedomCAR & Fuel Partnership Analysis Workshop, 25 January 2006, Washington, DC.

Refueling of MH Tank

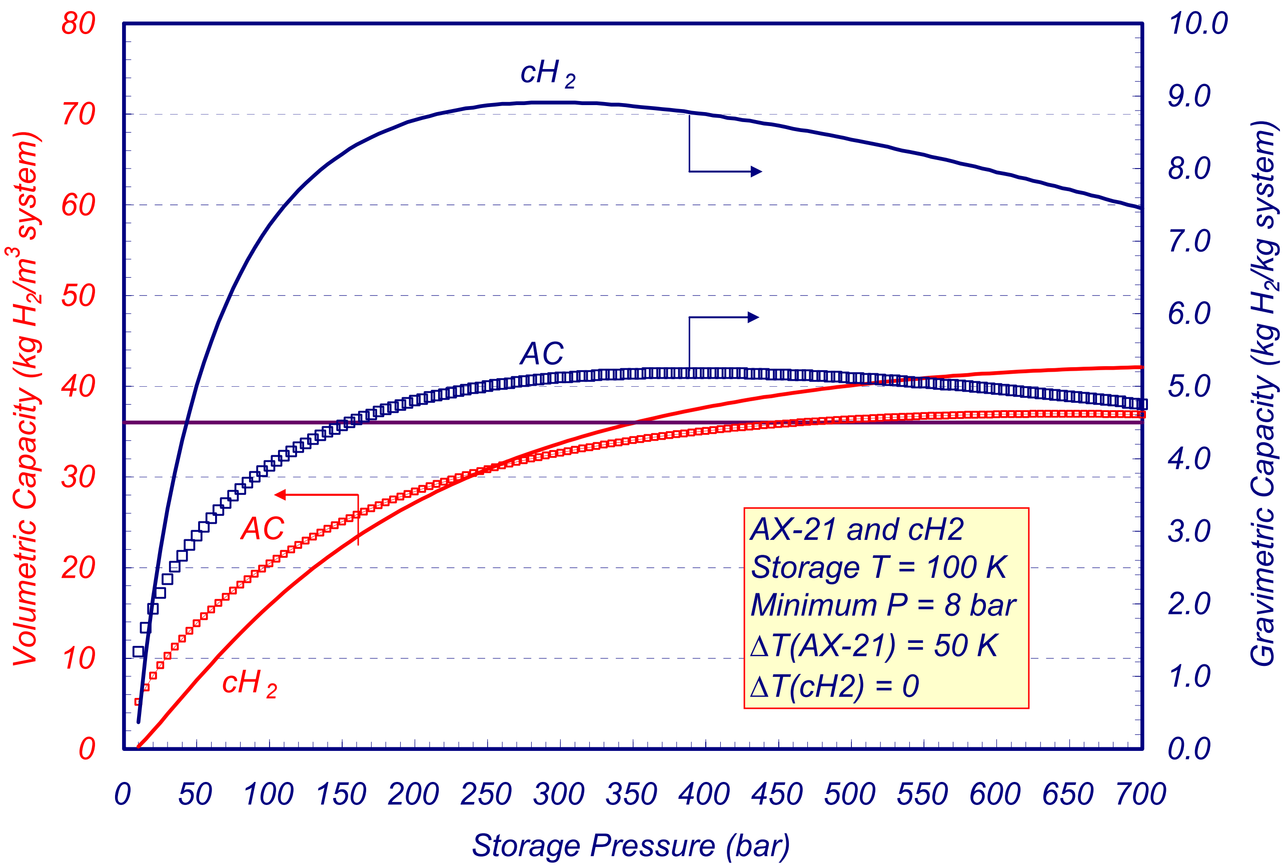
Refueling of MH medium depleted to maximum DOD, 115°C initial T

- Coolant flow rate varied to attempt to keep MH at 150-155°C
- Medium cannot be maintained at T at which charge rate is maximum
- Refueling time determined by intrinsic kinetics and heat transfer



Cryo-cH2 vs. AX-21 System

- Gravimetric capacity higher with cryo-cH2 storage
- Below 265-bar breakeven P, volumetric capacity higher with AX-21
- Cryo-cH2 simultaneously meets the 2007 gravimetric and volumetric capacity targets at lower pressure than AX-21



Storage System Parameters

Super AC powder medium
- AX-21: 2800 m^2/g, 300 kg/m^3, 0.1 W/m.K

Metal foam support
- 2-wt% Al 2024, 2.4 W/m.K

In-tank HX and manifolds
- Al 2024 construction
- 9.5-mm OD, 1.2-mm thick tubes
- 0.9-mm thick tube sheets

2-mm thick Al alloy liner

T700S carbon fiber
- 68%CF+32%resin, 1600 kg/m^3
- 2550 MPa tensile strength
- Fiber translation: 70% at 700 bar, 85% at 350 bar
- 2.25 SF

MLVSI
- Aluminized mylar sheets with Dacron spacer, 70 layers/in.
- 59.3 kg/m^3
- 10^{-5} torr
- $5.2x10^{-4}$ W/m.K
- 1 W heat transfer

3-mm thick Al alloy shell

System
- L/D = 2, 3:1 oblate ellipsoid head
- Miscellaneous: pipes, insulation supports, etc., 20 kg, 10 L
- LN2 cooling
- H_2 refueled at +100 bar, tank T
- 5.6 kg recoverable H_2 capacity
- 0.5-2 kg/min H_2 refueling rate