SRNL Technical Work Scope for the Hydrogen Storage Engineering Center of Excellence

Design and Testing of Metal Hydride and Adsorbent Systems

Theodore Motyka
Assistant Director and SRNL Project Lead

Bruce J. Hardy
SRNL Model Development Lead

Richard Chahine
UQTR

Kyle S. Brinkman
SRNL H2 Purification/Material Requirements

Savannah River National Laboratory

May 20, 2009

Hydrogen Storage Engineering
CENTER OF EXCELLENCE

Project ID#STP_06_Motyka

This presentation does not contain any proprietary, confidential or otherwise restricted information

Overview

Timeline

- Start: February 1, 2009
- End: January 31, 2014
- 3% Complete (as of 3/31/09)

Barriers

- System Weight and Volume
- H2 Flow Rate
- Energy Efficiency

Budget

- FY 08 Funding: $0 (new project)
- FY 09 Funding: $888,945* (authorized)

* Includes $241,200 for the University of Quebec Trois Rivieres (UQTR) as a subrecipient

Partners

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

SRNL's Major HSECoE Technical Activities

Hydrogen Storage Engineering Center of Excellence

D. Anton, SRNL
T. Motyka, SRNL

Materials Operating Requirements

D. Herling, PNNL

- Materials Centers of Excellence – SRNL, LANL, NREL
- Reactivity and Compatibility – UTRC
- Adsorption Properties – UQTR
- Metal Hydride Properties – SRNL
- Chemical Hydride Properties - LANL

Transport Phenomena

B. Hardy, SRNL

- Bulk Materials Handling – PNNL
- Mass Transport – SRNL
- Thermal Transport – SRNL
- Material Structure - GM

Enabling Technologies

J. Reiter, JPL

- Thermal Insulation – JPL
- Hydrogen Purity – UTRC
- Sensors – LANL
- Thermal Devices - OSU
- Pressure Vessels - PNNL

Performance Analysis

M. Thornton

- Vehicle Requirements– NREL
- Tank-to-Wheels Analysis – NREL
- Forecourt Requirements - UTRC
- Manufacturing & Cost Analysis - PNNL

Integrated Power Plant/ Storage System Modeling

D. Mosher, UTRC

- Off-Board Reversible - UTRC
- On-Board Reversible – GM
- Power Plant – Ford

Subscale Prototype Construction, Testing & Evaluation

T. Semelsberger, LANL

- Risk Assessment & Mitigation – UTRC
- Design Optimization & Subscale Systems – LANL, SRNL, UQTR
- Fabricate Subscale Systems Components – SRNL, LANL
- Assemble & Evaluate subscale Systems – LANL, JPL, UQTR

Technology Area

Technology Area Lead

- Technology Team – TT Lead
- Technology Team – TT Lead
- Technology Team – TT Lead

HSECoE

Relevance: Overall Project Objectives

Phase 1: 2009-2010

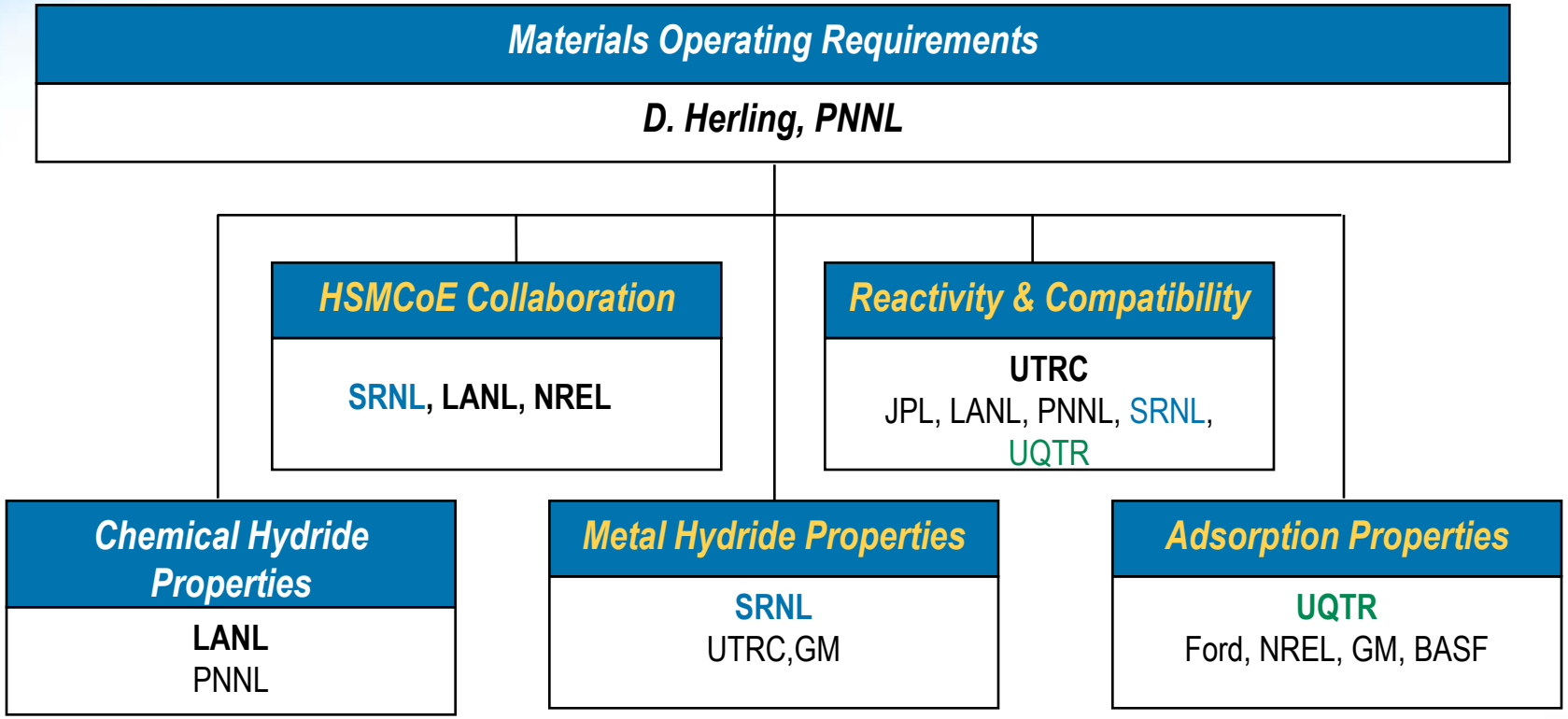
- Compile all relevant **metal hydride materials data** for candidate storage media and define future data requirements.
- Develop engineering and design models to further the understanding of on-board storage **transport phenomena requirements**.
- Develop practical and efficient **enabling technologies** in the areas of **hydrogen purification** and demonstrate **material compatibility** for various systems and components for adsorbent and metal hydride storage materials.

Phase 2: 2011-2012

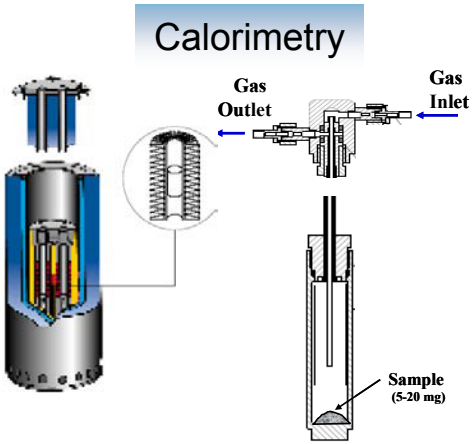
- Develop **innovative on-board system concepts** for metal hydride, and adsorption hydride materials-based storage technologies.
- Design components and experimental test fixtures to **evaluate the innovative storage devices** and subsystem design concepts, validate model predictions, and improve both component design and predictive capability.

Phase 3: 2012-2013

- Design, fabricate, test, and decommission the **subscale prototype systems** of each materials-based technology (adsorbents and metal hydrides storage materials).


Materials Operating Requirements
D. Herling, PNNL
HSMCoE Collaboration
SRNL, LANL, NREL
Reactivity & Compatibility
UTRC
JPL, LANL, PNNL, SRNL, UQTR
Chemical Hydride Properties
LANL
PNNL
Metal Hydride Properties
SRNL
UTRC,GM
Adsorption Properties
UQTR
Ford, NREL, GM, BASF

Phase 1 Objectives: Materials Operating Requirement – Metal Hydrides and Adsorbents



- **Collect Media Property Data for Metal Hydrides and Adsorbents**
  - **a. Kinetics data and models**
  - **b. Thermal and mass transport data**
  - **c. Evaluate completeness of available data**
  - **d. Propose experiments to obtain missing data**
  - **e. Liaison to MHCoE and independent projects**

- **Determine which existing <u>metal hydrides and adsorbents</u> have characteristics lying within the "acceptability envelope"**

Phase 1 Objectives: Materials Reactivity and Compatibility

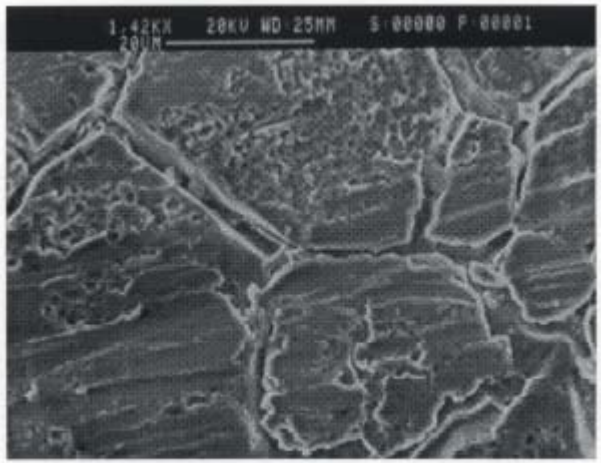
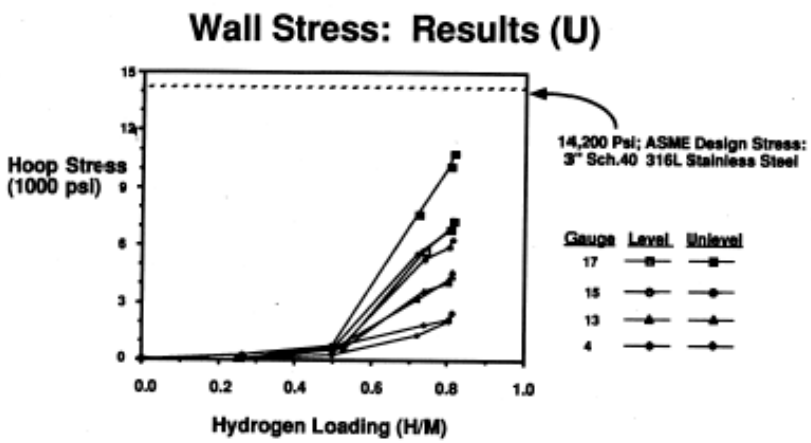


Figure 1. Interior surface of hydride bed container showing intergranular surface ditching



Materials Compatibility Studies

- **Chemical Interactions Between Hydrogen Storage Media and Vessel/ Liner Materials and System Components**
  - Surface Reactions
  - Characterization of Degradation Phenomenon

  Experiments

Coupon of vessel material placed in reactor vessel with storage media: Coupon characterization as a function of hydrogen charge/discharge cycles including XRD, XPS, Microstructure evolution and quantification of corrosion rates

- **Vessel/Liner/System Component Materials Hydrogen Permeability**
  - Hydrogen Transport Through Wall
  - Impact from Storage Materials

  Experiments

Hydrogen permeation rates measured on original as-received vessel materials and coupons exposed to storage material after hydrogen charge/discharge experiments.

- **Stress/Strain of Vessel/Liner Materials**
  - Small-Scale Tests
  - Storage Materials Expansion/Contraction
  - Expansion measurements on lab scale materials as a function of hydrogen charge/discharge cycles

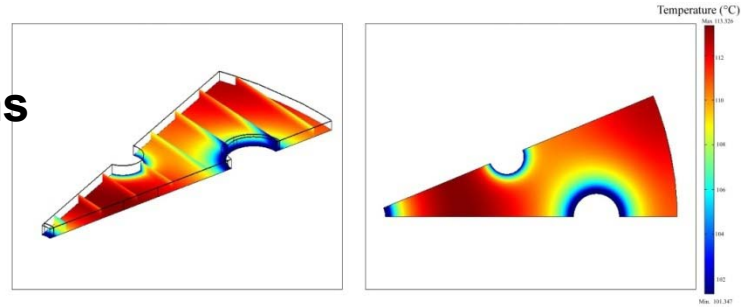
Technology Area Lead: Transport Phenomena

Transport Phenomena

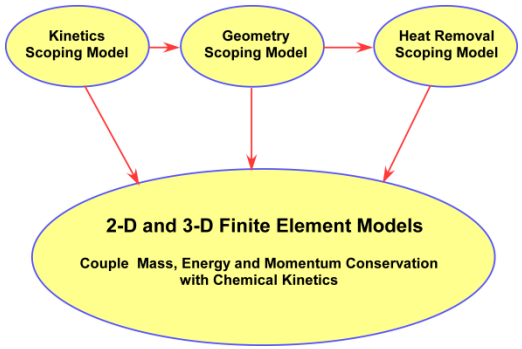
B. J. Hardy, SRNL, Technology Area Lead

Bulk Materials Handling	Media Structuring & Enhancement	Mass Transport	Thermal Energy Transport
PNNL LANL, UTRC, HSM, UQTR, Ford, GM	**GM** UTRC, UQTR, Ford, SRNL, PNNL	**SRNL** LANL, OSU, PNNL, UTRC, UQTR, Ford, GM	**SRNL** LANL, JPL, OSU, PNNL, UQTR, UTRC, GM, Ford

Phase 1 Objectives: Transport Phenomena and Storage System Model Development



- **Collect Operational Data for Storage Systems**
  a. Heat transfer
  b. Mass transfer
  c. Identify additional data required
- **Develop General Format for Models**
  a. Extension of "Hierarchical Modeling System"
  b. Apply preliminary system model boundary conditions
- **Assemble and Test Models**
  a. Preliminary validation
- **Identify "Acceptability Envelope" of Media Characteristics Based on 2010 & 2015 DOE Technical Targets**



Ultimate objective is the development of an "Acceptability Envelope" of Metal Hydride and Adsorbent Properties

Acceptability Envelope for Media Properties

Balance of Plant Parameters From System Models

For Example:

- H_2 at mass flowrate required by fuel cell or ICE
- Recoverable waste heat and temperature of discharge

"Black Box Storage System"

- Determine envelope of media properties required to meet Technical Targets along with BOP requirements & Forecourt operating parameters
- Use range of coolant temperatures & hydrogen temperatures & pressures from BOP analysis Forecourt operating conditions
- Media property envelope tied to storage vessel characteristics
- Feed media requirements back to BOP & Forecourt operating conditions

Forecourt Parameters

- H_2 pressure and temperature
- Controlled H_2 temperature (possible recirculation)
- Coolant flowrate & temperature required to control media temperature
  - Optimize kinetics
  - Optimize equilibrium capacity

HSECoE

Transport Phenomena Roles & Responsibilities

*Bulk Materials Handling**

PNNL - TTL

- Transport of solid chemical hydrides (PNNL, UTRC, HSM)
- Transport of chemical hydrides as liquids/slurries (LANL)
- Mechanical fuel element transfer system for chemical hydrides (PNNL)
- Adsorbent loading (UQTR, GM, Ford)
- Metal hydride loading (UTRC, HSM, GM, Ford)

** Media Transport*

Media Structuring & Enhancement

GM - TTL

- Identify media structures that improve operation of the stoarge system (SRNL, GM, Ford, UQTR, UTRC, PNNL)
- Investigate/develop fabrication methods that result in stable structures over a large number of cycles (UTRC, HSM, UQTR, Ford, GM)
- Investigate/develop additives, binders, etc. that enhance heat and/or mass transport in storage media (GM, Ford, UQTR, UTRC, PNNL)
- Investigate/develop media structures and additives that reduce thermal contact resistance to heat transfer surfaces (Ford, GM, UTRC, UQTR, PNNL)

*Mass Transport***

SRNL - TTL

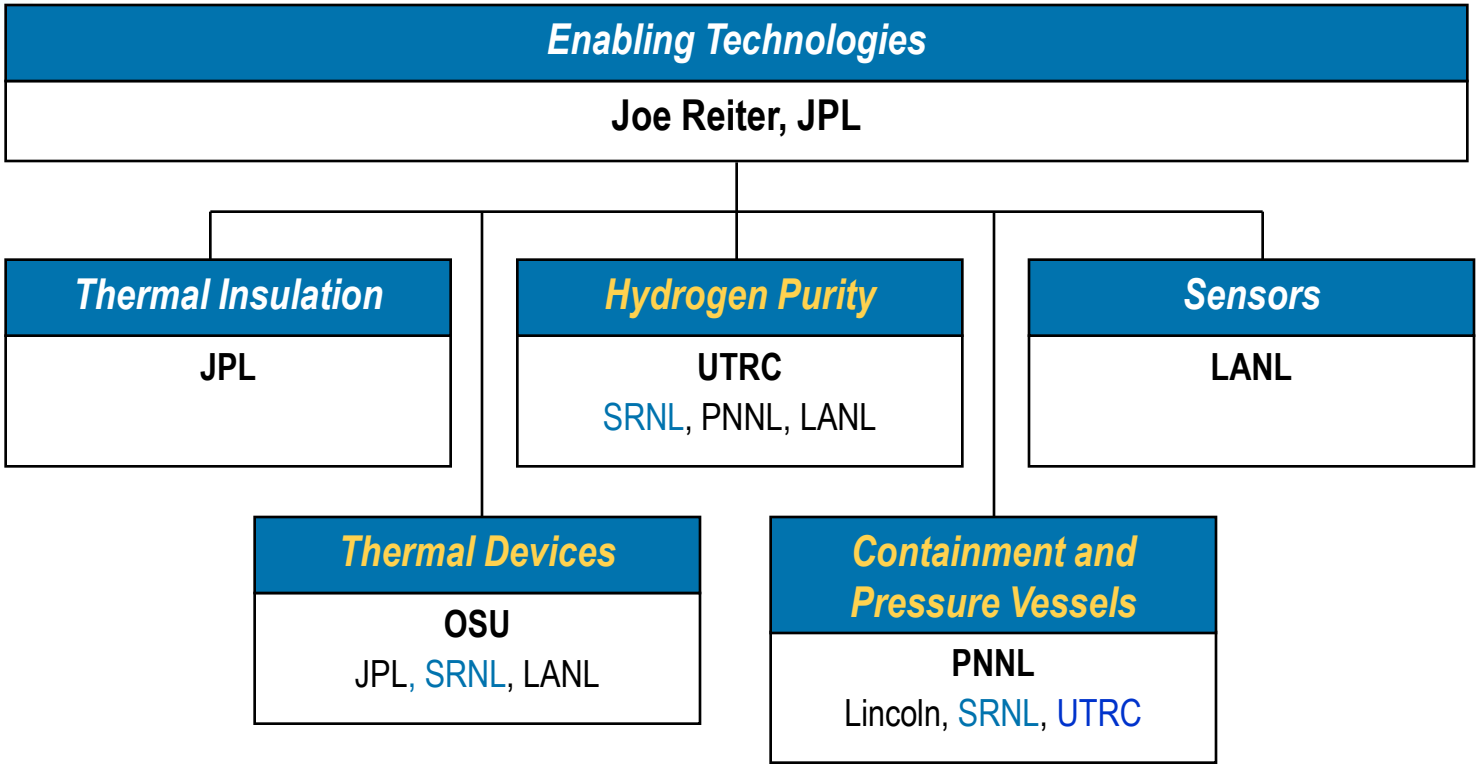
- Develop/incorporate models for gas transport in porous media and micro channels (SRNL, GM, Ford, UQTR)
- Transport in adsorbents and metal hydrides, including structured media and compacted powders (UTRC, UQTR, OSU, SRNL, Ford, GM)
- Transport in chemical hydrides, including solid structured media (LANL, PNNL)
- Transport in micro devices (OSU, SRNL)
- Transport in mini channel devices (UTRC, HSM)

*** Hydrogen Transport*

Thermal Energy Transport

SRNL - TTL

- Develop/incorporate models for energy transport & generation in media and transport to heat exchange systems (SRNL, GM, Ford, UQTR)
- Transport in adsorbents and metal hydrides, including structured media and compacted powders (UTRC, UQTR, OSU, SRNL, JPL , GM, Ford)
- Transport in chemical hydrides, including solid structured media (LANL, PNNL)
- Advanced and mini channel heat exchangers (UTRC, SRNL, JPL)
- Enhanced transport in micro devices (OSU, SRNL)
- Second Law optimization analysis (OSU)
- Advanced thermal insulation (JPL)


Enabling Technologies
Joe Reiter, JPL
Thermal Insulation
JPL
Hydrogen Purity
UTRC
SRNL, PNNL, LANL
Sensors
LANL
Thermal Devices
OSU
JPL, SRNL, LANL
Containment and Pressure Vessels
PNNL
Lincoln, SRNL, UTRC

Phase 1 Objectives: Hydrogen Purification

Hydrogen Purification Studies

- **Review of Existing Commercially Available Hydrogen Purification Systems**
  - **Through-put**
  - **Footprint**
  - **Cost**
  - **Product Quality**

- **Miniaturization of Existing Hydrogen Separations Technologies**
  - **Alternate manufacturing routes/ re-designs**
  - **Issues/Challenges w/Scaling**
  - **Alternate Materials**
  - **Replacement/Regeneration**

- **Understanding of Hydrogen Storage Media Secondary Impurity Effects on Operation**

Subscale Prototype Construction, Testing, & Evaluation

T. Semelsberger, LANL

Risk Assessment & Mitigation

UTRC
All Other Partners

Design & Optimize Subscale Systems

LANL, SRNL, UQTR
JPL, UTRC, PNNL, OSU

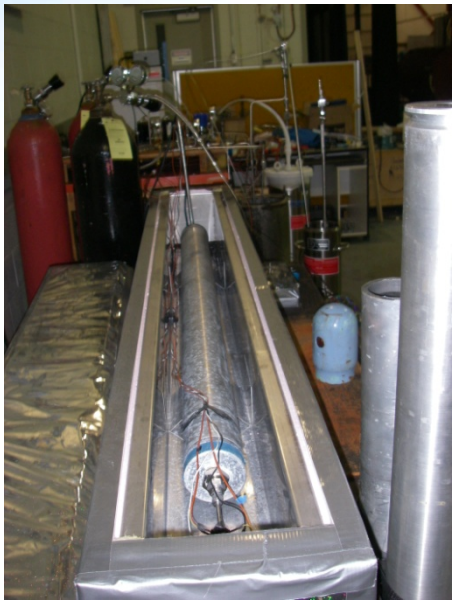
Fabricate Subscale System Components

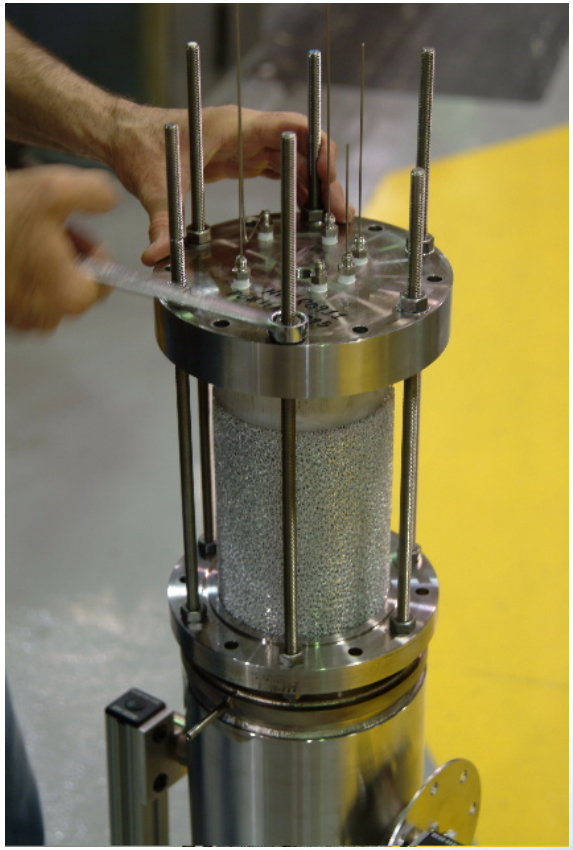
SRNL, LANL
Lincoln, OSU, PNNL, UTRC

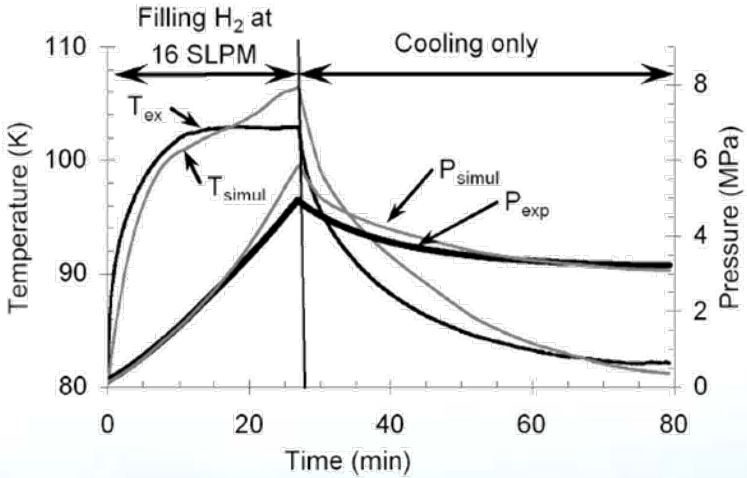
Assemble & Evaluate Subscale System

LANL, JPL, UQTR

Metal Hydride and Adsorbent Vessel Design, Fabrication and Adsorbent System Testing







Overall Objectives for Phase 3

- **Scale Design and Fabricate Metal Hydride and Adsorbent Based Prototype Vessels**
  - Use detailed models for to design prototypes that best represent full-scale systems
  - Fabricate vessels and ship to test facility for media loading
    - Metal hydride at SRNL
    - Adsorbent at UQTR
  - Test prototypes
- **Collect Data From Prototype Tests**
- **Apply Data to Models**
  - Validate and refine
  - Rank prototype designs
- **Use Refined Models to Predict Operation of Full-Scale Storage System (Metal Hydride and Adsorbent)**

Summary of SRNL Technical Accomplishments (as of 3/09)

- **Issued List of Data Requirements for Storage Media**
  - Overall list of media
  - Prioritized list (technical assessment)
- **Assembled SRNL Teams for HSECoE Tasks**
  - Including collaborative team efforts with UQTR
  - Detailed task list with individual assignments
- **Acquired Necessary Software and Aligned High Performance Computer Systems**
- **Initiated Microchannel Heat Exchanger Development Task With OSU Microproducts Breakthrough Institute**
  - In collaboration with UTRC, JPL and PNNL
- **Established Structured & Enhanced Media Technical Team, Led by GM**
- **Began Exchange of Data and Models for Adsorbents With UQTR, GM and UTRC**
  - Working with UQTR Ph.D. candidate on metal hydride model development

Collaborations

- **While SRNL is collaborating with virtually all Center members on this project our major technical collaborators include:**
  - UQTR, JPL, PNNL, UTRC, LANL and NREL
- **SRNL will also continue close collaborations with:**
  - MHCoE led by Sandia, SSAWG led by ANL as well as various national and international hydrogen groups such as the IPHE, IEA, AIST etc.

Approach: Phase 1 Milestones, Deliverables and Go/No-Go Criteria

Milestones

- **Compile Metal and Adsorption Hydride Data**
  - Chemical kinetics
    - Equilibrium hydrogen capacity
    - Model development
  - Heat transfer parameters
  - Mass transfer parameters
- **Develop Preliminary Hierarchical Model**
  - Use model to define "acceptability envelope" of metal and adsorption hydride properties to meet DOE 2015 goals
- **Develop Material Test Plan and Matrix**
- **Conduct Preliminary Purification Studies**

Deliverables (Programmatic Go/No-Go Criteria)

- **Preliminary Envelope of Properties for Acceptable Media**
- **Report Describing Phase 1 Activities and Results in Detail**

Technical Go/No-Go Criteria

- **Down Select Media Falling Within Acceptability Envelope**

Future Work: Phase 2 and 3 Milestones, Deliverables and Go/No-Go Criteria

Milestones

- **Identification of Subscale Storage System Designs for Testing**
- **Final Scaled Prototypes for Testing**
- **Predictive Capability for Full Scale Hydrogen Storage Systems**

Deliverables (Programmatic Go/No-Go Criteria)

- **Completed Modeling System**
  - Parametric sensitivity study
  - Identification and design of prototype storage systems meeting 2015 DOE Technical Targets
  - Test matrix & measurements
- **Material Recommendations for Prototypes**
- **Purification System Recommendations for Prototypes**
- **Prototypes**
  - Final scaled prototype design
  - Fabricated prototype vessel
  - Fabricate test station
- **Subscale Prototype Performance Report**
- **Prediction of Full-Scale Storage System Performance by Using Models Refined With Data from Prototype Tests**
- **Reports Describing Phase 2 and 3 Activities in Detail**

Technical Go/No-Go Criteria

- **Identify Prototype Designs That Meet the 2015 DOE Technical Targets**

Facilities

Savannah River National Laboratory

- **30,000 ft^2 Hydrogen Technology Research Laboratory (HTRL)**
  - 22 lab modules and a high bay area
    - Outfitted with centralized gas delivery system providing H_2, N_2, He, and Ar
    - Room and hood hydrogen monitors
  - Measurement of heat transfer parameters
    - Calorimeter
    - Thermal conductivity
  - A variety of hood configurations (including walk-in)
  - Computer network access
  - Atmospherically controlled gloveboxes
  - Clean room

Facilities

University of Quebec at Trois Rivieres

Hydrogen Research Institute (HRI), founded in 1994, is a research unit located at UQTR. HRI plays a strategic role in developing and evaluating reliable hydrogen technologies by fostering research activities on hydrogen storage material development, system design, and system safety.

- Automated high-accuracy gravimetric and volumetric hydrogen storage equipment for adsorption characterization
- Analytical tools for assessment of adsorption properties along with models for adsorption thermodynamics and system thermal effects.
- Test bench facilities are available for performing sub-kilogram scale adsorption-based system charging and discharging experiments
- Facilities available as needed for the production of custom-designed, high-surface-area activated carbon with optimized adsorption characteristics in kilogram quantities.
- Facilities for pelletization and post-production densification, which increase the volumetric capacity of granulated porous adsorbents

HSECoE

Key Personnel

Theodore Motyka	Ph.D. Chem. E.	SRNL Project Lead
Bruce Hardy	Ph.D. Nuclear/Chem. E.	Transport Phenomena and Modeling and Design Lead
Thad Adams	Ph.D. Matl. Sc. & E.	Material Compatibility Lead
Kyle Brinkman	Ph.D. Matl. Sc. & E.	Hydrogen Purification
Elliott Clark	Ph.D. Metalurg. E.	Materials Compatibility
Joshua Gray	Ph.D. Chem. E.	Material Op. Requirements
Leung Kit Heung	Ph.D. Chem. E.	Metal Hydride Prototype Vessel Design Lead
James Klein	Ph.D. Chem. E.	Prototype Vessel Fabrication
Richard Chahine	Ph.D. Energy/Physics	UQTR Lead, Adsorbents Material Requirements and Prototype Testing Lead

Project Summary

Relevance

As both the overall lead and a major technical contributor to the HSECoE project, SRNL is using its extensive expertise in metal hydride technology, hydrogen materials compatibility, transport phenomena modeling & analysis and hydrogen storage system & component design & fabrication to evaluate a solid-state hydrogen storage system for vehicle application that meets or exceeds DOE's 2015 goals.

SRNL, through a subcontract grant, is also utilizing the expertise of the UQTR, which has been internationally recognized for its work in hydrogen absorbent material and system development and testing.

Approach

In Phase I and II SRNL will:

- lead the overall project in Transport Phenomena modeling and analysis concentrating on metal hydride and adsorbent systems and components designs.
- lead in the collection and screening of material property and engineering data for metal hydride and adsorbent materials as well as help to analyze the reactivity and compatibility of these materials with vessel walls and other system components.
- lead in the development of hydrogen purification systems for metal hydride and adsorbent systems as required.

In Phase III SRNL and UQTR will be responsible for the final design and fabrication of a metal hydride and adsorbent based hydrogen storage system and subsequent testing of the adsorbent system at UQTR based on DOE GO/NO/GO decisions

SRNL will also continue to upgrade and refine the overall vessel model to be able to predict full scale storage system performance.

Technical Accomplishments and Progress (as of 3/09)

Beginning work in 2/09 progress has been limited mostly to establishing teaming arrangements and acquiring software/hardware tools.

Collaborations

HSECOE partners, Materials Centers, SSAWG, IPHE, IEA etc.

Proposed Future Work (Phase I)

- Compile Metal and Adsorption Hydride Data
- Develop Preliminary Hierarchical Model
- Use model to define "acceptability envelope" of metal and adsorption hydride properties to meet DOE 2015 goals
- Develop Material Test Plan and Matrix
- Conduct Preliminary Purification Studies