Advancement of Systems Designs and Key Engineering Technologies for Materials Based Hydrogen Storage

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United Technologies Research Center

C. Willson
HSM Systems

DOE Hydrogen Program

Annual Merit Review
Arlington, VA
May 20, 2009

HSECoE

Project ID: STP_08_Mosher

Overview

- **Timeline**
  - Start: Feb. 2009 (signed early March)
  - End Phase 1: Jan. 2011
  - End Phase 2: Jan. 2013
  - End Phase 3 / Project: Jan. 2014
  - Percent complete: 0.8% (spending)
- **Budget**
  - $6.86M Total Program
    - $5.32M DOE
    - $1.14M UTRC
    - $0.40M HSM
  - FY08: $0k
  - FY09: $600k
- **Barriers***
  - A – J
  - A. System Weight & Volume
  - D. Durability / Operability
  - E. Charging / Discharging Rates
- **Targets***
  - All
- **Partners**
  - Subcontractor:
    HSM Systems, Inc.
  - HSECoE Partners:

* DOE EERE HFCIT Program Multi-year Plan for Storage

HSECoE & Project Objectives

- In parallel with novel storage material development being pursued in DOE / world-wide research, advance technologies to support maximizing the performance of associated material based systems.
- Efforts will be focused on select storage material candidates (metal hydrides, adsorbents & chemical storage materials), with examinations also considering representative target materials.
- Three main objectives:
  - Analyses for more precise understanding of requirements
  - Conception, refinement and evaluation of novel technologies
  - Integration and optimization of components & sub-systems
- UTRC's efforts will involve each of these three main areas, building upon experience in the development of hydrogen storage systems and fuel cells to achieve system designs and process methods which result in the greatest overall system viability.

Primary Tasks

Range of novel and / or integrated technical elements:

1. System engineering / modeling & forecourt requirements
2. Material properties, kinetics & compatibility
3. System risk analysis
4. Component design modeling development
5. On-board separation / purification
6. Advanced heat exchangers
7. Hydride structured forms / compacts & integration
8. Chemical storage material transport
9. Reversible hydride & adsorbent prototyping support

Emphasis of specific concepts and tasks will evolve during the three Phases of the HSECoE.

Center Structure – Roles & Collaborations

Hydrogen Storage Engineering Center of Excellence

D. Anton, SRNL
T. Motyka, SRNL

Materials Operating Requirements

D. Herling, PNNL

- Materials Centers of Excellence Collaboration – SRNL, LANL, NREL
- **Reactivity & 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
- **Media 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, NREL

- 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 Rechargeable - UTRC**
- On-Board Rechargeable – GM
- Power Plant – Ford

Subscale Prototype Construction, Testing & Evaluation

T. Semelsberger, LANL

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

Leading / Project Tasks
Additional Project Tasks
Supporting

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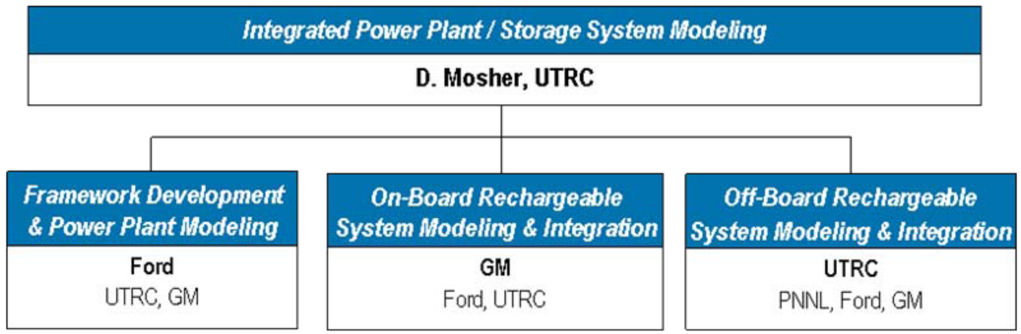
Task 1: System Engineering Modeling

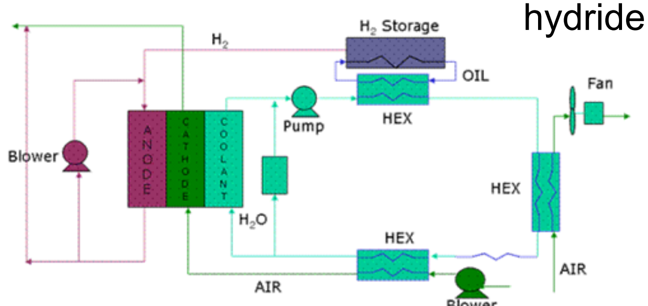
Modeling of the integrated power plant / storage system will provide detailed understanding of storage system requirements and prediction of overall performance.

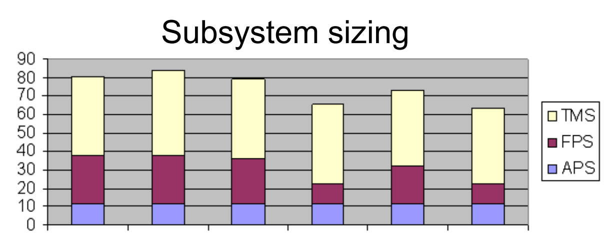
- Coordinate *Integrated Power Plant / Storage System Modeling* Tech. Area.



- Guide performance / cost requirements and evaluate design options for multiple vehicle operation scenarios.
- Assess forecourt requirements.

Example (simplified) integrated hydride / PEMFC study





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Interrelated Modeling Levels

Performance Analysis

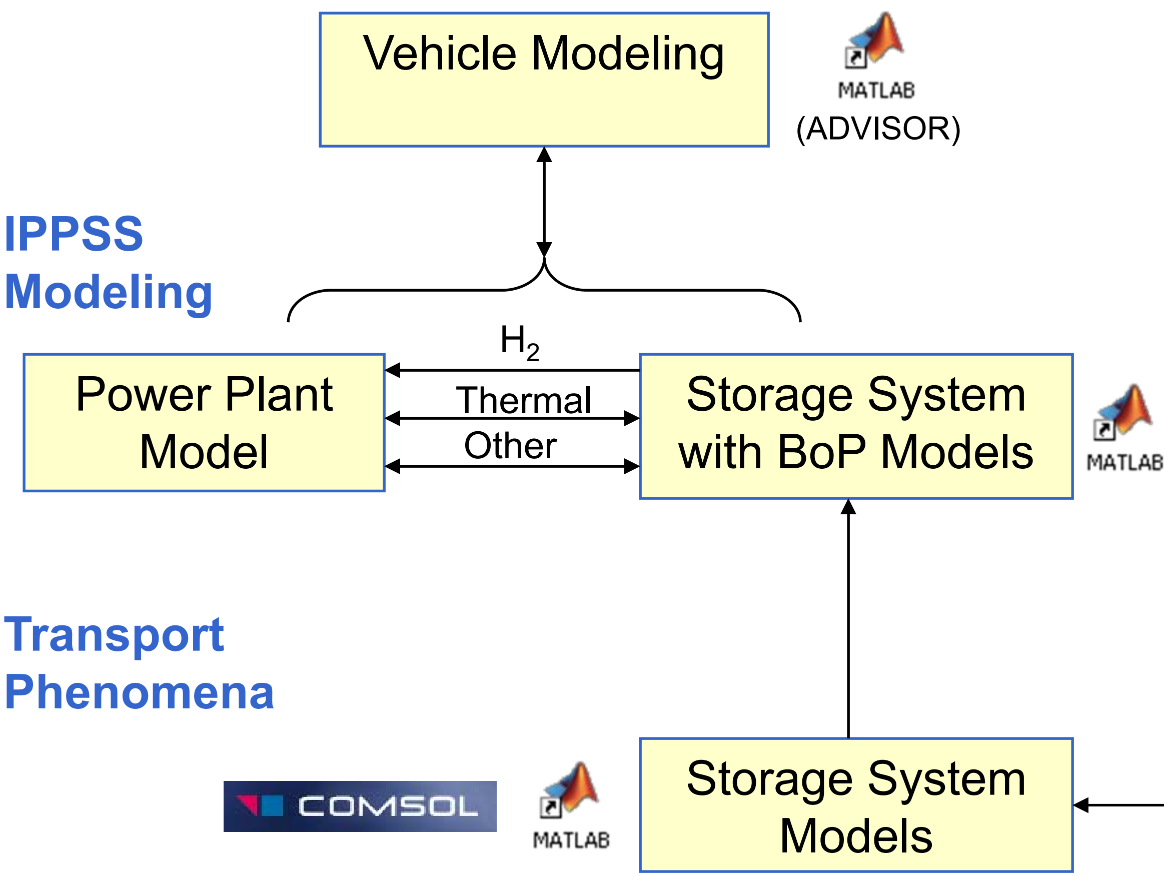
- Marketability
- Vehicle component opt.
- Refined power plant req.

IPPSS Modeling

- Integrated performance
- Storage system requirements
- SS component wt. & vol. opt.

Transport Phenomena

- Storage system design



Technology Area: Integrated Power Plant / Storage System (IPPSS) Modeling

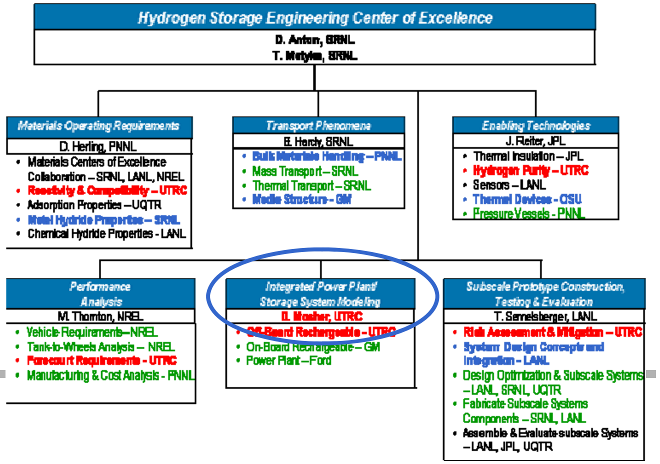
Technology Area Lead: D. Mosher

Objectives:

- Evaluate combined power plant / storage system configuration to determine hydrogen storage system requirements and to predict integrated performance (H2 supply, thermal management, weight and volume).
- Develop representations for on-board rechargeable adsorbent and hydride storage systems consistent with a common simulation platform and power plant model.
- Develop representations for off-board rechargeable chemical storage systems consistent with a common simulation platform and power plant model.

Accomplishments:

- Identified MatLab/Simulink as the common software platform.



Key Milestones:

1. Determine framework structure, vehicle interfacing and multiple integration level approaches. *(6/09)*
2. Construct FC model for baseline level IPPSS modeling. *(9/09)*
3. Construct baseline level storage system models and specify requirements. *(12/09)*
4. Develop detailed level model framework. *(3/10)*

Issues:

- Develop a common understanding of existing model structures.
- Proprietary data and software.

This and subsequent "quad-charts" provide information on Approach, Collaboration, Accomplishments (currently minimal) and Future Work.

Technology Area: Integrated System Modeling

Technology Team: Off-Board Rechargeable System

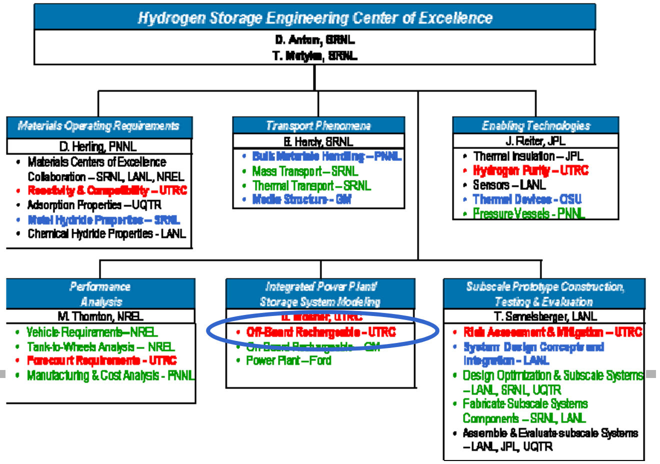
Technology Team Lead: D. Mosher

Team members: UTRC, PNNL, Ford, GM

Objectives:

- Develop representations for off-board rechargeable chemical storage systems consistent with a common simulation platform and power plant model.
- Determine storage system baseline requirements.
- Establish representations consistent with the modeling strategy for vehicle level optimization studies.
- Develop system simulation models for the prime material candidates and system configurations.
- Conduct simulations of integrated power plant / storage system performance for key operational conditions.

Accomplishments:



Key Milestones:

1. Identify materials and baseline configurations for hydrogen storage system simulation. *(6/09, UTRC / PNNL)*
2. Develop initial representations of system models. *(9/09, UTRC)*
3. Identify baseline hydrogen storage system requirements. *(12/09, UTRC / PNNL)*
4. Develop detailed representation consistent with power-plant and vehicle level models. *(3/10, UTRC)*

Issues:

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Technology Area: Performance, Cost & Energy Analysis
Technology Team: Forecourt Requirements

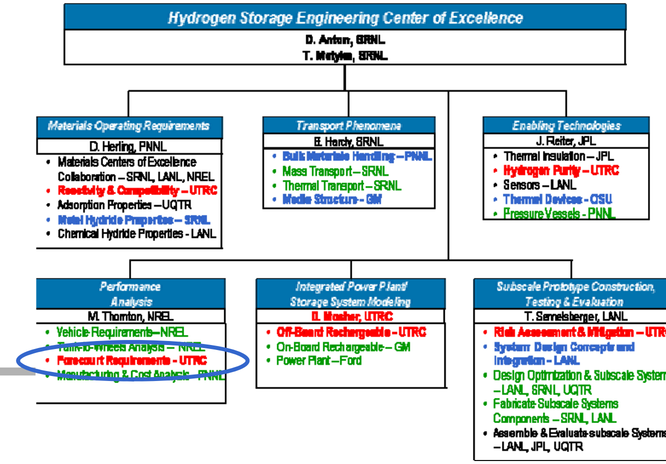
Technology Team Lead: D. Mosher
Team members: UTRC, NREL, PNNL

Objectives:

Develop an understanding of forecourt requirements for key storage system methods and assess impact on viability.

- Identify the primary requirement types and configurations for each class of storage system.
- Collaborate with the Well To Tank analysis efforts to expand information sources and ensure consistency.
- With input from storage system development efforts, assess infrastructure, energy and safety characteristics.

Accomplishments:



Key Milestones:

1. Compile forecourt requirement types for general representations of each major storage class. *(6/09)*
2. Provide WTT analysis efforts with energy utilization descriptions for at least one storage system. *(9/09)*
3. Evaluate prime storage system concepts and technologies for their strengths and weaknesses related to forecourt requirements. *(3/10)*

Issues:

- Develop an interface with Production & Delivery activities consistent with the broader DOE structure.

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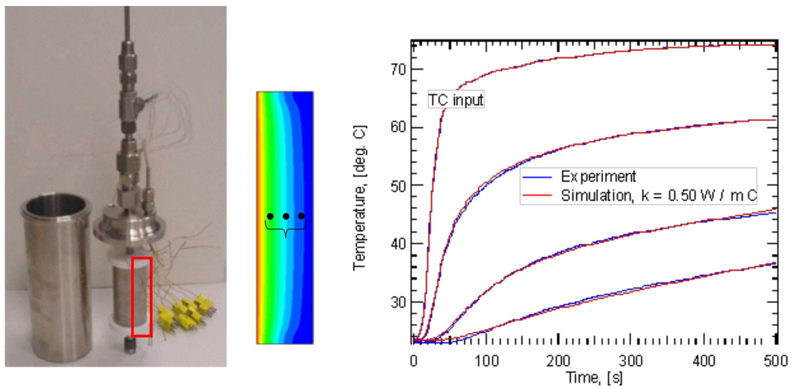
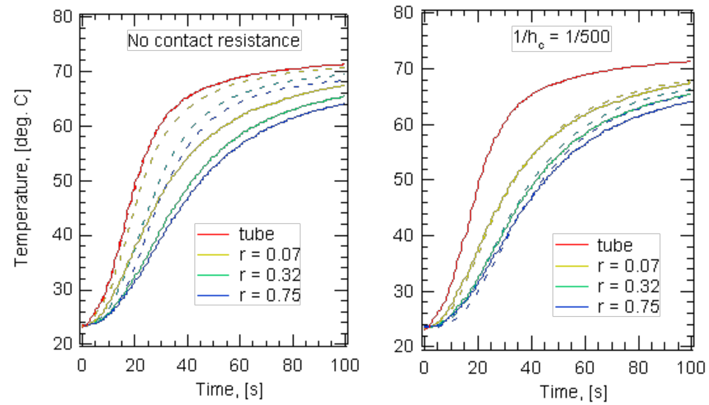
Task 2: Material Properties and Kinetics

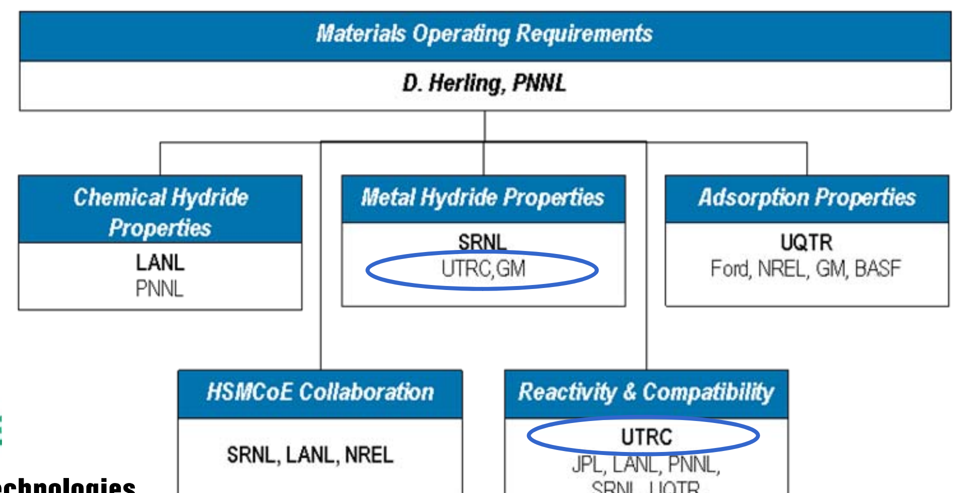
- Support measurement of chemical, thermal and physical properties with an emphasis on connections to other UTRC tasks (heat exchanger development, compacted / structured material forms and reactivity / compatibility)

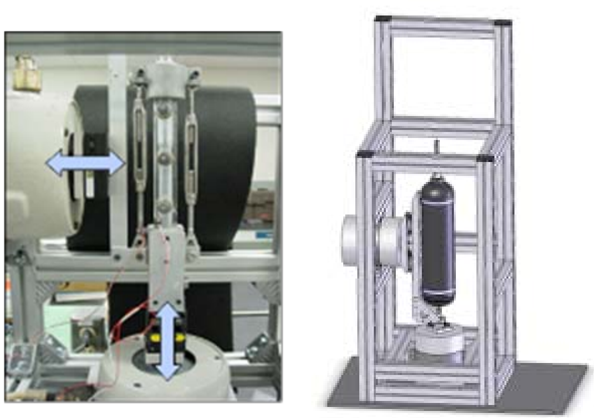


Thermal diffusivity / conductivity



Thermal contact resistance





Vibration effects for materials & sub-components

Technology Area: Materials Operating Requirements **Technology Team Lead:** D. Mosher

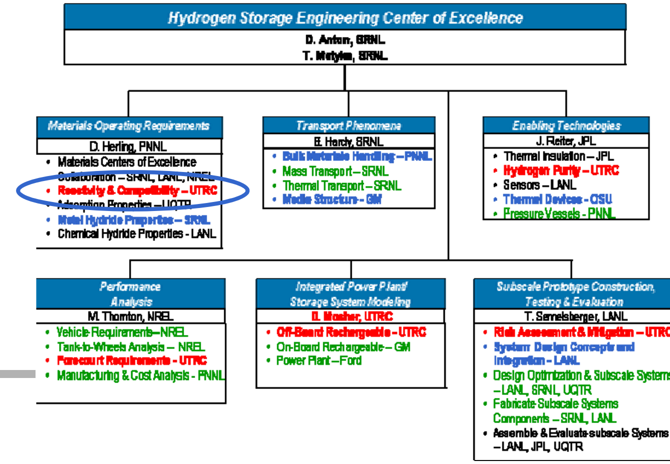
Technology Team: Reactivity & Compatibility **Team members:** JPL, LANL, PNNL, SRNL, UTRC, UQTR

Objectives:

Determine the effects from adverse reactivity/incompatibility of storage materials with system/component materials & potential contaminants.

- Collaborate with the DOE Reactivity Projects to evaluate the effects from exposure to contaminants (H2O, O2).
- Conduct cyclic or moderate endurance tests for storage material / system material combinations.
- Characterize H2 and storage materials compatibility with system components/materials (if data not available).
- Recommend and/or review materials for use in construction of prototypes for H2 compatibility.

Accomplishments:



Key Milestones:

1. Compile list of storage material candidates, potential system materials and operation conditions. *(9/09)*
2. Screen for compatibility of the top (potential & risk) material combinations under representative operation conditions. *(3/10)*

Issues:

- Determine the level of material CoE involvement in kinetics and composition tests.
- Establish initial guidelines for importance level of risk in the Phased development.

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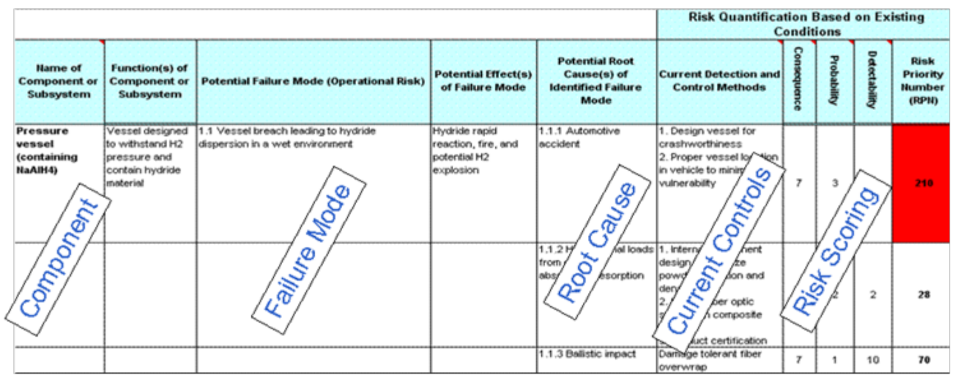
Task 3: Risk Assessment

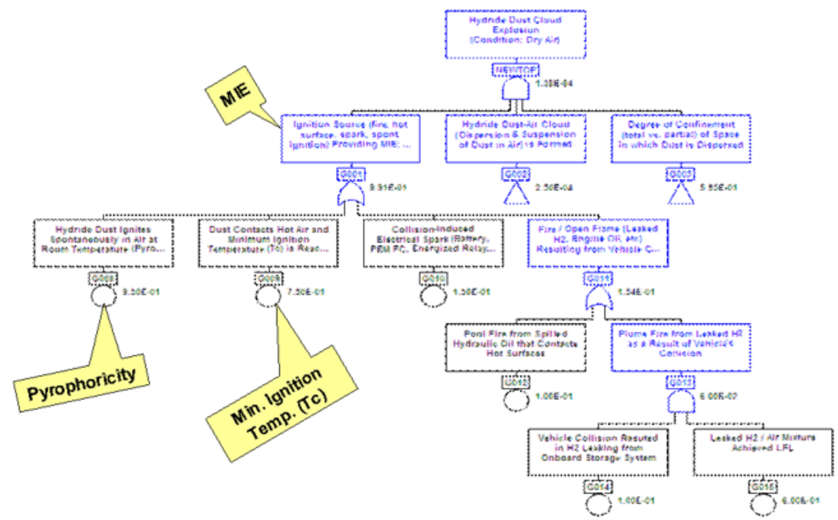
- Liaison to the three DOE Reactivity projects (UTRC, SRNL, SNL)
- Lead risk analyses of the innovative components, processes and systems at the appropriate level and time during concept / hardware development.
  - Understand potential risks at an early stage
  - Develop and incorporate risk mitigation methods

Qualitative risk assessment:
Failure Modes & Effects Analysis



					Risk Quantification Based on Existing Conditions				
Name of Component or Subsystem	Function(s) of Component or Subsystem	Potential Failure Mode (Operational Risk)	Potential Effect(s) of Failure Mode	Potential Root Cause(s) of Identified Failure Mode	Current Detection and Control Methods	Consequence	Probability	Detectability	Risk Priority Number (RPN)
Pressure vessel (containing NaAlH4)	Vessel designed to withstand H2 pressure and contain hydride material	1.1 Vessel breach leading to hydride dispersion in a wet environment	Hydride rapid reaction, fire, and potential H2 explosion	1.1.1 Automotive accident	1. Design vessel for crashworthiness 2. Proper vessel lo[illegible]tion in vehicle to minim[illegible] vulnerability	7	3		210
				1.1.2 H[illegible]al loads from [illegible] abs[illegible]esorption	1. Intern[illegible]nent design [illegible]ze powd[illegible]on and den[illegible] 2. [illegible]ber optic [illegible] composite [illegible]uct certification		2	2	28
				1.1.3 Ballistic impact	Damage tolerant fiber overwrap	7	1	10	70

Quantitative risk assessment:
Fault Tree / Event Tree Analysis



Technology Area: Subscale Prototyping

Technology Team: Risk Assessment & Mitigation

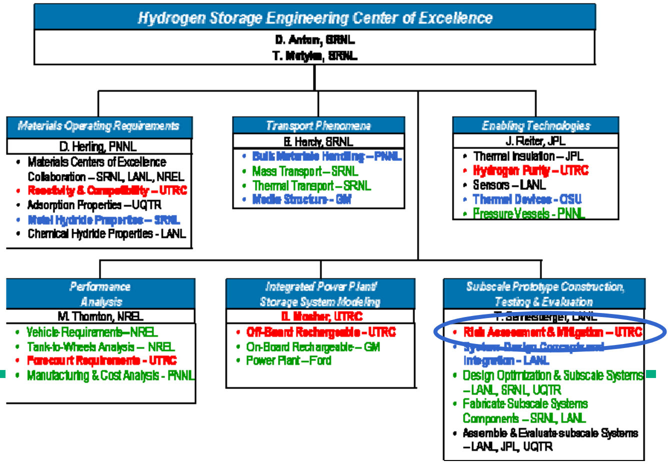
Technology Team Lead: D. Mosher

Team members: UTRC, All LANL, JPL

Objectives:

- Assess the risks of select novel approaches and system configurations under vehicle operation scenarios.
- Develop mitigation concepts to be advanced in association with the related technical area / team.
- Perform risk assessment of prototype fabrication, testing and decommissioning.
- Collaborate with the DOE Reactivity Projects in both the risk assessment and mitigation activities.

Accomplishments:



Key Milestones:

1. Develop an initial list of technologies / configurations of interest for risk / performance trade-offs. *(6/09, UTRC)*
2. Establish the risk analysis framework(s) to be used in novel concept evaluation. *(9/09, UTRC)*
3. Conduct qualitative risk analyses for select concepts. *(3/10, UTRC)*

Issues:

- Clarification: one portion of this TT focuses on novel concepts and the other on prototyping.

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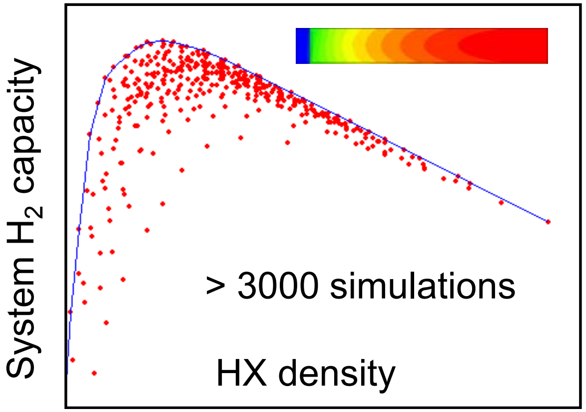
Task 4: Modeling Development Support & Application

- Support SRNL led effort in detailed model framework development. Share effective methods and experience for design analysis and optimization.
- Develop high level modeling and scripts with an emphasis on other UTRC tasks (heat exchanger development, compacted / structured material forms).

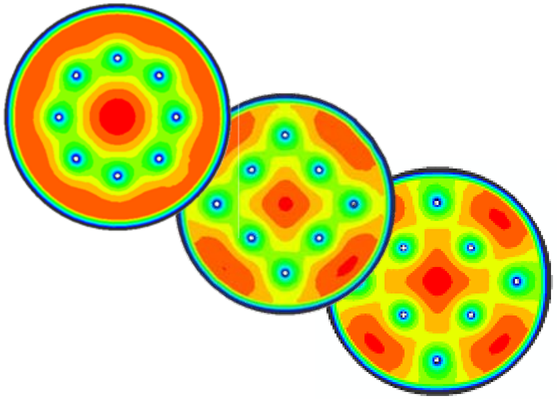
Build upon prior modeling methods

Fin unit cell model

Design variables:
- Fin thickness
- Fin spacing
- Tubing OD
- Tubing spacing



System cross-section model

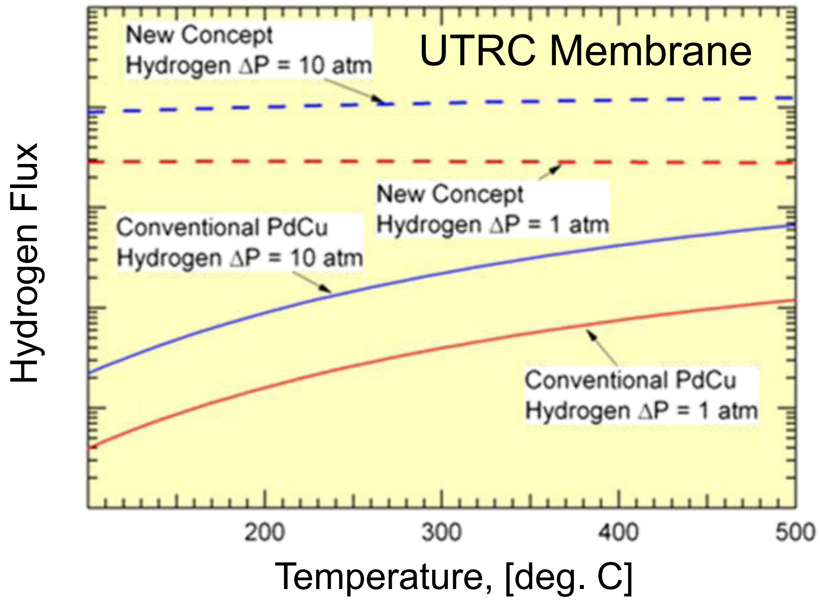


- Tubing positioning

Task 5: On-board Separation / Purification

- Primary objective is gaseous impurity separation / hydrogen purification.

  This could have substantial impact on the viability of many storage material candidates.
- Secondary objectives are to address solid / gas and liquid / gas separation.
- Distinct membrane materials & approaches: UTRC – ceramic; HSM – polymeric.
- Task will also examine molecular sieve methods and include efficient, robust system integration.



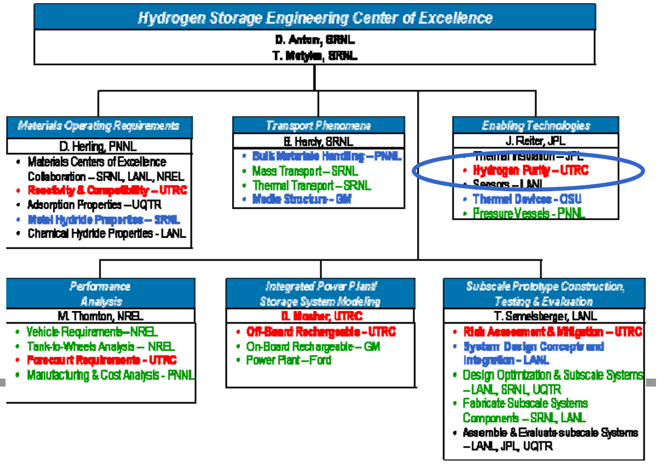
Technology Area: Enabling Technologies
Technology Team: Hydrogen Purity

Team Lead: D. Mosher
Team Members: UTRC, HSM, SRNL, PNNL, LANL

Objectives:

- Develop system methods to improve discharged hydrogen purity / quality for acceptable PEM fuel cell durability.
- Establish procedures for assessing hydrogen purity – moderate level & PEM FC durability level.
- Collaborate with material CoEs to identify existing purity data / concerns & gaps for future testing.
- Evaluate and advance separation method concepts (gas/gas and gas/particulate).
- Incorporate top separation candidate(s) into storage system designs.

Accomplishments:



Key Milestones:

1. Determine current purity concerns in materials CoE and select top 2 to 3. *(6/09, All)*
2. Compare initial evaluations of separation approaches. *(12/09, All)*

Issues:

- Storage materials & impurities are To-Be-Determined.

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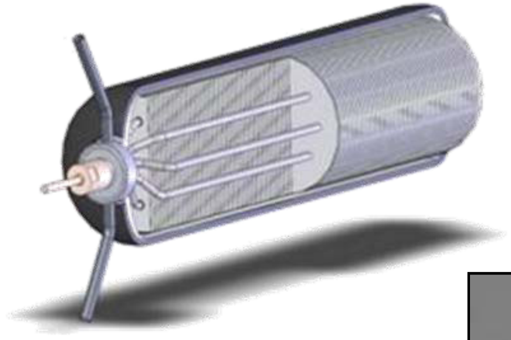
Task 6: Advanced Heat Exchangers

- Evaluate minichannel heat exchangers, phase change working fluids and alternate heat conduction enhancement configurations.
- Apply prior optimization and integration experience along with new CoE tools.
- Complement OSU microchannel development with commercially existing, low cost variation to current metal hydride systems.
- Collaborate with PNNL & Lincoln Composites for pressure vessel / overall system manufacturability including powder loading / compact installation.

Minichannel cross section

Low cost application in air conditioning



Build upon second UTRC $NaAlH_4$ prototype design

Task 7: Hydride Compacts and Integration

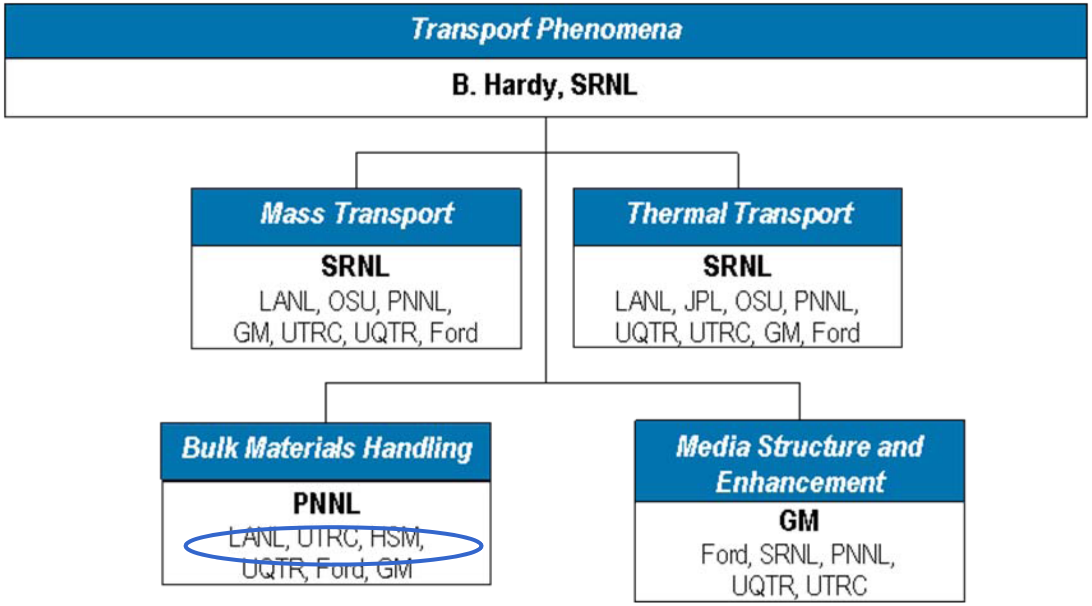
- Develop powder compaction and bed structuring methods to
  - Improve material volumetrics
  - Enhance heat transfer
  - Reduce undesired reactivity & risk
  - Provide adequate mass transfer
  - Ensure durability
- Integrate structured beds into overall system designs (heat exchanger, pressure vessel, system assembly procedure).

Optimally compacted $NaAlH_4$
Cycled through 100 cycles

HSM Systems

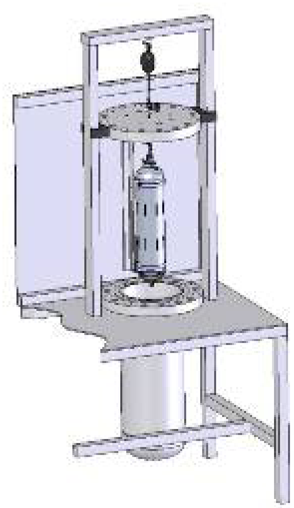
Task 8: Chemical Storage Material Transport

- Refine and evaluate novel concepts in solids handling and transport to complement PNNL led Technology Team.
- Leverage HSM efforts in alane system development.
- Include connection to Forecourt Requirements task.

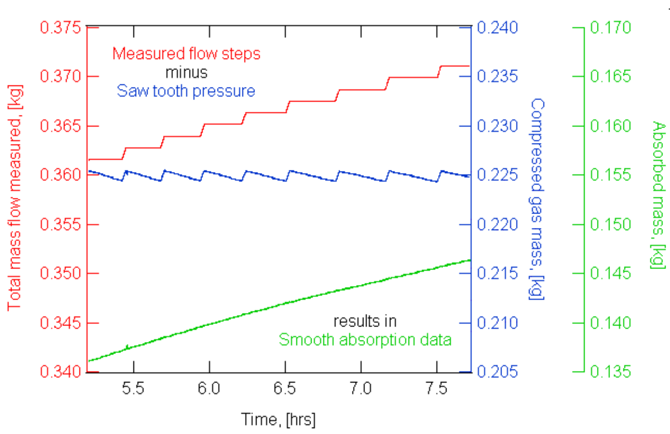


Task 9: Support Reversible Hydride & Adsorbent Prototyping

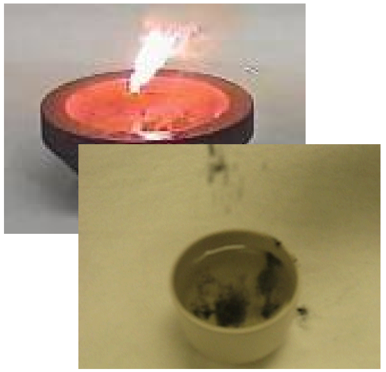
- Translate the component optimizations of tasks 5, 6 and / or 7 into detailed designs.
- Provide guidance on component manufacture and system assembly, particularly as they relate to the integrated designs involving UTRC components and system configuration development.
- Share experiences of prior complex hydride system fabrication, testing and decommissioning.



100 g H_2 scale prototype testing



"Burst flow" testing technique using Coriolis flow meters



Material tests associated with system decommissioning

Summary and Future Work

Objectives: Advance the state of materials based hydrogen storage systems through improved requirements understanding, refinement of novel concepts and demonstration of optimized components and systems.

Approach: The set of project tasks, in close collaboration with HSECoE partners, addresses the three main objective areas above. Emphasis will be placed on metal hydride systems with secondary efforts supporting adsorbent and chemical storage methods.

Future Work: Given that the project has just been initiated, the task slides and quad charts represent the future work to be performed. The more specific near-term milestones are specified in the quad-charts for the Technology Teams led by UTRC.