IV.D.1a Hydrogen Storage Engineering Center of Excellence (HSECoE)

Donald L. Anton
Savannah River National Laboratory
Bldg. 999-2W
Aiken, SC 29808
Phone: (803) 507-8551; Fax: (803) 652-8136
E-mail: DONALD.ANTON@SRNL.DOE.GOV

DOE Technology Development Manager:
Monterey Gardiner
Phone: (202) 586-1758; Fax: (202) 586-9811
E-mail: Monterey.Gardiner@ee.doe.gov

Subcontractor:
Universite du Québec, a Trois-Rivieres, Québec, Canada

Project Start Date: February 1, 2009
Project End Date: January 30, 2014

Objectives

- Develop system models that will lend insight into overall fuel cycle efficiency.
- Compile all relevant materials data for candidate storage media and define future data requirements.
- Develop engineering and design models to further the understanding of on-board storage energy management requirements.
- Develop innovative on-board system concepts for metal hydride, chemical 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.
- Design, fabricate, test, and decommission the subscale prototype components and systems of each materials-based technology (adsorbents, metal hydrides, and chemical hydrogen storage materials).

Technical Barriers

This project addresses the following technical barriers from the Hydrogen Storage section of the Hydrogen, Fuel Cells and Infrastructure Technologies Program Multi-Year Research, Development and Demonstration Plan:

(A) System Weight and Volume
(B) System Cost
(C) Efficiency
(D) Durability/Operability
(E) Charging/Discharging Rates
(G) Materials of Construction
(H) Balance of Plant Components
(J) Thermal Management
(K) System Life Cycle Assessments
(L) High Pressure Conformality
(P) Lack of Understanding of Hydrogen Physisorption and Chemisorption
(S) By-Product/Spent Material Removal

Technical Targets

This project is directing the work of a diverse team of engineering organizations to design, build and demonstrate prototype hydrogen storage systems for each metal hydride, chemical hydride and hydrogen sorption materials meeting as many of the DOE Technical Targets for hydrogen storage as possible. This project recently started in February of this year, and thus little quantifiable progress has been made towards meeting the DOE 2010 or 2015 Hydrogen Storage Goals. The technical targets of the center are to demonstrate hydrogen storage systems meeting and making progress towards meeting as many of the DOE Hydrogen Storage Technical Targets as possible. This can best be described with the Go/No-Go decisions established for the Center with DOE.

- Phase 1 Go/No-Go decision is to: Provide a system model for each material sub-class (metal hydrides, adsorption, chemical storage) which shows:
  - Four of the DOE 2010 numerical system storage targets met
  - The status of the remaining numerical targets must be at least 40% of the target
- The Phase 2 Go/No-Go decision is to: Provide at least one full scale system design concept (5 kg H_2 stored) where:
  - Six of the DOE 2015 numerical targets are met
  - The status of the remaining numerical targets must be at least 50% of the target

Approach

A team of leading North American national laboratories, universities, and industrial laboratories, each with a high degree of hydrogen storage engineering expertise cultivated through prior DOE, international, and privately sponsored research and development has been assembled to study and analyze the engineering aspects of condensed phase hydrogen storage as applied to automotive applications. The team is composed of Savannah River National Laboratory (SRNL), Pacific Northwest National Laboratory, Los Alamos National Laboratory, the National Renewable Energy Laboratory, NASA Jet Propulsion Laboratory, United Technologies Research Center, General Motors (GM), Ford, Lincoln Composites, Oregon State University, the University of Quebec at Three-Rivers, BASF and HSM Systems LLC. This diverse group will bring creativity and originality to the Center, especially in the early stages, when innovative concepts must be identified to develop hydrogen storage systems capable of meeting the stringent DOE goals. The technical activities of the Center are divided into six technology areas: Performance Analysis, Integrated Powerplant/Storage System Analysis, Materials Operating Requirements, Transport Phenomena, Enabling Technologies and Subscale Prototype construction, Testing and Evaluation. The organizational structure of the Center is depicted in Figure 1.

SRNL will coordinate and integrate all of the technical activities performed by the partners as well as those of the three existing materials centers of excellence. This collaboration will result in enabling DOE to transition seamlessly from materials-intensive discovery and analysis to validated and demonstrated subscale hydrogen storage prototype systems. SRNL will manage the interface between the HSECoE and the existing materials centers of excellence or any subsequent DOE sponsored materials development efforts. This will facilitate dialogue of the technical needs and ultimately result in enhanced productivity for all of the centers. Conduits will be established between other working groups that support DOE's hydrogen programs, including Manufacturing R&D, Office of Vehicle Technologies (OVT), Safety Codes and Standards, and the Hydride Reactivity groups.

Accomplishments

As the Center lead, the following accomplishments were achieved:

- Negotiated final Center work scope and Go/No-Go decisions with DOE.

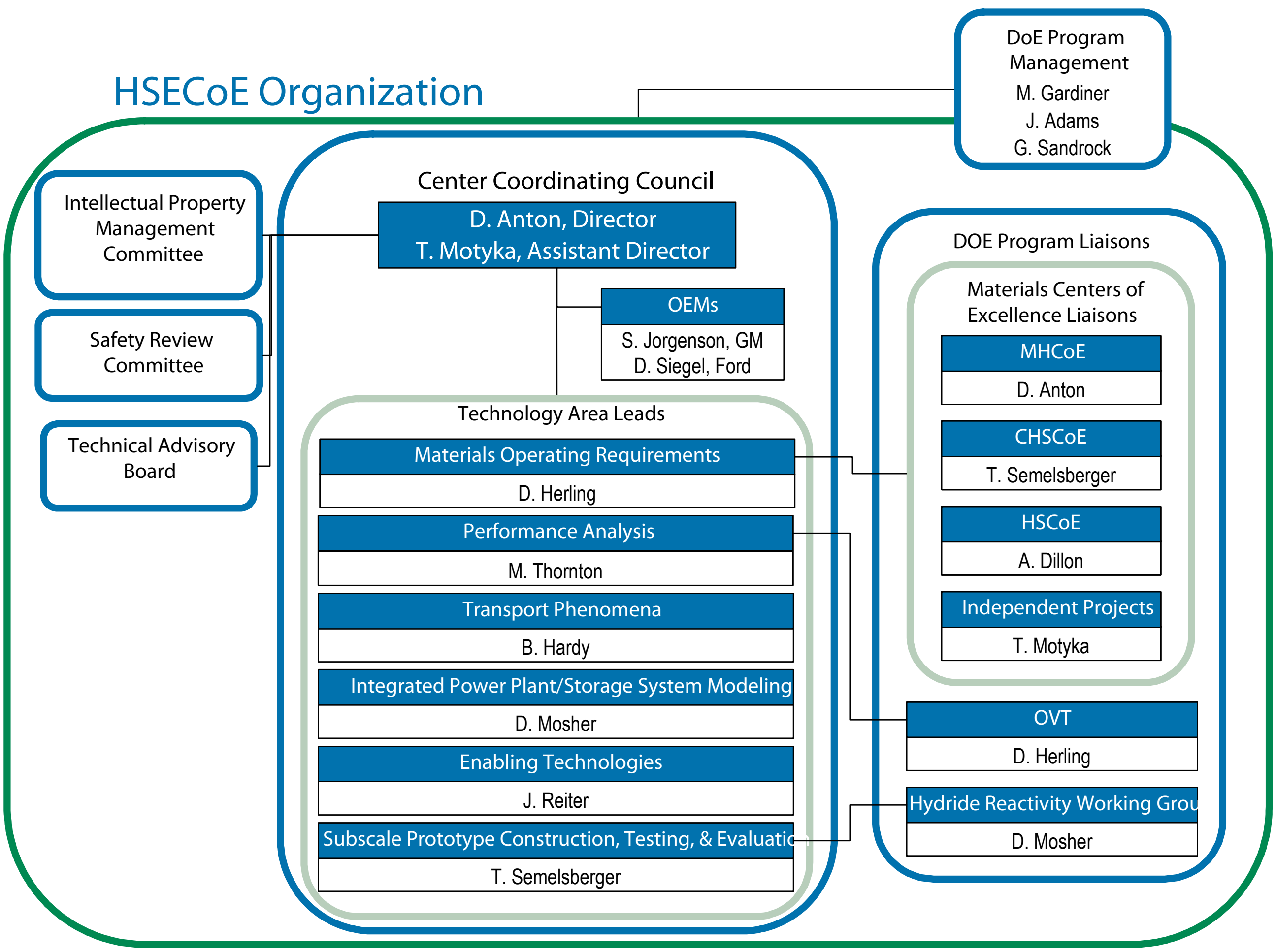

FIGURE 1. Organizational Structure of the Hydrogen Storage Engineering Center of Excellence

- Refinement of partners' roles and responsibilities.
- Established monthly technology area telecons to manage operation of the Center.
- Organized and led the kick-off meeting held in Washington D.C.
- Made two FreedomCAR Hydrogen Storage Tech Team Presentations in Dearborn, MI.
- Organized and led two Center-wide face-to-face meetings in Golden, CO and Arlington, VA.
- Completed and submitted a Safety Plan for the Center.
- Signed intellectual property agreement by all partners for the Center.
- Established public Web site for the center at www.HSECOE.org for the dissemination of data and technical challenges.

A summary of technical accomplishments the individual Technology Areas follows:

Performance Analysis

- Created a vehicle model framework to aid in the development and understanding of hydrogen storage system requirements for light-duty vehicles.
- Assess the base model accuracy by validating model outputs against compressed hydrogen fuel cell vehicles currently in operation.

Integrated Power Plant Storage System Analysis

- Refined structure of integrated system modeling. Developed simplified model of an on-board reversible storage system for inclusion in vehicle level modeling.
- Developed detailed modeling methods. Applied these tools to examine potential improvements in heat exchanger effectiveness.
- Constructed modeling framework for preliminary analysis of membrane separation methods. Compiled materials and impurities of interest.
- Developed compaction design concept which offers greater flexibility in optimization for heat transfer, simple/low-cost manufacturing and good potential for effective mass transport and durability.

Transport Phenomena

- Compiled and distributed a list of data requirements for storage media to the materials operating requirements technology area.
- Metal Hydride System:
  - Developed general model for $NaAlH_4$ metal hydride-based storage systems and validated model against heat transfer and kinetics data.
  - Conducted preliminary optimization studies with metal hydride model.
- Hydrogen Adsorbent System:
  - Began incorporation of adsorbent thermodynamic models into a multidimensional model.

Materials Requirements

- Obtained materials recommendations from the materials Centers of Excellence for consideration in prototype modeling.
- Identified $NaAlH_4$, AX-21 and $NH_3BH_{3(s)}$ as prototype materials to be used for initial model development and verification and obtained sufficient data for the two former materials.
- Identified $NH_3BH_{3(l)}$, AlH_3, $LiAlH_4$, as candidate off-board rechargeable materials, $2LiNH_2/MgH_2$ and $LiNH_2/MgH_2$ as candidate on-board rechargeable materials and metal-organic framework (MOF)-5 as a candidate adsorbent material and compiling data necessary parametric analysis.

Future Directions

Performance Analysis

- Link models/data to the Greenhouse gases, Regulated Emissions and Energy use in Transportation model.
- Obtain preliminary vehicle requirements results for base scenario.
- Evaluate prime storage system concepts and technologies for their strengths and weaknesses related to forecourt requirements.

Integrated Power Plant Storage System Analysis

- Refine simplified storage system models to include integration with power plant and vehicle level models.
- Construct fuel cell model for baseline level integrated power plant modeling.
- Construct baseline level storage system models and specify requirements.

Transport Phenomena

- Determine envelope of acceptability for metal hydrides and adsorbents utilizing backward calculation from system requirements.
- Develop initial adsorbent system design concepts.
- Develop advanced metal hydride design concepts.
- Develop initial chemical hydride reactor concepts.

Materials Requirements

- Obtain kinetic and materials data from the materials centers of excellence.
- Identify parametric equations specific to each storage material type.
- Perform statistical fits to materials data and pass parametric equations to the Transport Phenomena Technology Area.
- Assess the effects of bed structuring on kinetics.

Enabling Technologies

- Develop response surfaces to American Society of Mechanical Engineers pressure vessel code requirements.
- Assess the viability of membrane purification as well as alternate methods including adsorbents and scrubbers.