SAND2007-7547P

Sandia National Laboratories California

Hydrogen Storage Engineering at Sandia National Labs

Hydrogen storage engineering has been a major focus at the Sandia California laboratory for nearly 50 years. Our original mission focused on providing engineering design for hydrogen transfer and storage systems in non-nuclear components of the nation's nuclear weapons stockpile. The focus of this effort has expanded over time to encompass the ever-changing issues of energy and national security.

Sandia National Laboratories are managed for the DOE National Nuclear Security Administration by Lockheed Martin. Sandia conducts R&D work to meet national needs in four mission areas:

- Energy, Resources & Nonproliferation
- Homeland Security & Defense
- Defense Systems & Assessments, and
- Nuclear Weapons

Sandia actively maintains capabilities that are integral to the design, optimization and validation of hydrogen storage systems. A few of these capabilities are described below.

Engineering and material properties characterization

The engineering and material properties of candidate materials directly influence the efficiency, performance, safety, and cost of the entire hydrogen storage system. Therefore, these properties must be characterized prior to the realization of efficient storage solutions based on newly discovered materials. Capabilities at the California lab include:

- **Thermal properties characterization** test cells (Figure 1) which were designed and built to accommodate the complex decomposition and recombination reactions of hydrogen storage materials. The fully calibrated test cells are capable of measuring thermal conductivities ranging from 0.001 W/m-K to greater than 20 W/m-K as a function of sorption cycle, material phase, gas pressure, and system temperature. These test cells were recently utilized to measure the thermal properties of sodium alanates[i].
- Fully calibrated **mechanical properties** test cells (Figure 1) measure the pressure exerted on a vessel wall by volumetric expansion during phase change.
- Using measured **thermodynamic and chemical kinetic** data, we formulate physically-based kinetics models for the absorption and/or desorption of hydrogen storage materials. These models rigorously enforce thermodynamic constraints based on the measured equilibrium (plateau) pressures of the storage material.

An online storage materials properties database is maintained at Sandia that is regularly updated as new results are published. (http://hydpark.ca.sandia.gov/)

Figure 1 - Thermal properties test cell (left) and mechanical properties test cell (right).

Component modeling and simulation

We use modeling and simulation to (a) rapidly explore engineering concepts, (b) design experiments to quantify the role of complex physical behavior, and (c) design scale-up prototypes to validate numerical experiments. This allows for a timely and economical hydrogen systems development process and provides unique insight into the behavior of complex systems leading to novel engineering solutions.

Sandia has a modeling and simulation capability that is world-class due to a combination of three components: *people*, *software*, and *hardware*. In terms of *people*, we have technical staff with extensive experience in modeling and simulating a wide range of physical phenomena and experimentally validating those models. Our analysis capabilities include heat and mass transfer, mechanical design and stress analysis, computational fluid dynamics, chemically reacting and multi-phase flows, and molecular dynamics simulations. In terms of s*oftware*, our validated analysis tools include in-house and commercial codes for modeling steady and unsteady processes in spatial domains ranging from zero-dimensional to three-dimensional. Our in-house tools include multiphysics, massively-parallel codes developed under the DOE Advanced Simulation and Computing (ASC) initiative. We combine our software with world-class computational *hardware* resulting in a capability for high-fidelity simulations using very large models. Our computational hardware includes several massively-parallel Institutional Computing Clusters (ICCs).

Computational finite element models of hydrogen storage systems include measured engineering and material properties to accurately simulate the chemical kinetic, heat transfer, and mass transfer processes. Arrhenius expressions are used to predict the chemical processes as functions of temperature, hydrogen pressure, and chemical composition of the bed. Heat transfer by conduction, convection and radiation as well as contact resistances between the bed and containment vessel are included. These simulations generate results for the state of the bed including detailed hydrogen content and temperature distributions of the entire system (see Figure 2).

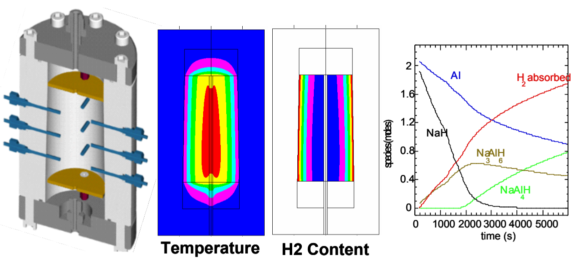

Figure 2 - Simulation of hydrogen absorption into a 200g sodium alanate sample resulting in temperature and hydrogen concentrations as a function of time.

System modeling and simulation

Sandia uses network codes to design, optimize, and define interactions between complex systems of components. These network codes have been utilized in the design of complex metal hydride systems[ii]. The network codes used for this application use fundamental rate expressions at the micro-scale that are combined with a model of the system geometry to give macroscopic relations that describe the absorption/desorption behavior of the bulk materials. The end result is a system model that describes the behavior of the storage material over a wide range of temperatures and pressures within the context of a hydrogen storage system.

Systems involving hydrogen flow networks are accommodated in tools we have developed for modeling flow, mixing, and heat transfer of hydrogen. The computer code TOPAZ is used to model high-speed compressible flows in arbitrary arrangements of vessels, valves, piping, and flow branches. TOPAZ is our primary tool for analyzing flows in hydrogen gas transfer systems (GTS) and has been utilized to design high-rate hydrogen re-fueling manifolds (Figure 3).

Sandia also has expertise in analysis of systems for distributed hydrogen production and stationary power. We developed a library of component models in the Matlab/Simulink software environment (H_2Lib), which provides a flexible tool for simulation of hydrogen systems. The models are based on fundamental physics, and validated against data from demonstration facilities. Components in the library include reformers, electrolyzers, fuel cells, compressors, pumps, turbines, heat exchangers, mixers, and separation devices.

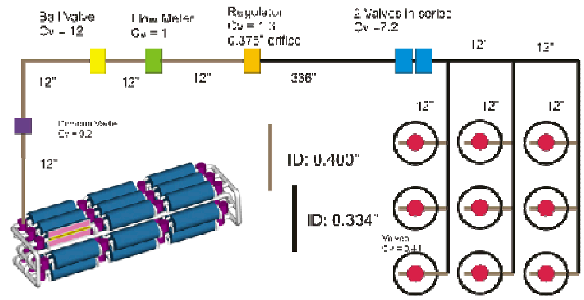

Figure 3 - Hydrogen refueling flow network optimized with TOPAZ.

Hydrogen storage test facilities

Sandia has several facilities that accommodate the storage, handling, and testing of hydrogen storage materials. These facilities utilize remote operation and sensing for operations with high hydrogen pressure or large quantities of hazardous materials. All of Sandia's hydrogen facilities are equipped with flammable gas detection systems that are integrated with our fire suppression systems and the site fire protection system.

For storage and handling of water reactive and/or pyrophoric materials, a number of inert gas glove boxes are available for use. These facilities can be used for preparation of test specimens and assembly of prototype systems (Figure 4).

Figure 4 - Inert glove box utilized for the production and handling of reactive hydrogen storage materials

For component or prototype testing, Sandia maintains a suite of test stations that cover a broad range of hydrogen capacities, hydrogen pressures, and operating temperatures. Sieverts-type stations can accommodate hydrogen pressures up to 15 MPa (2200 psi) and active temperature control up to 350ºC. Small stations can accurately measure the sorption of up to 1 gram of hydrogen. Larger stations (Figure 5) have an increased capacity of up to 100 grams of hydrogen.

Figure 5 - Large Sieverts-type hydride station with prototype solid-state hydrogen storage systems

If higher hydrogen pressure is required, Sandia operates unmanned test cells that can accommodate hydrogen pressures up to 700 MPa (100,000 psi) with remote sensing and control capability. If increased hydrogen capacity is necessary, a refueling manifold exists (Figure 6) that can deliver hydrogen at pressures up to 15 MPa (2200 psi) at precisely measured flow rates exceeding 50 gm/sec. This manifold can also be used to simulate fuel cell demands with continuously variable flow rates up to 2 gm/sec. In addition to hydrogen supply, automotive-scale heat exchange systems are available to accommodate the rapid re-fueling of hydrogen storage systems.

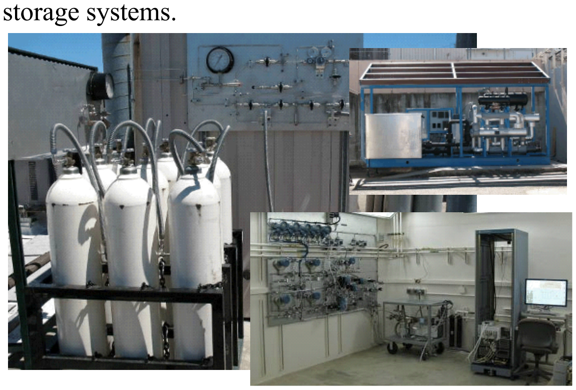

Figure 6 - High capacity, high rate, hydrogen fueling manifold

H_2 materials compatibility

Hydrogen can significantly affect the properties of materials. Sandia has expertise in characterizing and selecting structural materials for hydrogen service. Our expertise includes the following:

- **Effects of hydrogen on properties of materials**
  Sandia has over 40 years of experience in designing stainless steel pressure vessels for storage of gaseous hydrogen isotopes. To support this mission, Sandia maintains capabilities for measuring tensile and fracture-mechanics properties of materials exposed to high-pressure hydrogen gas. Capabilities include two experimental stations designed to measure effects on structural properties, six stations dedicated to measuring hydrogen-assisted crack growth at low and high temperature, and a station that is designed to measure structural properties in a hydrogen environment under dynamic loading.
- **Hydrogen permeation**
  We maintain a series of validated codes to predict hydrogen isotope ingress into materials. To support these codes, we maintain a database of parameters that control hydrogen ingress, including diffusivity, solubility, permeability, trapping concentrations, and trap energies.

Materials characterization

Sandia also has expertise in bulk and surface characterization. An abbreviated list of capabilities includes the following:

- **Electron Microscopy** - Our state-of-the-art facilities include optical metallography (OM), scanning electron microscopy (SEM), electron microprobe analysis (EMPA), and high-resolution transmission electron microscopy (HRTEM).
- **Auger Spectroscopy** - Our scanning Auger electron spectrometer can perform elemental surface and depth analyses of all elements different from hydrogen and helium.
- **X-ray Microscopy** - Capabilities are established that perform phase identification and crystal structure determination using Rietveld refinement with in-situ low pressure hydrogen sorption with high and low temperature control.

Hydrogen storage systems safety

Safety efforts at Sandia include both research and development projects and system hazard assessments.

Sandia is funded through the US DOE Hydrogen Storage program to quantify the reaction processes between hydrogen storage materials, such as metal hydrides, and contaminants, such as water.

Sandia's expertise in hazard assessment methodologies meets DOE policies for integrated safety management. All operations at Sandia undergo a rigorous hazards screening process which determines the need for a Hazard Analysis (HA). If an HA is required, site safety engineers in coordination with Sandia's Safety Basis personnel will perform the appropriate analysis. HA methods include "What If" techniques, hazard operability studies (HAZOPS), and failure mode effects and criticality analyses (FMECA). The result of this process is an overall hazard assessment and the development of controls to prevent or mitigate identified hazards.

Systems Design, Optimization, and Demonstration Examples

Our engineering approach for hydrogen storage involves (a) experimental characterization of engineering and material properties, (b) transport modeling for component design, (c) system simulation for optimization and integration, (d) automated controls with safety interlocks to perform experiments, and (e) a secure collaborative environment for data exchange and communication between remote locations (see Figure 7). Some examples of this approach are described below.

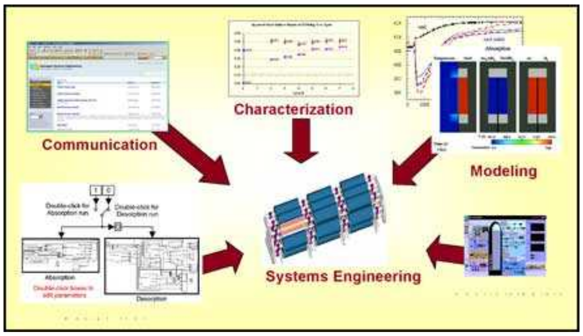

Figure 7 -Science-based systems engineering approach

General Motors H_2 storage project

We are working in partnership with General Motors on a multi-year program to develop and demonstrate an automotive scale hydrogen storage system using the complex metal hydrides. The goal of this effort is to develop a prototype solid-state hydrogen storage tank as well as a suite of engineering tools to enable design of follow-on systems based on new hydrogen storage materials.

We are currently fabricating a vehicle-scale hydrogen storage system which is the culmination of several years of research and development efforts. These efforts have included the following:

- characterization of thermal and mechanical properties of sodium alanates
- development of a unique chemical kinetics model of sodium alanates
- development of finite-element models with coupled chemical kinetics, heat transfer, and mass transfer for component design
- design, fabrication, and testing of prototypes
- development of system level simulation tools for component integration and system design
- assembly of large-scale hydride production lab
- final design optimization
- fabrication of a refueling and delivery facility
- demonstration of optimized storage system

Hydrogen fueled locomotive

Sandia National Laboratories and the Fuel Cell Propulsion Institute developed a hydrogen-powered mining locomotive. The project required Sandia to design, optimize and integrate a locomotive power plant including heating/cooling/air supply systems, a hydrogen storage unit using metal hydrides, and a control system to monitor and control overall operations through a touch-screen panel[iii]. For the final technology demonstration, the power plant was integrated onto a commercial underground mining locomotive (Figure 8).

Figure 8 - View of the fuel cell stack and hydrogen storage bed, integrated into an existing locomotive platform

In September 2002, the vehicle became the first hydrogen fuel-cell-powered locomotive to be operated underground, successfully pulling five loaded cars weighing 20 tons at Val d'Or, a former metal mine in Quebec. Earlier that year, the mining industry gave the locomotive a "best of show" award at the Canada Mining Expo.

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[i] Dedrick, D. E., M. P. Kanouff, et al. (2005). "Thermal properties characterization of sodium alanates." Journal of Alloys and Compounds **389**: 299-305.

[ii] Johnson, T., D. Dedrick, et al. (2007). Effects of Metal Hydride Properties on the Performance of Hydrogen Storage Systems. Materials Science & Technology 2007, Detroit, MI, USA

[iii] Chan, J. P., W. C. Replogle, et al. (2003). Hydrogen Powered Locomotive. NHA Annual Hydrogen Meeting. Washington DC.