

Thermal/Fluid Science and Engineering Department Physical and Engineering Sciences Center

Solving Complex Transport Problems

Sandia's Thermal/Fluid Science and Engineering Department is a multidisciplinary team specializing in the engineering science of heat and mass transfer. We provide systems engineering and computational analysis to develop prototype systems from conceptual design through testing.

Our theoretical expertise encompasses:

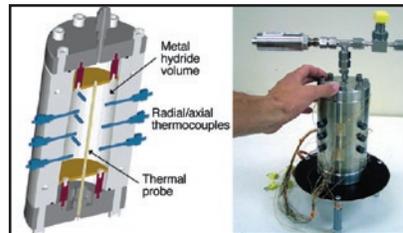
- Conduction, convection, and radiation heat transfer
- Fluid mechanics for turbulent and multiphase flows
- Multicomponent transport, chemistry, and kinetics
- Computing technology for multiphysics simulations

Our ability to solve complex, multiphysics engineering problems brings us a wide variety of work involving heat transfer and fluid flow. A sampling of our current projects, summarized below, illustrates the breadth of our capabilities.

Thermal Engineering for Hydrogen Storage

To advance the use of hydrogen in the transportation sector, we have teamed with General Motors to develop an automotive-scale hydrogen storage system based on a complex metal hydride (solid state) storage medium. Engineering property experiments form the basis for our computational models, which include detailed finite-element reaction/diffusion calculations for the hydride bed design, computational fluid dynamics calculations for the heat exchanger design, and dynamic system simulations for predicting combined storage bed and fuel cell performance. Full-scale systems are tested in a test cell designed for high-pressure hydrogen operations.

Our unique glove box and milling operation can produce 1 kg of metal hydride per day and load it into a pressure vessel in an inert environment.



The thermal properties of a solid-state metal hydride bed are quantified for use in engineering analyses.

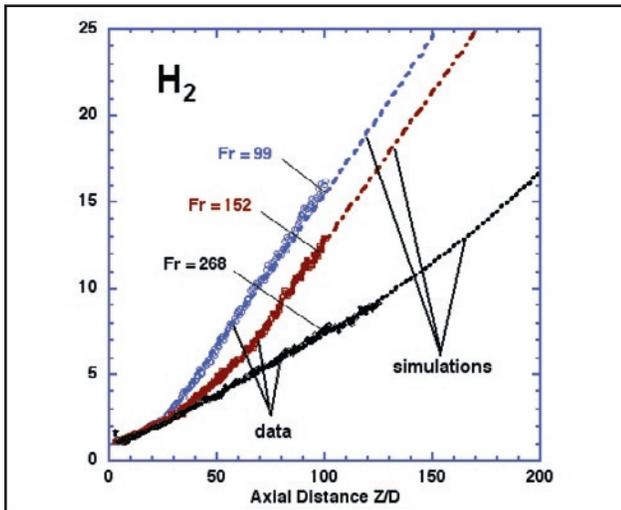
Hydrogen Safety

As hydrogen assumes a greater role in the nation's energy infrastructure, it becomes imperative to ensure its safe handling and storage. We are developing engineering models of hydrogen behavior in hypothetical leak scenarios. For unignited hydrogen releases, the models predict mean concentration and vapor cloud extent; for ignited releases, they predict



Technologists measure the thermal and kinetic performance of hydrogen storage system prototypes with a Sieverts apparatus. These experimental results are used to validate computational models of a vehicular fuel system.

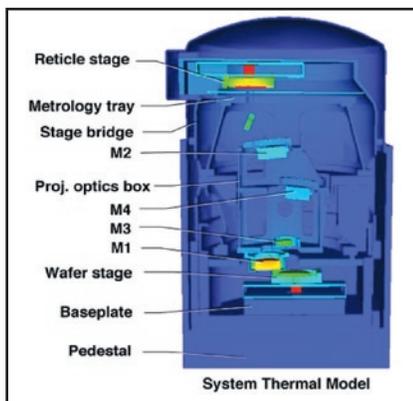
flame characteristics and thermal radiation effects. Validated by experiments in Sandia's Combustion Research Facility, these consequence models are used in conjunction with quantitative risk assessments to inform the codes and standards development process.



Our hydrogen leak analyses, validated by experiments, show how the hydrogen concentration decay rate in a buoyant plume increases as buoyancy becomes stronger relative to the mean flow (i.e., the Froude number decreases).

Thermomechanical Engineering for Lithography

We are conducting a thermomechanical engineering analysis for an optical maskless lithography (OML) tool. OML does not require a fixed mask set; rather, patterns are adjusted on the fly via microscopic mirrors called digital light processors, which have thermal and mechanical effects on the instrument. We are predicting these impacts using a computational approach similar to our previous characterization of an extreme ultraviolet lithography (EUVL) prototype. For EUVL, we built large finite-element models to simulate the illumination and projection systems. Heat conduction and thermal radiation analyses provided transient temperature distributions, while structural analysis enabled prediction of thermal strain displacements and optical analysis translated displacement to optical errors. EUVL used reflective optics; the next-generation OML system employs projective optics.



Colors indicate temperature distributions within the projection chamber for a prototype EUVL tool characterized by our group. We are currently working on the next-generation tool: an optical maskless lithography system.

Microfluidic Design

Mixing reagents is one of the most time-consuming operations on microfluidic platforms. With partners at Cornell and the University of Louisville, we have developed a unique microfluidic mixing device based on the principle of induced-charge electroosmosis (ICEO). ICEO creates microvortices within a fluidic channel by application of alternating current (AC) electric fields. The microvortices are driven by electrostatic forces acting on the ionic charge induced by the field near polarizable (metal) materials. By enabling mixing to be turned on or off, this approach prevents sample dilution, a common problem with other sample-mixing strategies. High-performance computation of electric field, fluid flow, and mass transport in multispecies liquids enabled us to rapidly prototype a wide range of device designs and to identify the geometries promising the best performance, such as the octagonal design pictured below.



Micrographs of the "octagon" device after loading it with liquids containing either red or green dye (left) and after applying a rotating electric field to drive the ICEO flow and mix the liquids (right).

Scientific Computing

We develop, verify, and validate massively parallel, multiphysics computational tools to model fluid flow and heat transfer. For example, we are members of the development team for Sandia's Fuego code, which uses an unstructured finite-volume method to solve turbulent, chemically reacting flows, including thermal radiation transport and conjugate heat transfer.

We also specialize in multiscale modeling. The most difficult problems in computational mechanics often involve modeling the interaction of material behavior observed at the macroscale with phenomena occurring at the atomic scale. We are developing multiscale simulation techniques where the continuum behavior of the material is modeled with finite elements, coupled to molecular dynamics simulations that model the atomic-scale phenomena.

Learn more at: <http://public.ca.sandia.gov/8700>

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