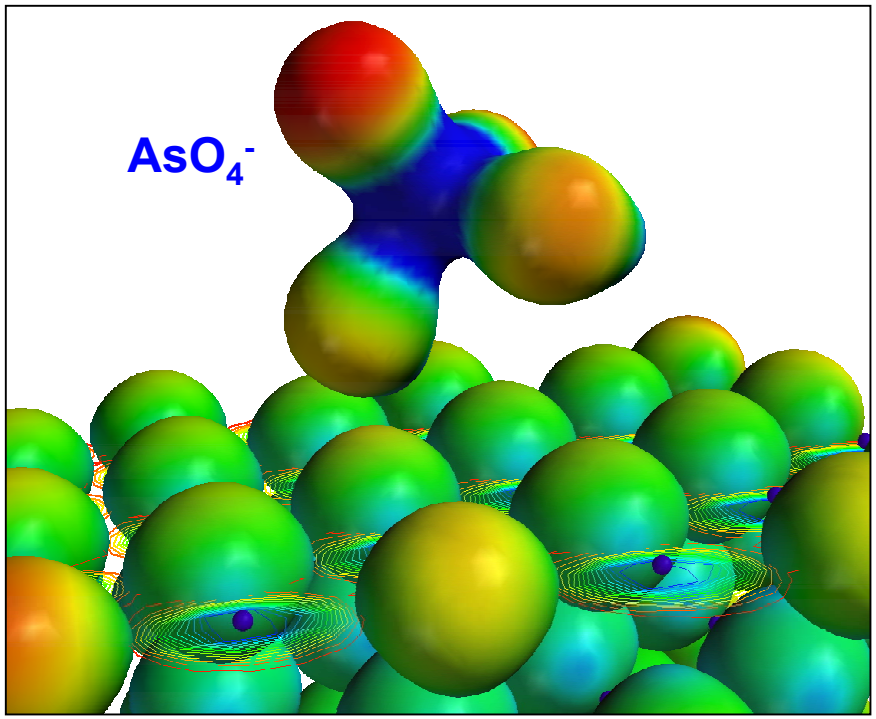
Water Treatment for Arsenic Contamination



QM Simulation of Arsenic Sorption on Oxide Surface

Problem: Arsenic (As) contamination in drinking water.

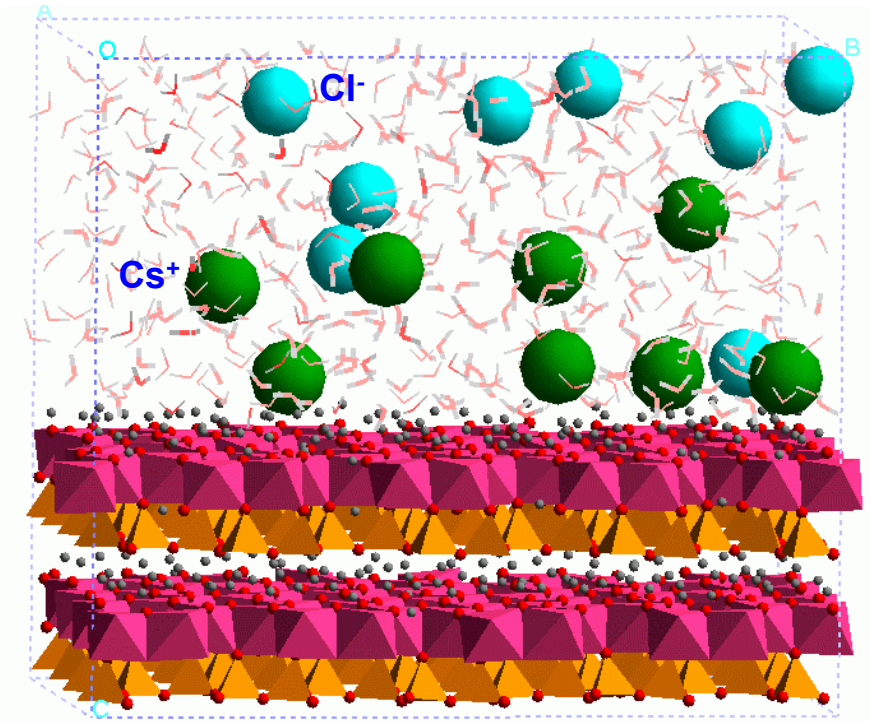
Approach: Use of quantum mechanics (QM) codes and aqueous geochemistry to develop new, efficient As getters.

Impact: Simple, economical, and effective water treatment.

Sponsor: Laboratory Directed Research and Development
Partners: University of New Mexico
CH2M Hill

Sandia National Laboratories

Metal and Radionuclide Sorption on Clays



(001) surface

Molecular Dynamics Simulation of Kaolinite with CsCl Solution

Problem: Radionuclide and metal contamination in soils.

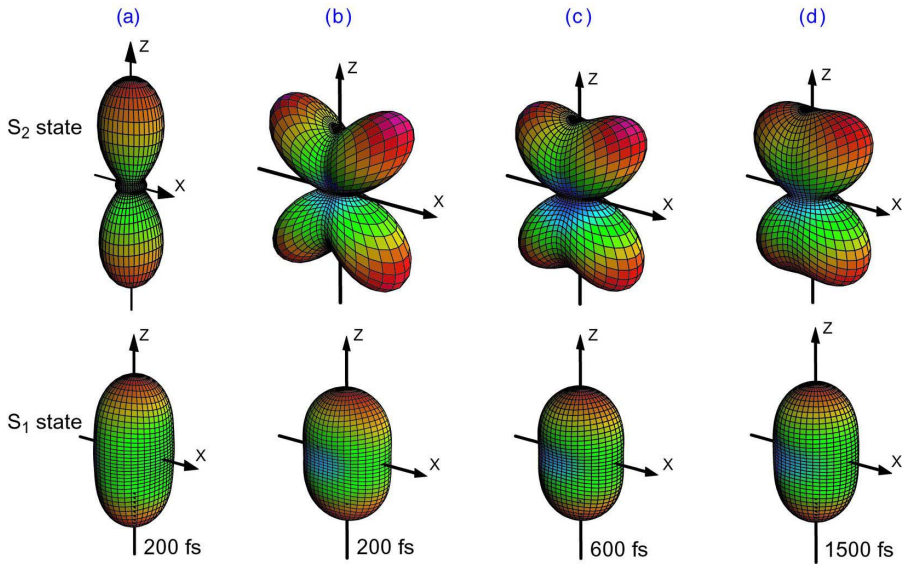
Approach: Use of quantum mechanics and molecular mechanics (QM/MM) codes and synchrotron analyses to predict metals sorption and release from soils.

Impact: Efficient cleanup of contaminated sites.

Sponsors: DOE/Office Basic Energy Sciences
Nuclear Regulatory Commission
Partners: University of California – Davis
University of Illinois – Urbana/Champaign

Sandia National Laboratories

Femtosecond-Resolved Photoelectron Angular Distributions



Photoelectron Angular Distributions of Excited Triethylenediamine

Problem: Improve use of photoelectron angular distributions as probes of dynamics in molecules.

Approach: Ionize molecules with femtosecond pulses so that the photoelectron angular distribution can be measured while the ions are still oriented.

Impact: The features of excited states give clues to how larger molecules are formed.

Sponsor: DOE Office of Basic Energy Sciences
Partner: University of Nottingham

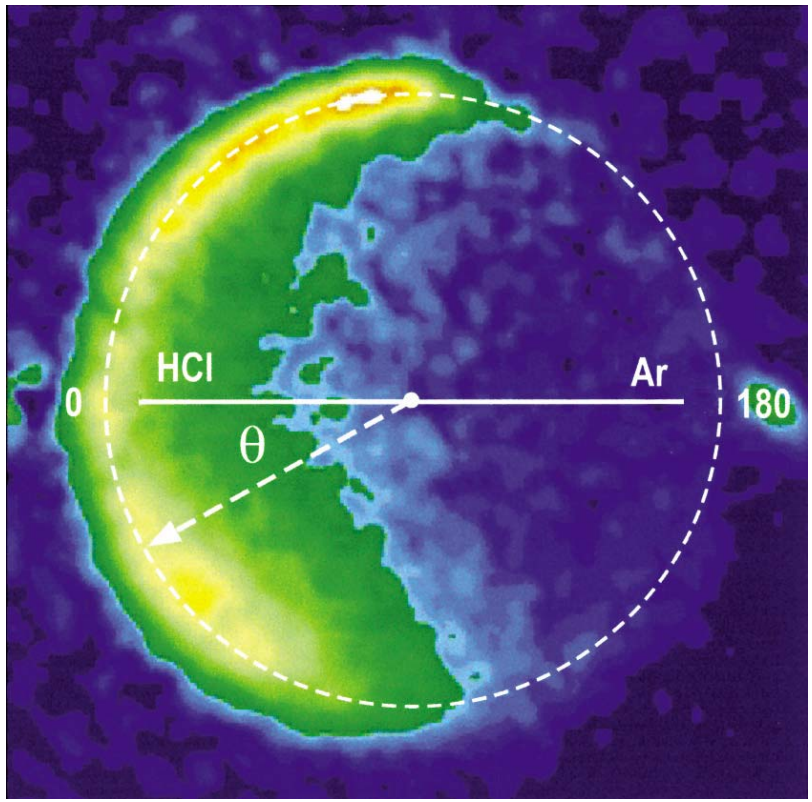
Sandia National Laboratories

Ion Imaging

Problem: Understand rotational energy transfer processes.

Approach: Establish the intermolecular potential energy surface for argon/HCl collisions by colliding HCl with argon and determining the angular distribution of products by ion imaging.

Impact: Rotational energy transfer processes serve as an important pathway for the redistribution of energy in the equilibrium of combustion products.



Ion Image of HCl Scattered Off Argon

Sponsor: DOE Office of Basic Energy Sciences

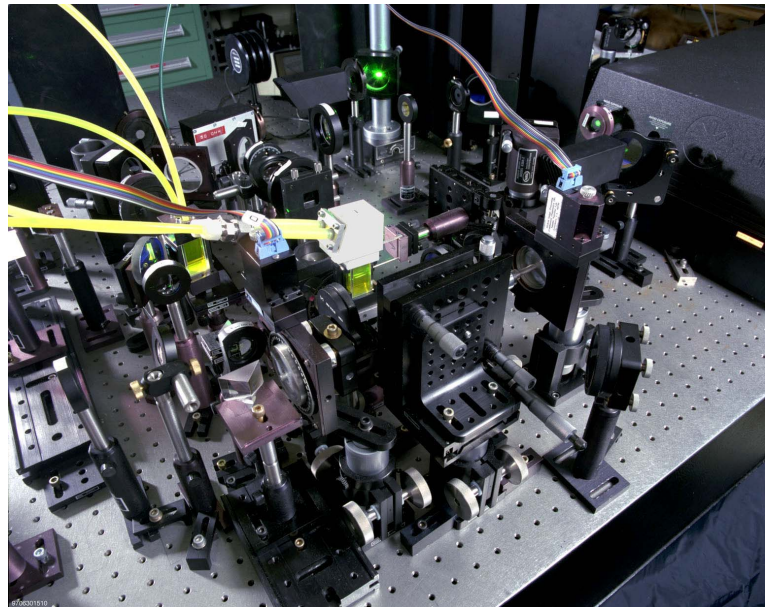
Sandia National Laboratories

Tunable Distributed-Feedback Dye Lasers

Problem: Visible and ultraviolet lasers with subnanosecond time resolution and moderate spectral resolution are needed for determining rotational energy transfer rates.

Approach: Combine a distributed-feedback dye laser with bow-tie amplifiers and a Nd:YAG pump laser, and use the system to determine the populations of electronic states in OH radicals.

Impact: Knowing the rotational energy transfer rate improves the accuracy of laser spectroscopic measurements of combustion systems.

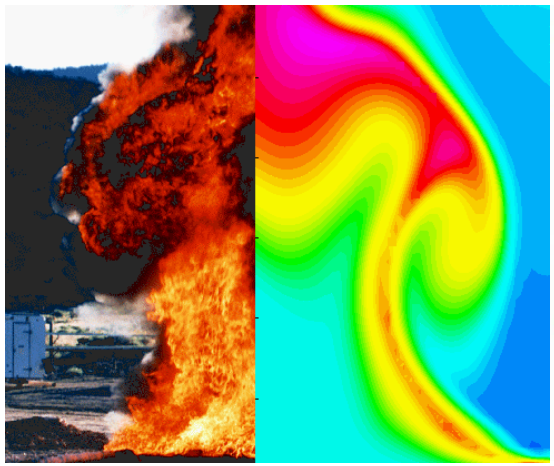


Distributed-Feedback Dye Laser

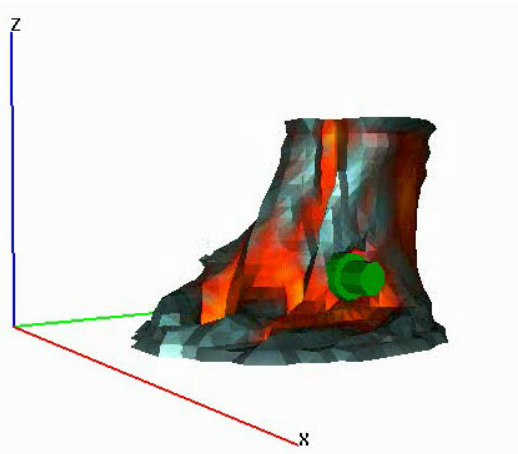
Sponsor: DOE Office of Basic Energy Sciences

Sandia National Laboratories

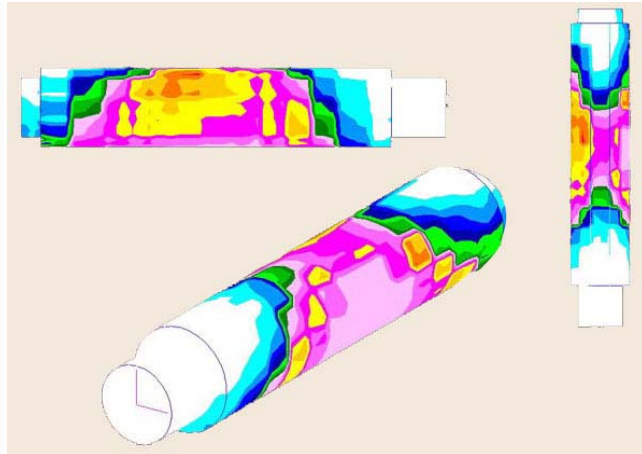
Thermal Analysis of Spent Fuel Cask



Comparison of a CAFE 2D Fire with a Real Fire; Contours Show Fire Puffing*



A CAFE 3D Fire Engulfing a Legal Weight Truck Transportation Cask



Computational Results from the CAFE 3D Fire Environment Coupled with PATRAN/Thermal software

Problem: Ensure integrity of radioactive waste containers during transportation.

Approach: Use finite element codes and measurements in extreme tests to predict and confirm cask response to accidents.

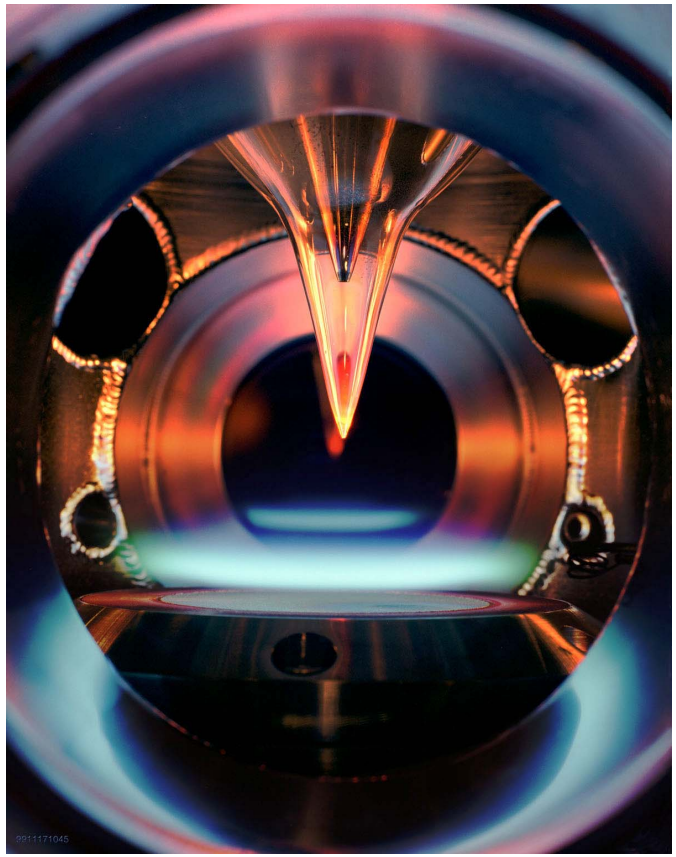
Impact: Demonstrated safety of nuclear spent fuel shipping casks.

Sponsor: DOE/Environmental Management
Partner: University of Nevada – Reno

**Container Analysis Fire Environment (CAFE) computer code*

Sandia National Laboratories

Details of Flame Chemistry



Quartz Flame Probe

Problem: Determine if the detailed kinetic model of dimethyl ether combustion agrees with experiment.

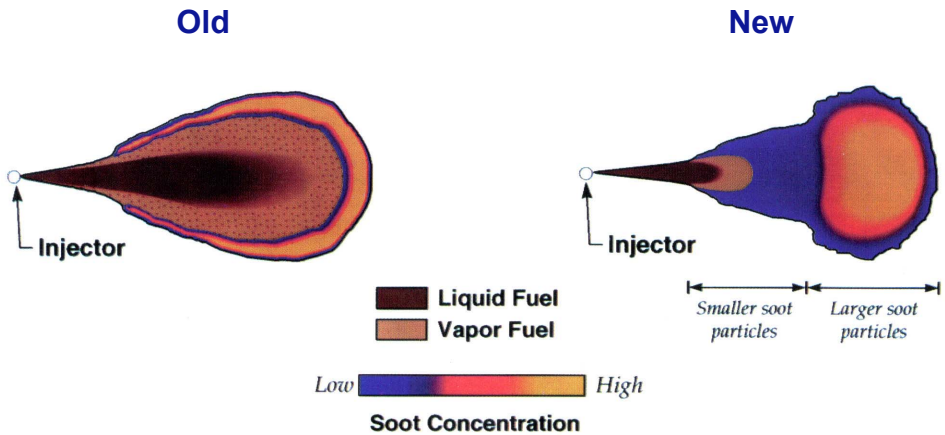
Approach: Measure concentrations of chemical species in a dimethyl ether /oxygen/argon flame in a molecular beam sampling instrument.

Impact: Dimethyl ether addition to diesel fuel can improve ignition and reduce emissions in diesel engines.

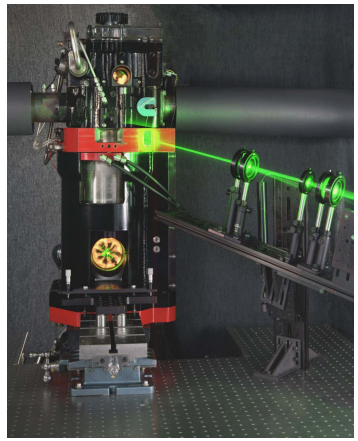
Sponsor: DOE Office of Basic Energy Sciences

Sandia National Laboratories

Soot Formation in a Heavy-Duty Diesel Engine



Old and New Ideas of Soot Formation



Heavy-Duty Optical Diesel Engine in Operation

Problem: Build a predictive model of combustion in a heavy-duty diesel engine.

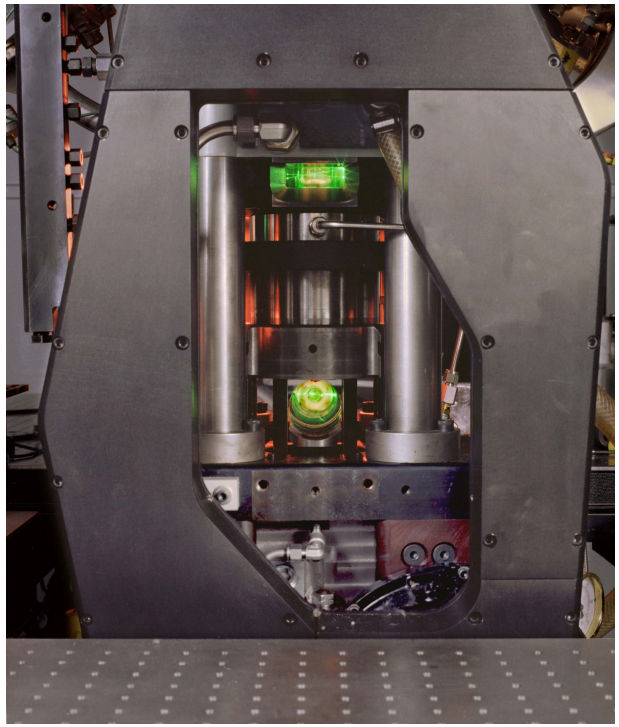
Approach: Use laser diagnostic techniques in an optical research engine to gather the data necessary to decrease the number of assumptions required for the diesel combustion model.

Impact: Completely changes the idea of how soot was formed in a combusting diesel fuel jet.

Sponsor: DOE Office of Transportation Technologies
Partner: Cummins Engine

Sandia National Laboratories

Late-Cycle Soot Measurements in a High-Speed Direct-Injection Diesel Engine



Optical High-Speed Direct-Injection Engine in Operation

Problem: Reduce NO_X and particulates in diesel engines at their source.

Approach: Capture and study images of combustion luminosity to verify models and gain a better fundamental understanding of in-cylinder diesel processes.

Impact: Soot can be oxidized late in the power stroke reducing particulate emissions.

Sponsor: DOE Office of Transportation Technologies
Partners: Wayne State University
University of Wisconsin

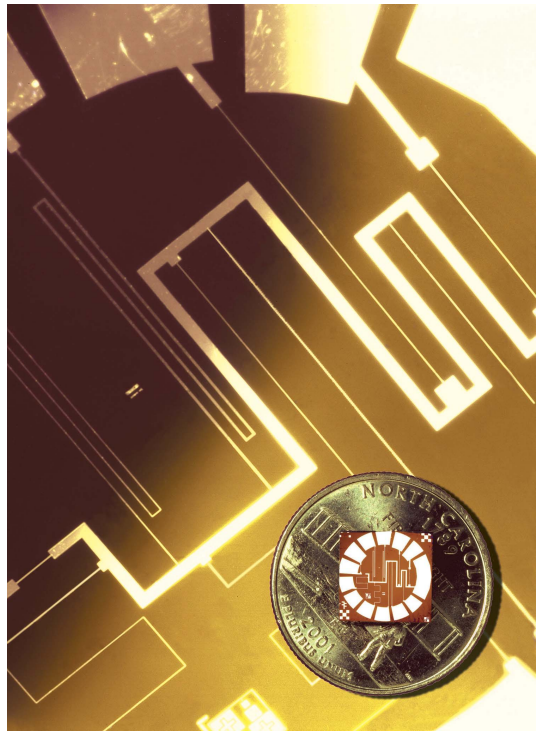
Sandia National Laboratories

Robust Hydrogen Sensors

Problem: Inexpensive, robust hydrogen sensors are needed to reduce the environmental impact of steam-forming.

Approach: Test usefulness of Pd-alloy chemiresistor strips as hydrogen sensors in a variety of configurations on small chips.

Impact: Rapid monitoring of hydrogen concentration in steam-forming process streams enables process strategies to reduce energy consumption.

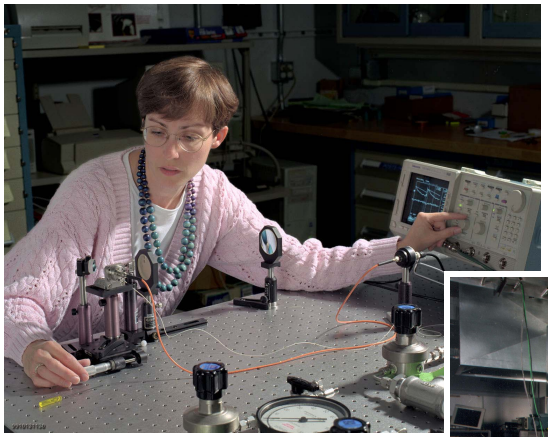


Magnified Photograph of Chemiresistor Chip

Sponsor: DOE Office of Industrial Technologies
Partners: Pennsylvania State University
Air Products and Chemicals
DCH Technology

Sandia National Laboratories

Steel Industry Sensors



Bench-Top Experiments

Calibrating Sensor Beam for Field Trial

Problem: Develop sensors that the steel industry can use for real-time process control in high-temperature particle-laden streams.

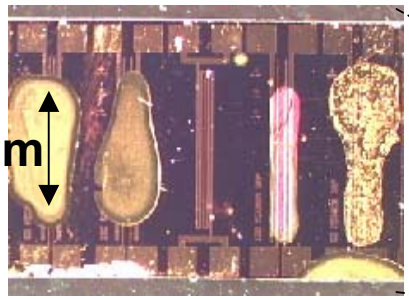
Approach: Create laser-based sensors to measure CO, CO_2, and H_2O concentrations and average line-of-sight temperatures in furnace off-gas.

Impact: Better process control can improve energy efficiency and emissions control.

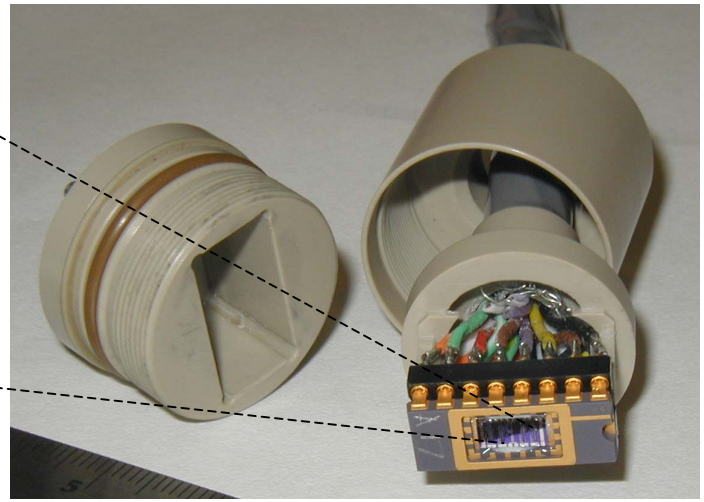
Sponsors: DOE Office of Industrial Technologies
American Iron and Steel Institute
Partners: Bethlehem Steel
Weirton Steel
Timken Company

Sandia National Laboratories

Subsurface Contaminant Sensors



Chemiresistor μsensor Arrays



Waterproof Sensor Package

Problem: Remote measurement of subsurface contaminants.

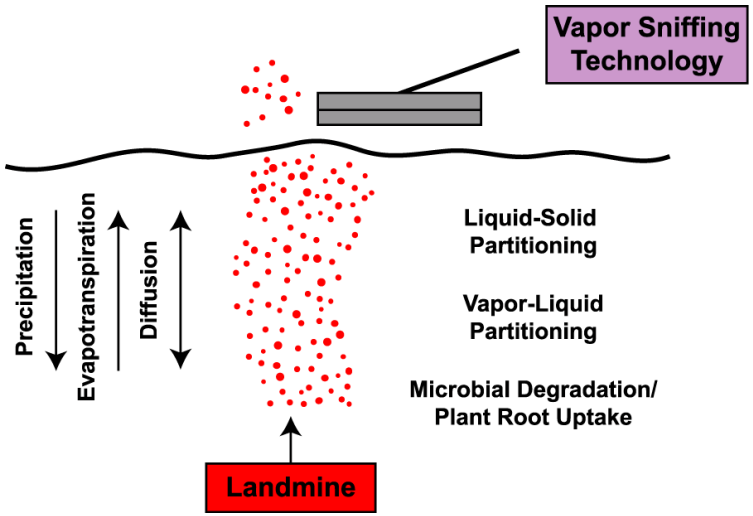
Approach: Development and testing of microsensor arrays to characterize volatile organic compounds (VOCs) in soils.

Impact: New, *in situ* sensors and packaging for subsurface applications.

Sponsor: Laboratory Directed Research and Development
Partner: University of New Mexico
Brigham Young University
NTS (Bechtel Nevada)
Edwards Air Force Base

Sandia National Laboratories

Detection of Unexploded Ordnance in Soils



Rapid Detection of Ultra Trace Explosive Residues

Problem: Detection of buried landmines.

Approach: Development of performance requirements for ultra-trace vapor detection of explosive residues in soils.

Impact: Optimization of sensor design and field application to detect buried landmines.

Sponsors: US Army and Defense Advanced Research Projects Agency
Partners: New Mexico Tech
California Institute of Technology
Massachusetts Institute of Technology
Nomadics, Inc.

Sandia National Laboratories

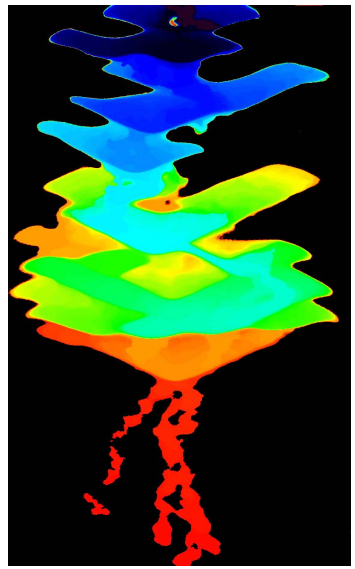
Multiphase Flow Modeling in Porous Media

Problem: Migration and remediation of subsurface dense non-aqueous phase liquid (DNAPL) plumes.

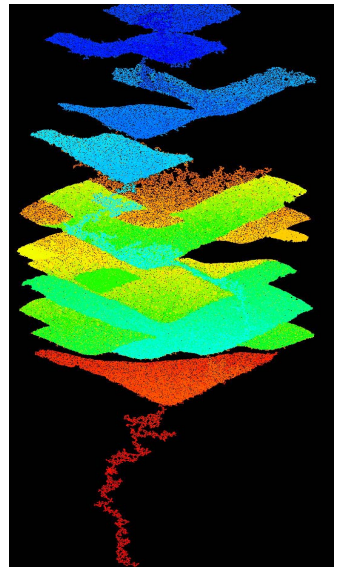
Approach: Combined numerical simulation and experimental verification of multiphase flow in porous media.

Impact: Improved models to predict the DNAPL migration in vadose zone.

Experiment with Heterogeneous Sand



Multiphase Flow Experiment

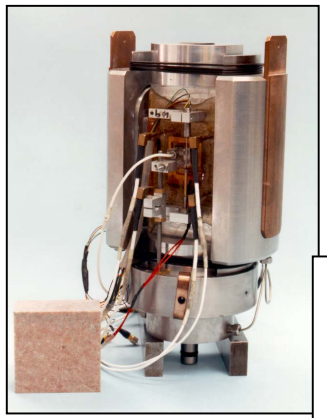


Percolation Theory Simulation

Sponsors: DOE/Office of Basic Energy Sciences
DOE/Environmental Management Sciences Program
Partners: New Mexico Tech
University of Colorado – Boulder
University of Idaho

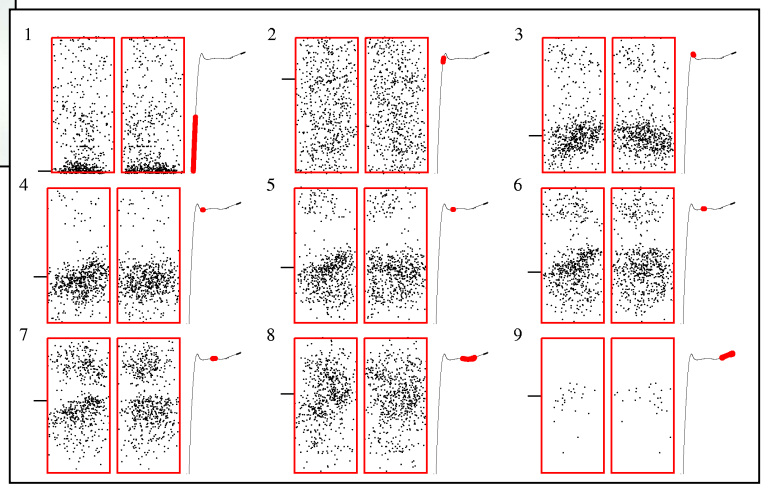
Sandia National Laboratories

Deformation of Porous Media



True Triaxial Assembly to Apply Realistic Stress Fields to Rock Samples

Problem: Origins of inelastic deformation and fracturing of rocks and porous media.



Acoustic Emission Measurements Show the Spread of Compacting Regions During Confined, Axisymmetric Compression Experiments on Castlegate Sandstone

Approach: Combined experimental and theoretical study of deformation structures under triaxial compression.

Impact: Improved prediction of rock deformation and compaction that influence fluid migration.

Sponsor: DOE/Office of Basic Energy Sciences
Partner: Northwestern University

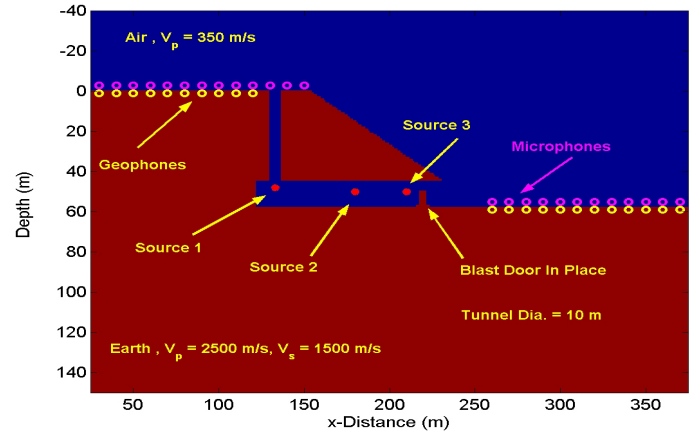
Sandia National Laboratories

Seismic Imaging of Underground Structures

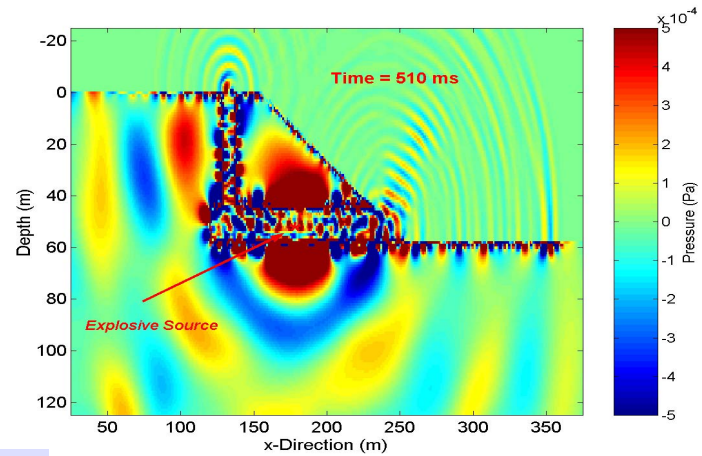
Problem: Accurate characterization of underground structures.

Approach: Use of 3D seismic and acoustic modeling to identify size, shape, depth and function of subsurface structures.

Impact: Improved planning strategies for defeat or battle damage assessment of underground targets.



Cross Section of Tunnel with Vent



Seismic and Acoustic Pressure Waves from Explosive Source

Sponsors: Defense Advanced Research Projects Agency
Defense Threat Reduction Agency
DOE/Office of Basic Energy Sciences

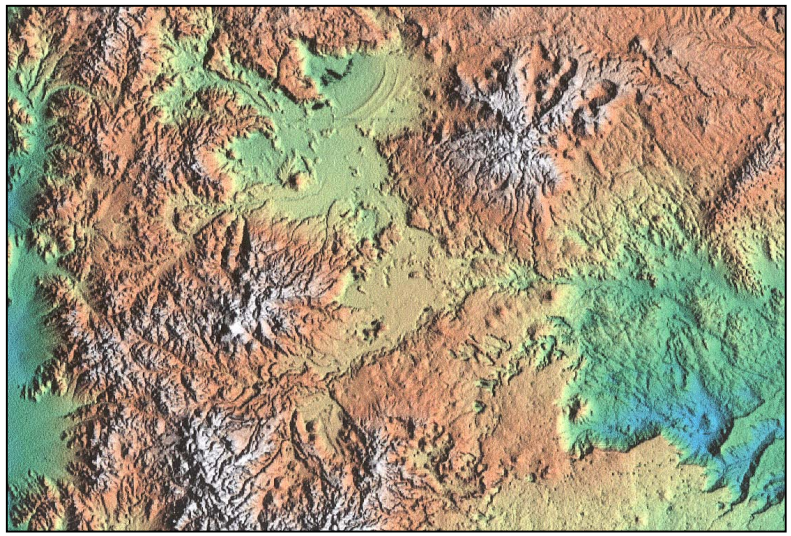
Sandia National Laboratories

Remote Sensing for Geologic Characterization

Problem: Determining rock characteristics and local geology at sites of interest in denied territory.

Approach: Process satellite imagery (spectral, SAR, panchromatic) for comparison with ground-truth field geology and mineralogy.

Impact: Improved characterization of inaccessible sites.



Multispectral Image of Hydrothermally Altered Region Showing Variation in Surface Mineralogy

Sponsor: **Laboratory Directed Research and Development**
Partner: **Springfield Research Facility**

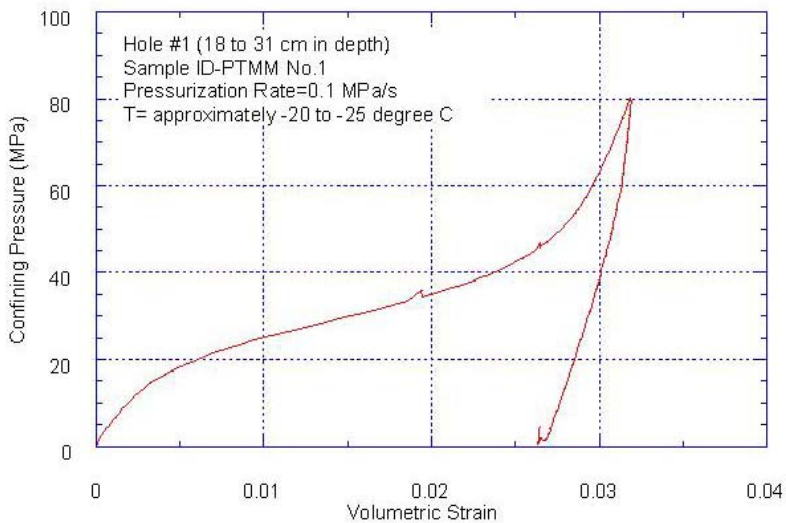
Sandia National Laboratories

Frozen Soils Constitutive Testing and Modeling

Problem: Prediction of projectile penetration into earth materials.

Approach: Experimental measurement of deformation and failure of rock and soils over range of pressure and temperature.

Impact: Improved materials data for inclusion into ASCI rock and soil penetration models.



Alaskan Frozen Soil Test

Recovery of Instrumented Penetrator

Sponsor: DOE/Defense Programs
Laboratory Directed Research and Development

Sandia National Laboratories