EES Division

Research Summaries

ACRONYMS AND ABBREVIATIONS

AIRS	Atmospheric Infra-Red Sounder
ARCS	Atmospheric Radiation and Cloud Stations
ARM	Atmospheric Radiation Measurement
CART	cloud and radiation testbed
CGRP	Cerro Grande Rehabilitation Project
C-INC	Isotope and Nuclear Chemistry Group
CRP	Containment Review Panel
CSSA	Camp Stanley Storage Activity
CST-11	Nuclear and Radiochemistry Group
DOE	Department of Energy
EBS	Engineered Barrier System
EES-2	Atmospheric, Climate, and Environmental Dynamics Group
EES-6	Hydrology, Geochemistry, and Geology Group
EES-7	Geotechnical Engineering Research Group
EES-9	Environmental Geology and Risk Analysis Group
EES-11	Geophysics Group
EES-12	Carlsbad Operations Group
EPA	Environmental Protection Agency (US)
ER	environmental restoration
ESF	Exploratory Studies Facility
ESH	Environment, Safety, and Health Division
ESRI	Environmental Systems Research Institute
FIRETEC	full-physics wildfire behavior simulation
FTE	flux-transfer events
FWO-WFM	Facility & Waste Operations, Waste Facility Management Group
GIS	Geographic Information System
GISLab	Geographic Information System Laboratory
HE	high explosives
HIPPO	high-pressure preferred orientation
HRS-4	Health Physics Measurements Group
IGPP	Institute of Geophysics and Planetary Physics
InSAR	interferometric synthetic aperture radar
LANSCE	Los Alamos Neutron Science Center
LANSCE-12	Manuel Lujan Jr. Neutron Scattering Center
LIDAR	Light Detection and Ranging
MCL	maximum concentration level
MDA G	Material Disposal Area G
MKAR	Makanchi array
MOS	Monin-Obukhov Similarity
MST-8	Materials Science and Technology Division, Structure/Property Relations Group
MTI	multispectral thermal imaging
NA	Office of Nonproliferation Policy (DOE)
NASA	National Aeronautic and Space Administration
NIS-2	Nonproliferation and International Security, Space and Remote Sensing Sciences Group
NTPO	National Petroleum Technology Office
NTS	Nevada Test Site
PA	Performance Assessment
PIMS	phosphate-induced metal stabilization
POP	Parallel Ocean Program
PRB	permeable reactive barrier
RRES-WQH	Risk Reduction & Environmental Stewardship, Water Quality & Hydrology Group
SAR	synthetic aperture radar
SDE	Software Development Environment
SNM	special nuclear materials
SODAR	Sound, Distance, and Ranging
SST	sea-surface temperature
T-3	Computational Fluid Dynamics Group (Theoretical Division)
TA-11	Technical Area 11, Martin Canyon
TA-16	Technical Area 16, Cañon de Valle and Martin Canyon
TA-60	Technical Area 60, Sandia Canyon
TCLP	toxicity characteristic leaching procedure
TCO	Test Coordination Office
THC	thermohaline circulation
TSM	test site monitoring
TSPA	Total System Performance Assessment
TWP	tropical western Pacific
USGS	US Geological Survey
UV-Vis	ultraviolet-visible (absorption spectrum)
WIPP	Waste Isolation Pilot Plant
X-4	Primary Design and Assessment Group, Applied Physics
XAFS	x-ray absorption fine structure
XANES	x-ray absorption near-edge structure
XAS	x-ray absorption spectroscopy
X-DO	Applied Physics Division Office

Advanced Measurement Capabilities and Their Applications to Ecosystem Monitoring

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Advanced measurement systems are currently being developed and applied to various ecosystem, atmospheric, and soil systems. The measurements will provide significant insights into the complex interactions between these systems and will enable improved management of natural resources through a more thorough understanding of fundamental processes.

Application of advanced measurement systems promises to unravel some of the intricate and complex relationships that control the interactions between ecosystems, the soils that support the ecosystems, and the atmosphere. Understanding these diverse relationships provides Los Alamos with the tools needed to address national problems in energy, environment, and national security.

Recent developments in carbon measurement (Cremers et al., 2001; Ebinger et al., in press) and ecosystem monitoring (Breshears and Allen, 2002) continue to provide fundamental understanding of interactions between the carbon cycle and terrestrial systems. In addition, new work in water-vapor-flux mapping significantly improves our understanding of atmospheric processes (Cooper et al., in press).

Fig. 1. Mobile scanning raman LIDAR unit in the field.

We have used the unique mobile-scanning Raman light detection and ranging (LIDAR) system for the past two decades to map 3-D water-vapor fields in the atmosphere. We extended these measurements to map water-vapor flux with a spatial resolution of 50 m. This capability allows EES scientists to probe and characterize the surface-atmosphere interface over any location, day or night. In addition, mobile-scanning LIDAR gives an unprecedented insight into the transfer of mass and energy in varied environments, for resolving questions related to nonproliferation, environmental stewardship, and homeland security.

Because mass and energy exchange is an inherently spatial process, an ability to map the scalar and flux of water vapor addresses many assumptions made when researchers rely on point sensors alone. It is now possible to verify atmospheric dispersion models with direct intercomparisons using LIDAR-generated data. The following two examples illustrate these capabilities: We can evaluate how different tree species use surface water in riparian zones of the Southwest, and we are beginning to understand how mass is exchanged between the Earth's surface and the atmosphere in urban nocturnal boundary layers.

We also have made recent major advances in addressing source areas for water vapor and have developed a major assumption about turbulent mixing length, two areas in which our previous lack of knowledge had limited our applications of LIDAR. In collaboration with university researchers, EES has addressed the first unknown, the source area, by developing a method to characterize source areas for water vapor and flux mapped by LIDAR (Cooper et al., 2003). Previously, all other source-term analysis was done with models not yet verified; now, we can use LIDAR to estimate directly those contributions of the source area. The second unknown was addressed by directly measuring turbulent mixing length for the first time. These two advances make flux mapping possible with LIDAR-based sensors completely independent of point-sensor technology. ■

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Finding the Roles of Ocean Physical and Biogeochemical Processes in Global Climate Variation

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A dream of human society and one of the goals of the scientific community is developing the capability to make reasonably accurate forecasts of weather and short- and long-term climate. Accurate forecasting benefits public preparedness for hazards and disasters caused by severe weather. Applied to long-term planning, forecasts help us set appropriate policies for energy exploration and consumption, transportation systems, environmental pollution prevention, and agricultural activities. From the perspective of national defense, this capability benefits military planning and exercise. However, this capability can exist only if we have a reasonably reliable and complete hierarchy of climate observation, analysis, and forecast systems.

To maintain quality in forecasting over a broad spectrum in space and in time, systems must include and represent, in reasonable detail and with accuracy, the atmosphere, the oceans, the land, the ecosystems, and all physical, chemical, and biological processes. At the present time, the

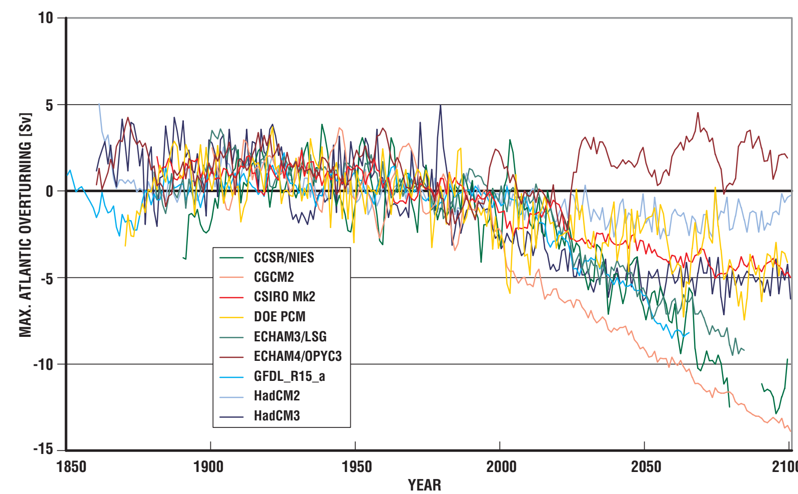

Fig. 1. Simulated water transport of the Atlantic "conveyor belt" computed by different climate models. Shown is the annual mean relative to the mean of years 1961–1990. Units are106 m^3/s. The future-forcing scenario is IS92a (gradual doubling of CO_2 at the rate of 1% per year). The ECHAM4-OPYC model combination showing no decline in conveyor belt strength involves an isopycnic coordinate (OPYC) similar to the MICOM Model.

systems' ocean component requires much research attention because of (1) the dominant role ocean water has in the climate system as a result of its larger heat capacity and greater inertia in comparison with air; and (2) the complexity of the oceans' physical, chemical, and biological processes, which are far more complicated than the processes in the atmosphere and far less understood.

The overall goal of this project is to build a complete ocean modeling system that includes physical and biogeochemical processes. The current objectives include (1) comparing the effects of the choice of an isopycnal coordinate on model simulations of physical processes like currents and thermohaline circulation; (2) verifying our capability to simulate some fundamental biogeochemical process components; and (3) enhancing our understanding of some global climate variation mechanisms by analyzing ocean observational data.

In the development of ocean models that sustain and represent thermohaline circulation (THC), our isopycnal coordinate ocean model and its hybrid-coordinate version have provided advantages over conventional Z-coordinate models. This is important because THC is the mechanism that transports heat around the globe and modulates atmospheric temperature and regional climate (Fig. 1). Most Z-coordinate models are predicting a weakening in Atlantic overturning after 2000.

Our effort to expand the biogeochemical model component has put us at the forefront of the scientific community. Our model now includes the chemistry of nitrogen, iron, carbon, silicate, and sulfur cycles, and an ecodynamics system for the ocean's top 200 meters. The model is coupled to Los Alamos' Parallel Ocean Program (the Ocean General Circulation Model). We have completed several simulations including an iron fertilization experiment for carbon sequestration studies and a simulation of chlorophyll distribution (phytoplankton abundance) in the tropical Pacific during the onset of El Niño from December 1996 to December 1997. Figure 2 shows that the simulation results match satellite observation images very well.

El Niño is the dominant interannual climate variation and has tremendous impact on weather for most of the globe. However, the scientific community still has not identified the mechanism or trigger that shifts an El Niño into the La Niña phase (or vice versa). We investigated the relationship between the Antarctic Circumpolar Current (and the associated atmospheric-ocean coupled wave) and the variation in tropical oceans. We found that so-called El Niño actually appears in all three major oceans—Pacific, Atlantic, and Indian. By filtering the global ocean sea-surface temperature (SST) monthly data series of 1900–1994 with several time windows, we identified the SST perturbation along the Antarctic Circumpolar Current to be one of the possible triggers for the El Niño phase shift. ■

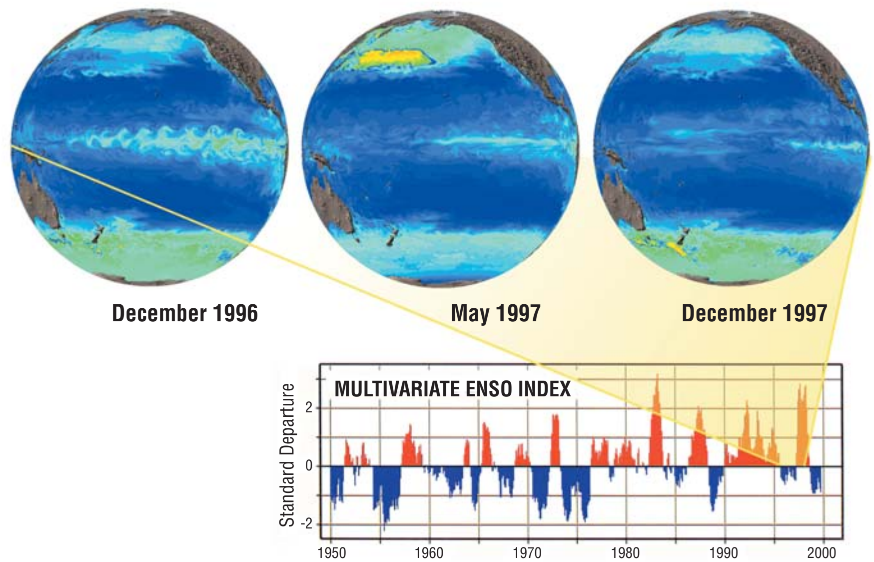

Fig. 2. Surface chlorophyll distribution in late 1996 (a La Niña year), May 1997 (onset of a strong El Niño), and late 1997 (full El Niño conditions). Biological activity is intense across the equatorial Pacific during La Niña (December 1996). The warm pool then shifts eastward, shutting off the supply of nutrient from the deep ocean (mid-97). Plankton growth slows, and the chlorophyll peak gradually recedes towards the east (December 1997). Plot of a multivariate El Niño Southern Oscillation index is superimposed for comparison.

Recent FIRETEC Developments and Applications

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Los Alamos has been developing a physics-based wildfire model, FIRETEC, for the purpose of assisting decision makers concerned with wildfires and controlled burns. FIRETEC models the driving processes in a wildfire by solving a coupled set of partial differential equations that describe the conservation of mass, momentum, energy, species, and turbulence. The philosophy behind the development of FIRETEC is that a physics-based model of this type will be applicable to a variety of complex wildfire situations that the empirically based wildfire models cannot represent. In addition, we envision using FIRETEC to explain thresholds in wildfire behavior and to help determine ideal fuel-thinning strategies of the future (Fig. 1).

The ability to model complex wildfire situations and study fundamental wildfire behavior meets a national need for a better understanding of wildfire behavior, including its response under varying environmental conditions. In addition to developing a wildfire modeling capability, the work leading to FIRETEC has increased EES capabilities in dispersion modeling and fine-scale atmospheric modeling.

In recent months, we have focused FIRETEC's developments in two areas. The first area of focus is the incorporation of US Forest Service data pertaining to individual trees. These data are being used to create stands of trees for use in fire simulations. This is an important step because it will allow us to examine specific thinning strategies and the thresholds that dictate a fire's ability to become a crown fire.

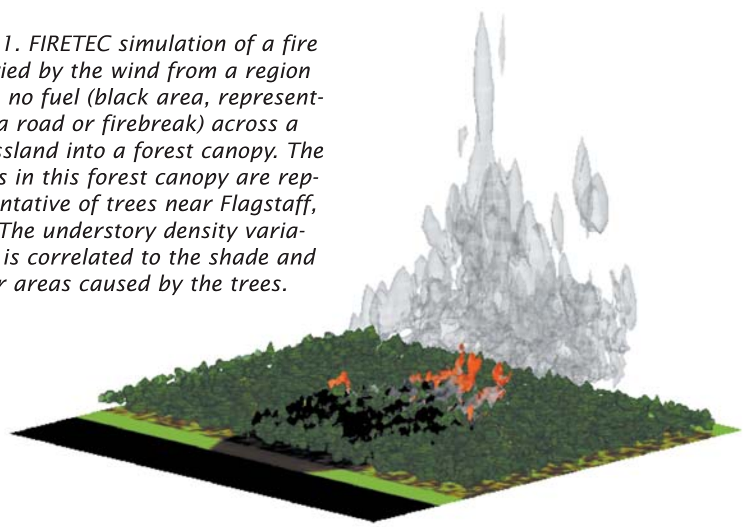

Fig. 1. FIRETEC simulation of a fire carried by the wind from a region with no fuel (black area, representing a road or firebreak) across a grassland into a forest canopy. The trees in this forest canopy are representative of trees near Flagstaff, AZ. The understory density variation is correlated to the shade and litter areas caused by the trees.

The second focus area is the generation of a framework that allows for generalized rules regarding the grass density variations to be tested. This framework is important because our ability to model realistic stands of trees and the fires that occur on the floor of a canopy depends on knowledge of the ground fuels and their distribution with respect to the trees.

FIRETEC is an exciting example of science, part of which originated within the weapons program, serving society. Many aspects of wildfires that can be studied with FIRETEC cannot be studied with other operational models. ■

Assessment of Surface and Near-Surface Hydrologic Processes at Technical Area 54

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Material Disposal Area G (MDA G) is an active low-level radioactive waste repository that has been in operation since the 1950s. Maintaining operations at this site is vital to Los Alamos because closure would have major negative impacts on the Laboratory's weapons program as well as other R&D activities. DOE requires a Performance Assessment (PA) and periodic revisions to determine whether the site meets a specified set of risk criteria. The original PA was approved, and the first revision review will occur in 2004. The PA process requires update activities to (1) reduce uncertainties for the major risk pathways, and (2) address possible impacts of recent changes at the site. The surface pathway was found to be the highest risk driver. Thus, the EES-2 Hydrology and Ecology teams and collaborators have focused on surface and near-surface processes at MDA G. These efforts include assessing the impacts of runoff and gully erosion, wind erosion, changes in near-surface hydrology resulting from asphalt paving, and postclosure plant succession. In addition to supporting Laboratory institutional needs, recent work contributes to improved understanding of the eco-hydrology of semiarid environments.

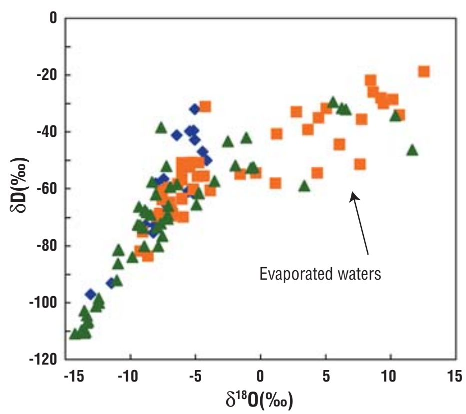

Fig. 1. Pore-water stable isotope values from asphalt boreholes (blue diamonds) show a large hydrologic shift compared to nonasphalt boreholes (green triangles and orange squares). All of the asphalt borehole data plot along the meteoric water line and lack the large isotopic values at the near surface that are characteristic of evaporation (as indicated in the figure).

Erosion is a major concern at the site because of the potential to expose waste and transport contaminated materials to potential receptors. Gully and wind erosion are of particular concern. Activities to date include the installation of Big Springs Number Eight wind erosion samplers and use of the SIBERIA code to model gully erosion at the site.

Substantial asphalt paving is probably the largest change that has taken place on the mesa top since the original PA was performed. This change affects not only the surface hydrology but also the hydrology under the asphalt by causing an increase in water content, partly because of a lack of normal surface evaporation (Fig. 1). Through borehole analysis of water content, chloride, and stable isotopes ($\delta^{18}O$ and δD), we are continuing to make significant improvements in our understanding of the impacts of asphalt at MDA G. Related ongoing projects include evaluating potential impacts of piñon and juniper growth on cover performance and percolation during the postinstitutional control period, and HYDRUS (Simunek et al., 1996) modeling of various cover scenarios. HYDRUS is especially useful for examining water balance and flow problems for complex near-surface environments and for evaluating landfill cover performance. ■

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Tropical Western Pacific

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Our important scientific progress this year focuses on the beginning of the 2002 El Niño and its effect on the Atmospheric Radiation Measurement (ARM) Program sites in the tropical western Pacific (TWP; Fig. 1). The combination of this event and supplemental remote-sensing data from DOE's multispectral thermal imaging (MTI) satellite and the more recent Atmospheric Infra-Red Sounder (AIRS) component of the NASA Aqua satellite are providing insight into the climatically important but poorly understood TWP region. The effect of the 2002 El Niño can be seen in the changes in the predominant wind directions at the island of Nauru. During 2000, the wind direction was almost always from the east. In 2002 during the El Niño, wind directions are almost evenly distributed between east and west.

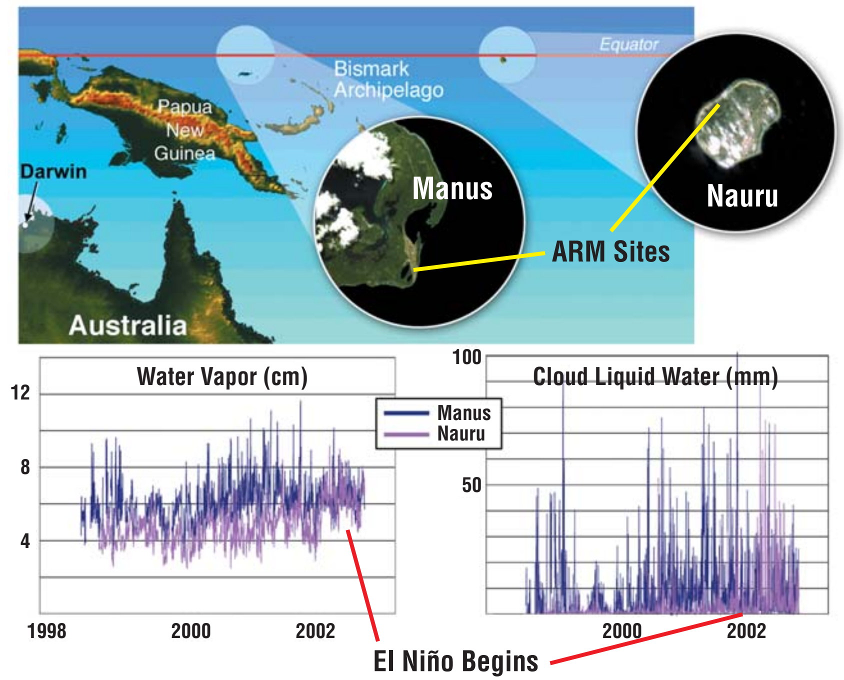

Fig. 1. Manus and Nauru sites in MTI satellite images and trends show the effect of the 2002 El Niño on vertically integrated water vapor and cloud liquid water.

During 2000, we combined MTI images of cloud trails from Nauru with numerical cloud modeling to improve our understanding of the sensitivity of boundary-layer clouds in tropical regions to perturbation. This model study showed that mechanical turbulence generated by the interception of the predominant wind by this small (3-km-diam, 65-m-high) island can be enough to generate a cloud trail under some circumstances. However, comparison of nighttime to daytime images of the Nauru cloud trail indicates that, in most cases, convective turbulence by daytime island heating is more effective in forming the island cloud (Fig. 2).

The ARM Program established a cloud and radiation test bed (CART) site in TWP in 1996, in order to obtain data to better understand phenomena that are important to global climate change predictions. The first TWP Atmospheric Radiation and Cloud Station (ARCS) began operations in Papua New Guinea in October 1996. The second ARCS started collecting data in November 1998. Two years later, in April 2002, the third ARCS began its operations in Darwin, Northern Territory, Australia. The ARM Program chose Darwin because its climate regimes (i.e., dry continental, monsoon, and transitional periods) are of specific interest for studies of atmospheric radiation and clouds. Darwin is also associated with existing scientific programs of the Australian Bureau of Meteorology and the Commonwealth Scientific and

Industrial Research Organization, a rich research collaboration that is beneficial to climate research. ■

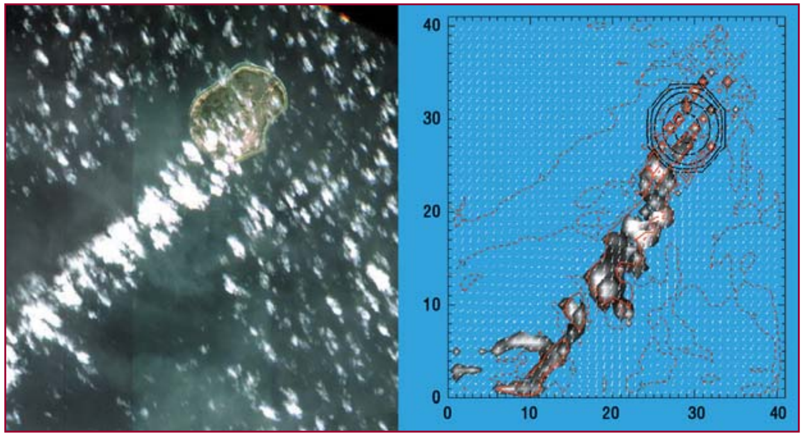

Fig. 2. Comparison of MTI satellite images and model results of clouds generated by Nauru on a day (Dec. 13, 2000) on which a cloud trail was observed.

Weapons Phenomenology and Infrasound

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The development of sensors to detect atmospheric nuclear explosions from space satisfies an important national security need to monitor and verify international test ban treaties. Design and successful operation of these sensors requires a basic understanding of the source and its associated emissions, propagation of the signals to the detector, and the detailed nature of the natural and anthropogenic background in which the detectors must operate. The Weapons Phenomenology Program at Los Alamos is focused on the development of models and computational tools to simulate all aspects of the treaty-monitoring problem from the source to the sensor. The present emphasis in EES-2 is on predicting the optical and electromagnetic pulses produced by a nuclear detonation, but we have also worked on various aspects of acoustic-wave propagation, simulations of bolide-atmosphere collisions, fireball physics, lightning and ionospheric physics, satellite-data analysis, satellite-system analysis, urban pollution analysis and modeling, and active space experiments such as chemical injections into the upper atmosphere.

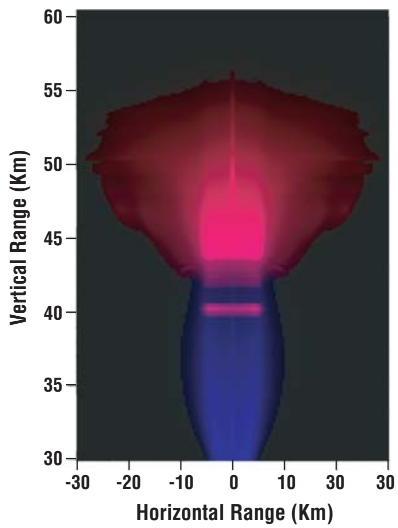

Fig. 1. True color synthetic picture of a sprite discharge. The image was obtained from a fully electromagnetic 2-D cylindrically symmetric simulation of a high-altitude discharge driven by runaway air breakdown. The emissions derive from electron-induced fluorescence of nitrogen. Sprites are routinely observed over large mesoscale convective systems that form over the midwestern United States. The observed emissions extend from 30 km to altitudes exceeding 80 km. The red emissions are eliminated at low altitudes by quenching.

The Infrasound Team supports DOE's Ground-Based Nuclear Explosion Monitoring Program by using the low-frequency acoustic signals generated by atmospheric explosions to detect and locate these sources. This technique compliments the US space-based optical and radio frequency sensors, which are the primary detection method for atmospheric nuclear explosions. The infrasound data can provide additional information on signals of interest that may not trigger the space sensors but still need to be understood and identified. This effort also includes the ability to reliably calibrate infrasound sensors.

Another relatively new effort of the team that is related to both efforts described above is that of modeling the optical emission of bolides and the associated fragmentation processes occurring during entry into the atmosphere. Comparisons between bolide light emission and the corresponding temporal emission from a nuclear explosion are also being explored. This effort is yielding an improved understanding of the variability of bolide emission resulting from the bulk porosity of the various types of bolide materials. ■

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Hydrogeology of the Pajarito Plateau

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In 1998, the New Mexico Environment Department approved the Laboratory's Hydrogeologic Work Plan, which describes activities to characterize groundwater flow beneath the 43-sq.-mi. area of the Laboratory and to assess the impact of Laboratory activities on groundwater quality. The centerpiece of the Hydrogeologic Work Plan is installation of up to 32 deep wells in the regional aquifer and 51 shallow wells in canyon-floor alluvium. The expected outcomes of the activities described in the work plan are

- Refined understanding of the Laboratory's hydrogeologic framework, including recharge areas, hydraulic interconnections, flow paths, and flow rates, that is synthesized by modeling simulations.
- Information sufficient either to design and implement a detection-monitoring program that meets applicable requirements or to demonstrate that groundwater monitoring requirements can be waived.
- Defined areas of existing or potential groundwater contamination, and the potential pathways of contaminant transport from the surface to the regional aquifer, with predictions of directions and rates of movement and of risk based on modeling simulations.

This project addresses a variety of state and federal environmental regulations and is vital to the continued operation of the Laboratory. EES Division provides technical leadership in geology, geochemistry, hydrology, and flow and transport modeling for this program. Our investigations include collection of stratigraphic, lithologic, and geophysical data; identification and characterization of perched water zones; collection of water quality and water-level data; collection of moisture and

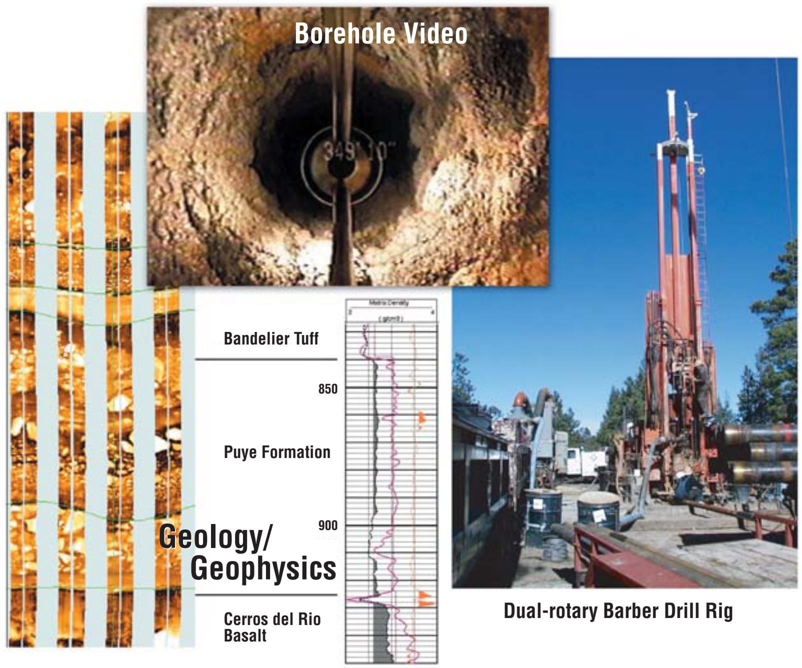

Fig. 1. EES Division scientists plan and execute a broad spectrum of hydrogeologic investigations across the Pajarito Plateau in support of the Laboratory's environmental programs. The EPA data-quality objective process is used to focus data-collection activities on key data needs.

contaminant profiles through the vadose zone; in situ hydraulic tests in wells; and mineralogic and geochemical studies of key hydrogeologic units (Fig. 1). In addition, groundwater is collected from installed wells on a quarterly basis to determine spatial and temporal variations in water quality (including contaminants) across the Laboratory. The data collected support refinement of the hydrogeologic conceptual model, and they provide input and constraints for the site-wide geologic model, geochemical models, and numerical flow and transport models (Fig. 2).

Our most significant finding to date is that high-explosive (HE) contamination occurs in concentrations above EPA health advisory limits in deep groundwater below a portion of TA-16 located in the southwestern part of the Laboratory. Equally important is the discovery of Laboratory-derived contaminants in deep perched groundwater beneath Mortandad Canyon. This groundwater contains elevated tritium activities, nitrate concentrations above the US Environmental Protection Agency (EPA) primary standard for nitrate, and perchlorate above the EPA draft provisional risk-based level for perchlorate. The occurrence of deep groundwater contamination at these two sites indicates that nonsorbing contaminants such as HE, tritium, nitrate, and perchlorate in surface water are capable of relatively rapid transport through the vadose zone, particularly down-gradient of Laboratory sites releasing large volumes of effluent into canyon systems. ■

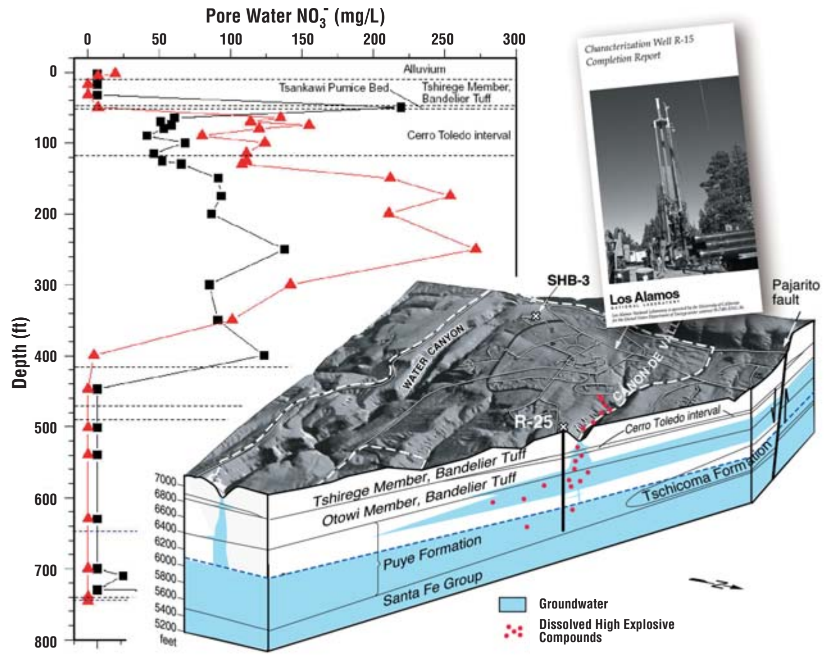

Fig. 2. Data from hydrogeologic investigations are used to develop conceptual models for groundwater systems and to model contaminant transport as part of risk assessments and site decisions. Shown are a pore-water nitrate profile from a drillhole in Mortandad Canyon, and a conceptual model block diagram for high-explosives transport at TA-16.

Tracing Ecologic Processes with Stable Isotopes

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We have been using light stable isotopes to identify ecologic processes relevant to issues of natural attenuation of contaminants as well as to carbon sequestration in terrestrial, aquatic, and oceanic environments. This research uses EES Division capabilities in geochemistry, ecology, and hydrology and supports Laboratory missions related to human health and environmental security.

Natural Attenuation

We have used nitrogen isotopes to identify the occurrence of microbial denitrification in wetlands in Sandia Canyon (Technical Area 60, also designated TA-60), Martin Canyon (TA-16 and TA-11), and Cañon de Valle (TA-16). Denitrification is a process in which microbes reduce nitrate to nitrogen gas under oxygen-poor conditions, resulting in the release of nitrogen from sediments. The Sandia Canyon wetland (Fig. 1) receives treated sewage effluent from the Laboratory. This effluent contains nitrate that is highly enriched in the heavy isotope of nitrogen, nitrogen-15, with a $\delta^{15}N$ of 32.4‰. The delta notation is the ratio of $^{15}N/^{14}N$ relative to an international standard and expressed as parts per thousand or parts per mille. Cattail stems in the wetland were measured for $\delta^{15}N$. Cattails near the head of the wetland have values up to nearly 38‰, the highest values that we are aware of for plants. Denitrification is a fractionating process in which the residual nitrate available for plant uptake is progressively enriched in nitrogen-15. The high $\delta^{15}N$ values for the cattails relative to the value of input sewage nitrate, and trends towards higher $\delta^{15}N$ in more oxygen-depleted sediments, indicate that denitrification is an important natural attenuation process in this wetland (Fig. 2; Heikoop et al., 2002).

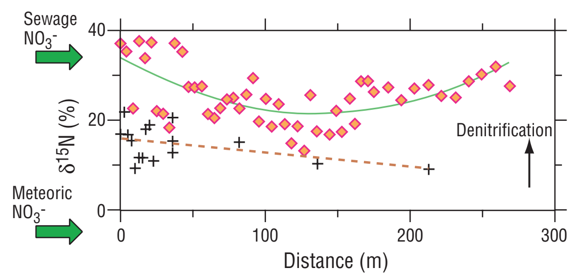

Fig. 1. Trends in cattail $\delta^{15}N$ with distance, Sandia Canyon wetland. Red diamonds are cattails from the longitudinal access of the wetland, while black crosses are cattails from the periphery. Photo shows a Sandia Canyon wetland.

In Martin Canyon and Cañon de Valle, the nitrogen-bearing contaminants are nitrate and high explosives associated with the production of barium nitrate, RDX, and HMX at TA-16. Although the value of $\delta^{15}N$ of the explosives is unknown, we know that the value must be close to 0‰ because nitric acid is used in their production and typically has a value near zero. Despite the input of isotopically light nitrogen, grasses and cattails associated with wetlands and springs have enriched values of up to nearly 12‰, again suggesting that denitrification is an important natural attenuation process.

These studies are designed to develop a quick, cost-effective technique to map the spatial variability in processes that can naturally attenuate contaminants without the need for the application of expensive, invasive cleanup technologies.
This research was funded as part of a postdoctoral fellowship to Jeffrey M. Heikoop and as part of the Laboratory's Environmental Restoration Project.

Carbon Sequestration

As part of an IGPP-funded project, we have been examining the isotopic composition of the deep-sea coral *Primnoa resedaeformis* (Fig. 3). This coral has a skeleton made of both calcite and a proteinaceous material called gorgonin, arranged in annual layers (Risk et al., 2002). The $\delta^{15}N$ and

$\delta^{13}C$ of the gorgonin fraction of the skeleton reflects the isotopic composition of plankton that have sunk from the surface and been consumed by the coral (Fig. 4; Heikoop et al., 2002). The $\delta^{15}N$ and $\delta^{13}C$ of the plankton reflect the productivity of plankton in surface waters. Plankton productivity is an important component of the oceanic biological pump that takes carbon dioxide from the atmosphere and sequesters it in the deep ocean. We are using this signal to measure the isotopic composition of gorgonin layers in *Primnoa* back through time, in order to reconstruct the history of this biologic pump in various areas of the oceans. At one site near the boundary of the Pacific and Southern oceans, for instance, plankton productivity appears to have decreased through time.

In the terrestrial realm, we have recently begun a project to look at the effects of drought on terrestrial carbon sequestration. Drought-related mortality and reduced growth of ponderosa pines and piñon pines on the Pajarito Plateau will affect the carbon sequestration potential of these forests. We are using carbon isotopes, which reflect water availability to plants, in tree rings to reconstruct drought history and its impact on tree growth in this region. ■

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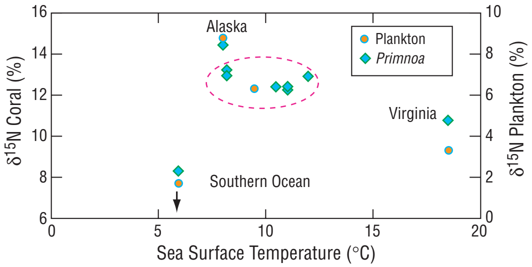

Fig. 2. $\delta^{15}N$ *of* Primnoa *and plankton from overlying waters. Low* $\delta^{15}N$ *values for a coral from the Southern Ocean indicate low-productivity waters, and high values from an Alaska coral indicate high-productivity waters. The deep-sea coral* Primnoa resedaeformis *is shown in the photo.*

Three-Dimensional Model of the Española Basin Aquifer

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The Española Basin contains the principal aquifer supplying drinking water to a rapidly growing population in northern New Mexico. The development and analysis of the 3-D numerical model of the Española Basin aquifer is an important aspect of the Laboratory's Groundwater Protection and Environmental Restoration programs. The project addresses major issues related to sustainability of groundwater resources in the region and the potential impact of previous and current Laboratory activities on the subsurface environment and on groundwater quality and quantity. Our regional groundwater study recently attracted substantial interest from local environmental groups, legislators, stakeholders, and DOE and Los Alamos management.

The unique capabilities at Los Alamos that are brought to bear on this project include integration of large data sets (hydrologic, geologic, geophysical, and geochemical) through flow and transport modeling; use of inverse methods to discriminate between alternative conceptual models, particularly with respect to hydrostratigraphy; application of nonlinear optimization methods to explore uncertainty associated with model predictions; coupling Site-Scale and Basin-Scale models using novel approaches; and application of new methods to simulate dispersion in the contaminant transport.

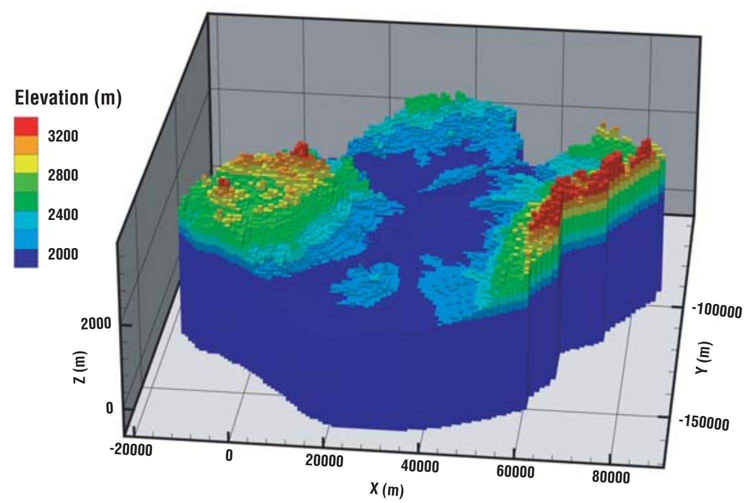

Fig. 1. Basin Model computational domain showing local topography.

We have presented our results in Laboratory reports, conference proceedings, and peer-reviewed journals.

Our current objectives are quite varied. First, we are supporting a risk-assessment project by evaluating potential contaminant transport in the regional aquifer in a probabilistic framework. Second, we are completing our capture zone analyses for water supply wells in the vicinity of Los Alamos, which includes robust estimation of model uncertainties. We are initiating a study of coupled heat flow and geochemical processes using the basin flow and transport models. This study, which is continuing, will be used to estimate possible deterioration of existing water quality problems in the region as a result of heavy pumping. We are also supporting a new Laboratory-Directed Research and Development project that started in October 2002 by using the basin model to interpret high-precision, repeat-gravity measurements to derive new insights into aquifer storage and recharge rates.

Many of our modeling applications are very computationally intensive. A predominant portion of the model simulations has been performed implementing the existing multi-processor supercomputers at Los Alamos.

Our major accomplishments have been related to capture zone analysis of the Buckman wellfield and a new horizontal collector well, both of which supply Santa Fe with water. The research demonstrated that the capture zones extend on both sides of the Rio Grande River and that some of the pumped water flows in the aquifer beneath Los Alamos. We also estimated the groundwater flowpaths, travel times, and dilution factors from potential contaminant sites to the wells. Further, we analyzed some aspects of the uncertainty in these predictions. We assessed the impact of uncertainties in the aquifer recharge distribution and in the geologic structure on the capture zone and groundwater transport predictions.

The research addresses fundamental R&D issues associated with using numerical models for analysis and interpretation of physical processes. It relates directly to the Laboratory's mission to solve national problems in energy, environment, infrastructure, and health security. Our research is highly relevant to at least two of the Laboratory's institutional goals. One of our objectives is to develop predictive tools with an integrated experimental and computational approach. Our research directly supports the goal to establish a major Los Alamos initiative in civilian science and technology. Some of our efforts also tie to a number of the Strategic Research Directorate program goals, such as (1) providing scientific leadership and nucleating new programs in energy and environment; (2) in high-performance computing, to lead in exploring and developing new approaches to modeling simulation, and calibration (inversion); and (3) fostering and championing excellence in basic and applied research. The work on this project relates the division's Water Thrust to the following key EES-6 capabilities: hydrology, national security science and technology, and computational science and mathematics. ■

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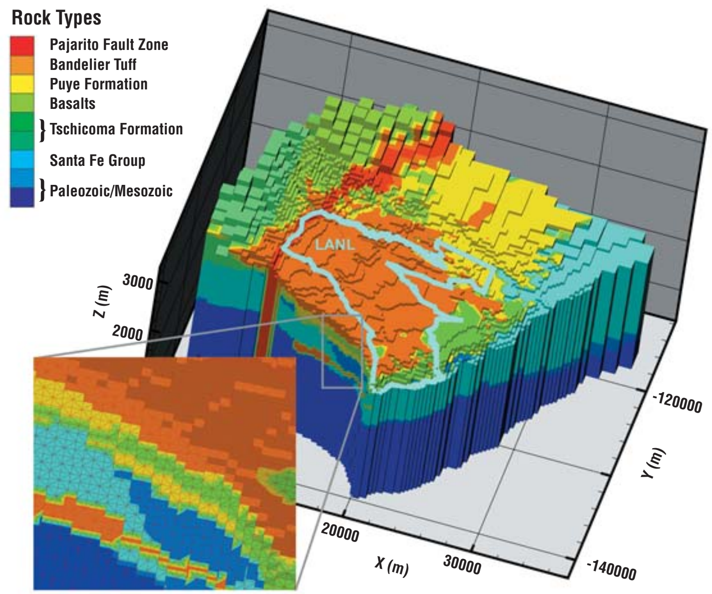

Fig. 2. Geologic structures within the submodel domain beneath the Pajarito Plateau.

Colloid-Facilitated Radionuclide Transport

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Laboratory and field observations indicate that plutonium and other reactive radionuclides may migrate faster in groundwater when colloids are present than would be predicted with simple groundwater solute-transport models. Prediction of colloid-facilitated radionuclide transport may be necessary for assessment of contaminant boundaries in systems for which radionuclides are already in the groundwater and for the performance assessment of potential repositories for radioactive waste. Therefore, a reactive transport model is developed and parameterized using results from controlled laboratory fracture-column experiments and from field observations.

The computer model used in this study builds upon capabilities developed in EES Division for assessment of potential high-level radioactive waste repositories. However, the application is directed toward the assessment of the migration of radionuclides already in the subsurface at the Nevada Test Site (NTS) as a result of previous underground nuclear weapons testing. The capabilities developed in this project are readily applicable to other groundwater solute-transport problems within the division's water thrust, particularly as water quantity and water quality issues become more coupled.

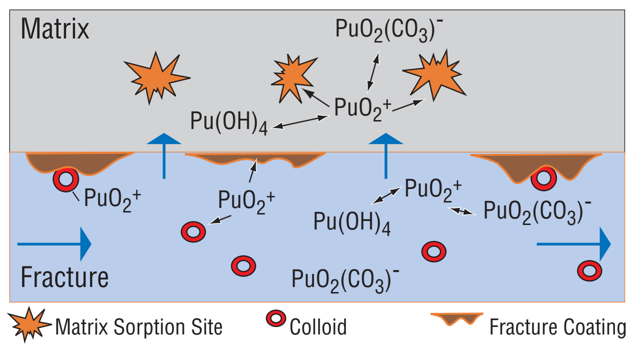

Fig. 1. Schematic of processes affecting solute and colloid mobility in a fracture matrix system. The processes include speciation, sorption to mobile colloids, sorption to immobile minerals, and diffusion between fracture and matrix.

In the laboratory component of this study, silica, montmorillonite, and clinoptilolite colloids are used in column experiments along with plutonium and tritium. The goal of the numerical model is to identify and define the parameters for the physical and chemical processes that affect the colloid-facilitated transport of plutonium in the fractures. The model is then extended to the field scale and is used to explain recent field observations and to provide capabilities for determining the location of the maximum contaminant boundary in ongoing studies.

Some key findings in this study are (1) colloids appear to be necessary in the explanation of plutonium, cesium, europium, and americium migration in NTS groundwater; (2) kinetic reactions in which desorption rates are much slower than sorption rates are necessary to explain the transport in both lab and field observations; and (3) desorption rates, although slow for some colloids, are much greater in a flowing fracture than in a laboratory batch experiment. ■

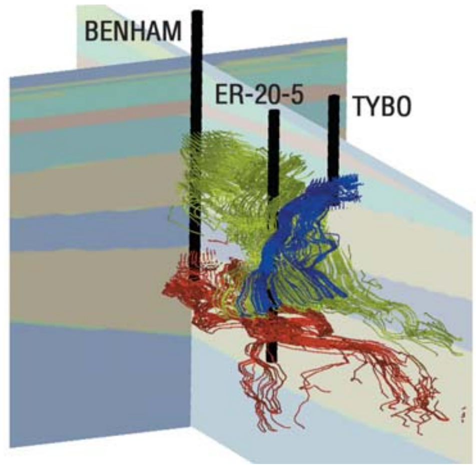

Fig. 2. Solute and colloid pathways in NTS groundwater. Sources at BENHAM and TYBO are shown relative to ER-20-5 observation wells.

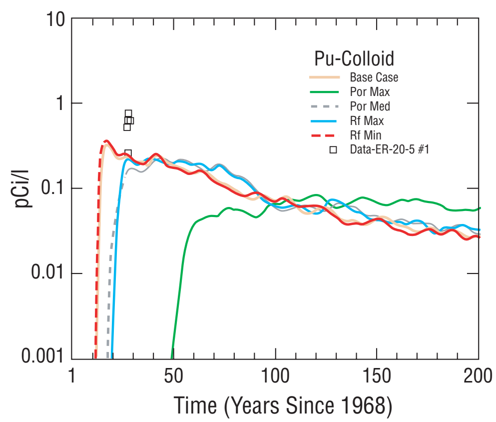

Fig. 3. Model predictions and field observations of plutonium concentration in well ER-20-5 #1 at the NTS. Different curves show results for various simulations in the transport parameter sensitivity study. These simulations show little sensitivity to retardation to fractures (Rf) but reasonable sensitivity to porosity (Por).

Geochemistry of Carbon Capture and Sequestration

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Fossil fuels represent an abundant and cheap domestic resource for energy, yet the increasing level of atmospheric carbon dioxide (CO_2), which is by far the largest byproduct of fossil-fuel combustion, is challenging their continued use. Responding to this challenge, President Bush announced in early 2002 a "new environmental approach" to the use of fossil fuels and set the goal of reducing the intensity of greenhouse gas emissions (particularly CO_2) while sustaining economic growth. Achieving this goal will require new approaches to capturing CO_2 and storing it permanently and safely.

To meet this challenge, EES Division has been leveraging core theoretical and experimental capabilities to identify new approaches to improve the efficiency of the carbon fuel cycle while minimizing its environmental impact. In collaboration with other Los Alamos divisions, EES has become a scientific leader and innovator of new solutions to many aspects of carbon control. These solutions include energy conversion with integral separation of CO_2 (for example, the zero-emission coal process), carbon monitoring and analysis (use of laser-induced breakdown spectroscopy to analyze soil carbon), and sequestration of CO_2 (geochemical efforts to understand the CO_2 mineralization process). These efforts tie directly to the nation's goals in energy and the environment. Moreover, they support scientific needs for the core Los Alamos missions in defense by providing a scientific challenge to stimulate new approaches to prediction of complex systems, monitoring and remote sensing of gases, environmental fate and transport of carbon compounds, and geoengineering the subsurface to contain high-pressure gases.

Several of the EES carbon research efforts focus on exploiting our geochemistry and geomaterial capabilities to develop novel concepts related to the long-term storage of CO_2 and the direct capture of CO_2 from the atmosphere.

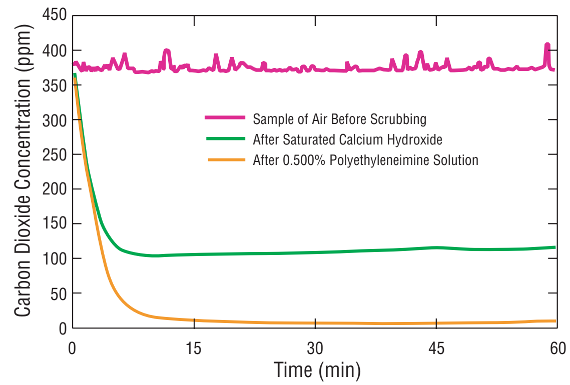

Fig. 1. Experimental determination of CO_2 collection efficiency for various aqueous sorbents.

Air Extraction

Most efforts in CO_2 capture for sequestration are focused on large point sources such as power plants. This focus neglects over half of the CO_2 emissions that come from automobiles, home heating, and other sources. Current approaches also require extensive pipeline networks and cannot address past CO_2 emissions. Los Alamos recently proposed a novel concept that addresses these issues by removing CO_2 directly from the air. The challenge is to concentrate CO_2 from about 370 ppm in the air to a purified CO_2 stream. Our efforts are focused on identifying mechanisms that enable this process to proceed rapidly, efficiently, and inexpensively.

We have begun studying the CO_2 collection efficiency of a variety of different adsorbents (Fig. 1). Atmospheric CO_2 concentrations were measured both before and after the adsorbent. We used infrared CO_2 sensors to quantify the collection efficiency. Our initial studies focused on alkali and alkaline-earth hydroxide solutions that react rapidly with CO_2 in air. Gram-scale quantities of CO_2 have been extracted from Los Alamos air using calcium hydroxide solutions, which have a high (>50%) collection efficiency. Depending on the fuel type, the theoretical energy needed for CO_2 recovery from the solid calcium carbonate is about one quarter to one half of the energy produced by burning the fossil energy, which indicates that this could be a viable approach. The search for new absorbents that would significantly reduce the energy penalty is underway. Recent experiments with new amine polymers are very encouraging: very dilute polyethylinineimine solutions demonstrate almost 100% CO_2 uptake with a lower binding energy and, hence, smaller energy needs for recycling and recovery.

CO_2 Mineralization

Conversion of CO_2 to a solid is a concept introduced by Los Alamos in 1995 as a means of safe, permanent storage of large volumes of CO_2. The concept relies on exploiting a natural carbon cycle in which magnesium silicates are converted to magnesium carbonates and silica. The challenge is to achieve industrially meaningful amounts of conversion. This requires speeding the natural process by orders of magnitude while using minimal external energy input. Los Alamos research is focused on understanding the geochemical mechanisms and, therefore, identifying novel routes to speed the reaction while avoiding energy-intensive processing. This work has relied on combining high-pressure experimental facilities with our theoretical geochemical capabilities including reactive transport.

We have recently demonstrated rapid dissolution (the first step in the process) of serpentine in the presence of a variety of organic-acid chelators. We are currently working to understand the precipitation process (the second step) to determine mechanisms for enhancing its rate. Recent successes also include exploiting our reactive-transport codes for chemical reactions in geological systems, in order to develop a model that can explain observations in dynamic experimental studies of olivine carbonation. This model will be used to guide new experimental studies and to determine if olivine carbonation is theoretically possible at industrially meaningful rates. ■

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Yucca Mountain Saturated-Zone Flow and Transport

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Because of the complexity of the Yucca Mountain system, model predictions that are required for performance assessment contain uncertainty. The activities we perform are intended to increase confidence that the Site-Scale Saturated-Zone Flow and Transport Model provides a representation of saturated-zone (SZ) flow and transport processes that is sufficiently accurate to allow us to properly evaluate the role of the SZ as a component of the natural barrier system. Additionally, we intend for the activities to validate the appropriateness of the use of the SZ site-scale flow model to perform the SZ abstractions for Total System Performance Assessment (TSPA).

Our work relies on data that have not been directly incorporated into the calibration of the model in order to establish a basis for evaluating model reliability. As part of building confidence in the model, we made qualitative and quantitative comparisons between measurements not used in the calibration and the model's predictions for those quantities. These activities may include but are not limited to (1) the comparison of system-properties measurements such as hydraulic head or tracer concentrations (which were not used in the development or calibration of the model) with model predictions; (2) collection of new data for comparison with model predictions; and (3) the development of independent lines of evidence for process descriptions such as flow paths that were modeled using geochemical data to test against predictions.

Confidence-building activities affect the flow model, the transport model, and the abstraction of flow and transport in support of TSPA. These are described below.

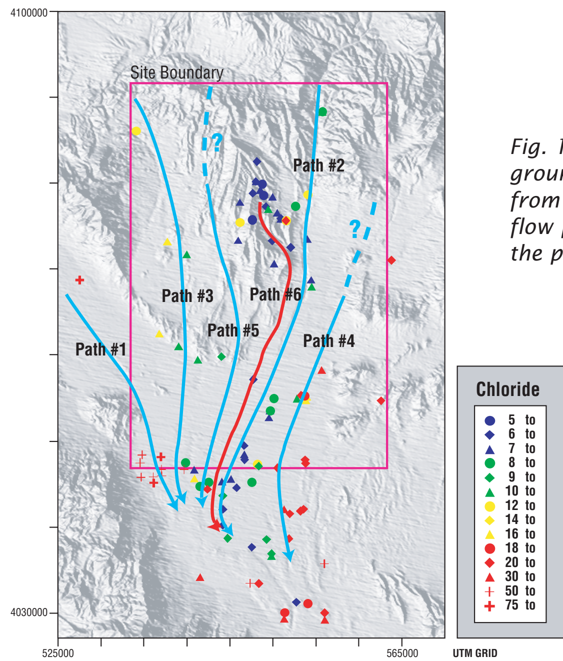

Fig. 1. This figure illustrates groundwater flow paths inferred from geochemical data. The dark flow path originates just beneath the proposed repository.

Flow Model Validation

Use of Water-Level Data. Model simulation predictions were made, and predicted water-level data were compared to measured data not used in the calibration.

Thermal Modeling. Temperature data from the Yucca Mountain area are potential indicators of flow patterns, particularly in terms of vertical flow components. We completed a quantitative comparison between measured temperature and model predictions. Predicted temperatures were within 10 degrees of measured temperatures in more than 90% of the wells.

Hydrochemical Analyses. Like temperature, groundwater hydrochemical and isotopic data provide a means of tracing groundwater movement. The evaluation involves (1) the analysis of spatial patterns in the data in map view and in three dimensions; (2) the examination of scatterplots that show the relation between relevant chemical and isotopic species; (3) the creation of quantitative mixing and reaction models with hydrochemical software (PHREEQC) to explain chemical and isotopic trends identified in the graphical analyses; (4) forward runs with the calibrated SZ flow and transport model, to predict the concentrations of selected nonreactive and reactive species at measurement locations, for comparison with data. These analyses will incorporate new groundwater chemical and isotopic data from Nye County and other Yucca Mountain Project activities as it becomes available. Figure 1 shows the model-generated path and the path inferred from hydrochemistry. The trajectories of particles originating at the potential repository can be compared to Path 6 in the figure. Path 6 follows Dune Wash before turning southwestward near the intersection of Dune Wash and Fortymile Wash. The figure indicates that the general direction of groundwater movement predicted by the numerical models from the potential repository area is in agreement with the flow direction determined from the hydrochemical and isotopic data.

Use of New Hydrogeological and Boundary Fluxes Data. The incorporation of new data involves updating the development of the flow model by using a new hydrologic framework model and new boundary fluxes, extracted from the 2001 revision of the USGS model. Flow paths and travel times of the revised model are compared to those of the validated model within less than 10% of each other.

Transport Model. This work provides a transport-process model to validate abstraction models for performance assessment. The model will allow us to test various assumptions and simplifications employed in the performance assessment particle-tracking model, and to incorporate physical and chemical processes more fully. The work for this model includes the development, testing, and quality assurance of the model software, followed by analyses of processes such as sorption, climate change, and colloidal transport. Improvements to the particle-tracking model include a method of obtaining in situ concentrations from particle-tracking results.

Transport Properties. Confidence building in the transport properties includes (1) documentation of the basis for the radionuclide K_d distributions used in TSPA, and (2) analyses to determine whether radionuclide K_d values are correlated between different units and between the unsaturated and saturated zones. ■

Data-Management Team Continues to Expand Services

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New challenges are a constant stimulant for the Test Coordination Office's (TCO) Data Management Team, which continues to provide the Yucca Mountain Project scientific community with prompt, high-quality technical data services while complying with demanding procedures and requirements in a nuclear culture. Accomplishments for the past two years include providing data-acquisition and data-management services for numerous field tests. These tests include large-scale underground thermal conductivity testing; a series of Rock Modulus Slot tests; the Engineered Barrier series of testing at DOE's Atlas complex in North Las Vegas; the Natural Convection Test series, also in North Las Vegas; the United States Geological Survey (USGS) video camera network in the cross drift; the Laser-Strain Gage Test; and over 70 data loggers operated underground by USGS and Lawrence Berkeley National Laboratory. The team has also created and developed a baseline for more than 20 software programs used for the automated transfer of test data between the remote test location and the TCO Data Management Facility in Las Vegas.

In 1998, the TCO initiated a continuing project to build a fiber-optic-based local area network (Fig. 1) to service the underground Exploratory Studies Facility (ESF). We have since expanded the network to enable remote monitoring, control, and automated downloads of over 80 data-loggers and several computer-based data-acquisition systems. Scientists who use the network control in real time can now monitor most of the underground tests directly. Additionally, the automated data-collection activities for the prominent five-year-old Heated Drift Scale Test (with over 6,000 data channels) continue at a high level of reliability and accuracy. The team is currently designing and installing an Environment, Safety, and Health remote-monitoring system for several underground radon detectors and completing a network to provide remote access to the remaining dozen manually downloaded data-loggers in ESF.

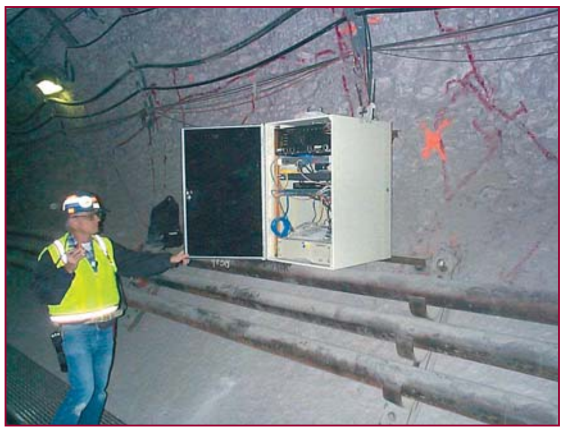

Fig. 1. One of the many fiber-optic-based local area network locations used to provide real-time interconnection of data collection systems underground in ESF.

The many demanding procedures and requirements of the project's nuclear culture require that we control and document all measuring and testing equipment, software, and data-management activities under a rigid quality-assurance program in an safety-conscious work environment. ■

Engineered Barrier Systems for the Yucca Mountain Project

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Since 1998, the Yucca Mountain Project (YMP) has performed pilot-scale tests to acquire data to evaluate features and components of the Engineered Barrier System (EBS). The data acquired from these tests have been used to develop and verify process models and input for computer models.

The EBS Test Facility is located in North Las Vegas, NV, in the DOE complex on Losee Road. The facility consists of 20-ton overhead cranes; three test assemblies of the following dimensions: 40.2 m length × 1.37 m diam., 11.1 m length × 1.37 m diam., and 18.57 m length × 2.44 m diam.; a test chamber 4 m wide, 4 m long and 2.5 m high; and several surrogate waste packages and drip shields.

The Test Coordination Office coordinates the following tests:

Phase 1—Quarter-Scale Ambient Inlet Air Ventilation Test. This test was performed to evaluate the cooling of emplacement drift from the ventilation during preclosure and to acquire data for the ANSYS computer program used for the design of the repository ventilation. In this test, we used 25 surrogate quarter-scale 21 pressurized water reactor waste packages having diameters of 40.64 cm. and lengths of 1.32 m. We performed the tests at a linear thermal load of 0.18 kW/m and at 0.36 kW/m. Four inlet air volumes with 0.5, 1.0, 2.0, and 3.0 cubic meters per second were used for each of the two power settings.

Fig. 1. The Ventilation Test Setup.

Phase 2—Quarter-Scale Conditioned Inlet Air Ventilation Test. The test was performed at linear line power loading of 0.22 kW/m and 0.36 kW/m. We used two intake air volumes, 0.5 and 1.0 cubic meter per second, for this test. We maintained the inlet air temperatures and relative humidity between 25˚C–45˚C and between 10%–50%, respectively. The calculated ventilation efficiencies, defined as the percentage of heat removed from the waste packages by the ventilating air, ranged from 80%–94%.

Acquired data from the tests was used to compare the test results with those computed using the ANSYS computer model.

Natural Convection Tests. Two tests were performed at geometric scales of 44% and 25% in comparison with the 5.5-m-diam emplacement drifts. These tests were performed to (1) evaluate the 3-D effects of distributed thermal load under postclosure unventilated conditions; (2) to assess the contribution of convection in transferring heat; and (3) to investigate the effect of scaling on heat-transfer coefficients. We used seven surrogate waste packages for these tests. We accomplished visual observations of the convection currents by injecting neutrally buoyant helium bubbles. We measured convection current velocities using an omni-directional hot-wire anemometer. We are using the acquired data as input for the FLUENT and ANSYS computer models.

Full-Scale Breached Drip-Shield and Waste Package Test. This test was performed to determine the flow of drip water into breached waste packages and the drip shield and to develop a flow-process model. We used a breach area of 0.072 m^2

(0.269 m × 0.269 m), consistent with general corrosion patches used by the total system performance analysis for the YMP, for this full-scale test.

Our current activities focus on coordinating Rock-Bolt pull tests in the Exploratory Studies Facility at ambient and elevated temperatures, and also on coordinating a Quarter-Scale Heat Dispersion Test for post-closure thermal environment.

The data collected from the Scaled EBS Testing Program has contributed to evaluating the suitability of engineered features and components to enhance the performance of the proposed repository in isolating high-level radioactive waste. ■

Fig. 2. Installing the Convection Test.

Fig. 3. The Breached Drift Shield Test.

Yucca Mountain Project Underground Field Testing Coordination

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Field testing, an important component of Yucca Mountain Project site research, is a way for scientists to test their theories in situ at analog sites in the Yucca Mountain area. Our team coordinates all underground field-testing activities within the Exploratory Studies Facility (ESF) and associated drifts, alcoves, and niches. The 7.8-km- and 2.8-km-long tunnels at the ESF include eight testing alcoves, five test niches, and various other locations within the drifts in which scientists conduct research on moisture monitoring, air permeability, liquid permeability, percolation, seepage, and rock mechanics. In addition, one alcove is dedicated to testing the changes that gas and water composition, rock mineralogy, rock mechanics, and hydrology experience during a long-term heating cycle to temperatures expected during repository operations.

Our emphasis in the past two years has been concentrated primarily on geomechanical testing, thermal testing, and flow and seepage testing in the lithophysal rock units that make up over 75% of the planned repository. Our staff is on-site at all field testing locations and is working directly with construction, engineering, and scientific staff to solve problems, ensure compliance with Integrated Safety Management principles and functions, and facilitate underground activities to ensure that the tests are conducted on schedule and within budget.

Over the past two years, underground testing has emphasized work that will be used to directly support the license application submission planned for late 2004. This work explicitly included the geotechnical rock properties testing, comprised of large-diameter core collection for lab work and large in situ slot testing for bulk modulus data (Fig. 1), conducted in the lower lithophysal unit of the repository horizon for which the data will be used in drift stability and ground-support analysis. Testing work also included the start of the four-year cooling phase of the Drift-Scale Thermal Test to support the coupled processes models, the completion of the mine-back portion of the transport tests at Busted Butte to support the unsaturated zone transport models, and the continuation of the underground cross-drift ambient hydrologic testing program to support the unsaturated zone flow and seepage models. Underground testing will continue as a performance confirmation program throughout the licensing phase and then throughout construction and waste emplacement. ■

Fig. 1. Operating a large saw in the underground to cut slots in the rib in support of the Geotechnical Rock-Properties Testing Program.

Geological Elements of the Laboratory's Seismic Hazards Program

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Los Alamos National Laboratory lies at the active western boundary of the Rio Grande rift, a major tectonic feature of the North American continent. The seismic hazards (in particular, ground motion and surface rupture) presented by the rift boundary faults could have major impacts on many of the Laboratory's existing and planned core mission-critical facilities. Thus, by quantifying the general and site-specific hazards, the Laboratory's Seismic Hazards Program plays a crucial role in design and planning for Los Alamos' national security efforts.

Our team of geologists brings a unique mix of expertise spanning structural geology, geomorphology, petrology, volcanology, pedology, and paleoseismology to bear on the seismic hazards issues. Detailed site-specific investigations of structural geology are done for existing nuclear facilities and the sites of future facilities, for evaluation of potential seismic surface rupture. For most critical facilities, we are required to identify, from natural exposures, faults with as little as 30 cm of vertical displacement in the last one million years. To achieve this, we have developed an innovative method of field-data acquisition and analysis referred to as "high-precision geologic mapping."

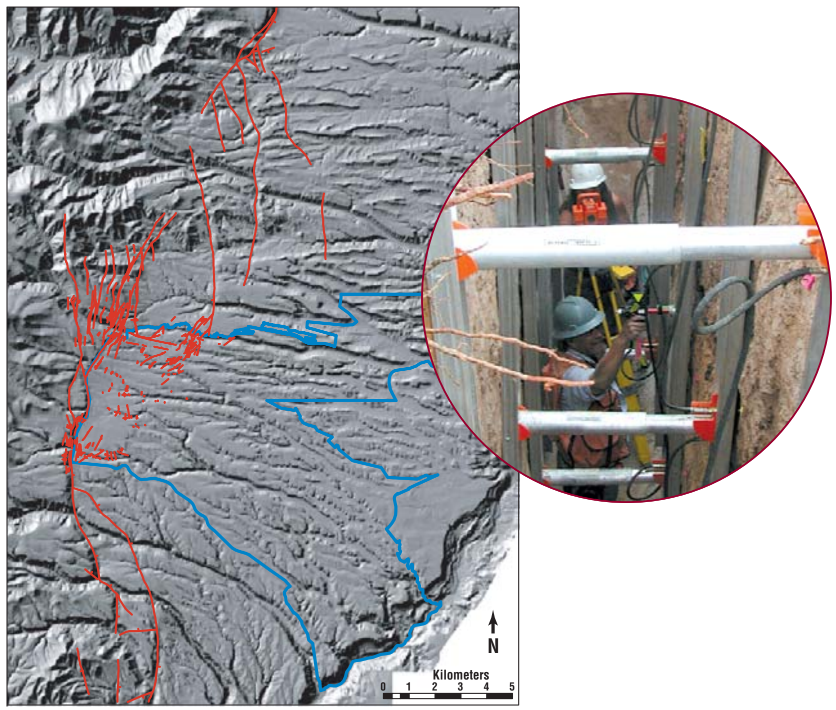

Fig. 1. Shaded relief map with detail of Rio Grande rift boundary faults (red) and outline of Los Alamos National Laboratory (blue). (Inset) Seismic Hazards Team geologists examine a fault exposed in a 5-m-deep paleoseismic trench.

We have now applied our high-precision mapping technique to about one-third of the Laboratory's area, for an unprecedented level of detail regarding the structural interactions between potentially active faults and the nature of ruptures at fault tips.

Significantly, ruptures at fault tips deviate from the predominant northern trends of the major faults and appear to pirate structural grains inherited from a period early in local rift development when the stress field was oriented differently. Additionally, detailed mapping combined with results from paleoseismic studies indicate that the major faults that form the local rift boundary are, in part, interdependent with three surface-rupturing earthquakes in the Holocene Epoch. These results indicate the short-term slip rate on these faults is about six times higher than the long-term rates, and will be used in recalculation of the probabilistic hazard. ■

A New Volcano at Yucca Mountain? What is the Risk?

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Disruptive events that could affect the Nuclear Regulatory Commission's licensing of Yucca Mountain as the nation's high-level radioactive waste repository include the probability of rising magma dikes penetrating the site and the effects of a volcanic eruption above the repository. Los Alamos volcanologists are addressing the probability of an eruption at the Yucca Mountain Project site and the physical effects of such an eruption.

Perry et al. (1998) determined that the probability of the repository being disrupted by dikes is 10^{-7} to 10^{-9} (intersections by dikes annually). New project objectives include study of the effects of rising magma intersecting the repository and of eruption processes that would scatter waste particles at the surface.

Modeling of magma that could intrude the repository under pressure is unique; parameters for these models include calculated magma properties and properties inferred from magmas erupted in the past near Yucca Mountain. The challenge is to determine if eruptions into the drifts would be explosive (pyroclastic) or passive (lava flows), and also to determine the corrosive effects of volcanic gases on waste containers. An existing multifluid, multiphase computational code is being qualified and will be used to analyze such eruptions.

Fig. 1. The Lathrop Wells volcano, viewed from the south. Los Alamos scientists are studying this 75,000-year-old scoria cone as an analog "Yucca Mountain volcano." Analysis of the cone and its surrounding tephra fall blanket supplies information needed to understand eruption processes and the depths of a conduit formation that would affect an underlying repository.

If a dike continues to rise above the repository and erupts at the surface, the percentage of waste particles in ash fall and lava flows must be modeled. We can glean information about eruption processes from the nearby 75,000-year-old Lathrop Wells cone. The eruption history is determined through the study of the cone and surrounding tephra sequences. Changes in particle types within tephra deposits provide an eruption history for the Lathrop Wells cone. Pyroclast characterization and inferred history are largely based on comparison with tephras from observed eruptions (Heiken and Wohletz, 1985).

To determine posteruption ash redistribution by erosion, two methods of study are used: (1) analysis of the percentage of ash per sediment volume in samples collected along the first-order channels north of the Lathrop Wells cone; and (2) measurements of bomb-pulse cesium-137 to evaluate erosion and deposition along the Fortymile Wash alluvial fan and beyond the mouth of the fan. Measurements at many sites across the fan should permit the creation of an erosion-and-accretion contour map of the fan for the last 50 years and an evaluation of exposure risk to the public and the environment. ■

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Environmental Investigations in Canyons at Los Alamos

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Radionuclides and other contaminants have been discharged into canyons at Los Alamos since World War II as a result of various research and processing activities. Once in the environment, they largely adsorb onto sediment particles, where they are subject to redistribution by floods, although some (e.g., tritium) remain in an aqueous phase and some (e.g., strontium-90) can be associated with either solid or liquid phases. Since 1995, EES Division scientists in collaboration with other divisions at Los Alamos, private companies, and universities have developed and applied a science-based approach for understanding the current distribution of contaminants in canyons at Los Alamos, the potential risk to human health or ecosystems, and the effects of future contaminant redistribution. This work is, in turn, used to guide remedial actions where deemed appropriate.

Recent progress includes

- Publishing a probabilistic model for the fate of sediment and associated pollutants in fluvial systems (Malmon et al., 2002). This model goes beyond traditional approaches to sediment transport that focus on in-channel processes and tackles the critical problem of interchanges between channels and floodplains, and the fate of individual particles. An initial application of this model to Los Alamos Canyon is shown in Fig. 1, and indicates that 92% of the cesium-137 that entered the canyon from outfalls has already left the site or decayed radioactively, and that 50% of the remaining cesium-137 will decay before being transported off-site.

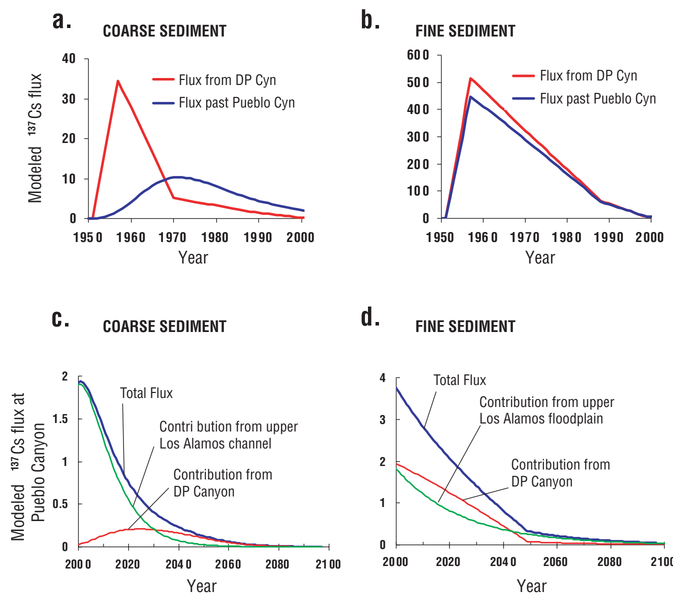

Fig. 1. ***(a, b)*** *Estimated cesium-137 fluxes (mCi/yr) into upper Los Alamos Canyon study reach from DP Canyon and modeled cesium-137 fluxes out of the study reach past Pueblo Canyon, 1950–2000. Flux is much higher and faster for fine sediment (b) than for coarse sediment (a).* ***(c, d)*** *Modeled future fluxes of cesium-137 at the confluence with Pueblo Canyon, showing relative importance over time of new sediment from DP Canyon (red) and remobilization of sediment currently present in Los Alamos Canyon (green). Model predictions are shown for coarse sediment fraction (c) and fine sediment (d).*

- Evaluation of plutonium transport in Pueblo Canyon. The upper Pueblo Canyon watershed was severely burned during the Cerro Grande fire, resulting in an increase in flood magnitude and frequency, and resultant transport of sediment and associated contaminants. We are sampling and analyzing storm water at a series of stations and using that data in combination with analyses of associated flood deposits to provide an improved understanding of the dynamics of plutonium transport in this system. ■

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Advanced Geographic Information System Capabilities in Support of EES

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The Geographic Information System Laboratory (GISLab) at Los Alamos is dedicated to excellence in Geographical Information System (GIS) science and technology. GISLab's mission is threefold: (1) to provide intellectual leadership concerning GIS science and technology; (2) to conduct basic and applied GIS research; and (3) to provide GIS services for Laboratory projects and operations. The GISLab staff consists of a team of highly skilled, multidisciplinary scientists and professionals knowledgeable in GIS technology, environmental and life sciences, geology, modeling, information science, project management, and emergency planning. The team brings more than 60 combined years of high-level GIS expertise to Los Alamos' most sophisticated GIS capabilities—cutting-edge enterprise GIS technologies for data warehousing and delivery, 3-D modeling and visualization, and rapid development and support of custom GIS applications.

Major Projects

Cerro Grande Rehabilitation Project (CGRP) GIS—A spatial data clearinghouse for institutional and fire-related datasets.

Environmental Systems Research Institute (ESRI) Partnership—3-D GIS, Earth system modeling, and GIS tools.

Fig. 1. The CGRP GIS provides Web-based access to geospatial data for the May 2000 Cerro Grande fire.

Environmental Restoration (ER) GIS Project—Spatial information management, analysis, and mapping support; management of ER spatial database.

University of California at Santa Barbara (UCSB) Cooperative Agreement Project—"Influences of topography and plant canopies on surface climate variability" (with Jeff Dozier, UCSB).

Other Projects—3-D modeling and visualization of contaminant transport; Laboratory floodplain mapping and hydrological modeling, demography, and air quality; Yucca Mountain Project GIS support; Laboratory infrastructure security.

GIS Services

GISLab offers a full suite of GIS services and consultation in support of Laboratory projects and operations, including cartography (hard copy and Internet), data service through Software Development Environment and Oracle, custom GIS applications, global positioning system mapping, spatial and numerical modeling, Internet GIS, and consultation on spatial information management and GIS technology. By the end of 2002, GISLab had produced more than 11,000 original maps and more than 31,000 map copies for customers within and outside the Laboratory.

Honors and Awards

GISLab and colleagues received the ESRI Special Achievement in GIS Award in recognition of work on the CGRP GIS. ■

For more information about GISLab and the CGRP GIS see http://gislab.lanl.gov *and* http://cgrp-gis.lanl.gov.

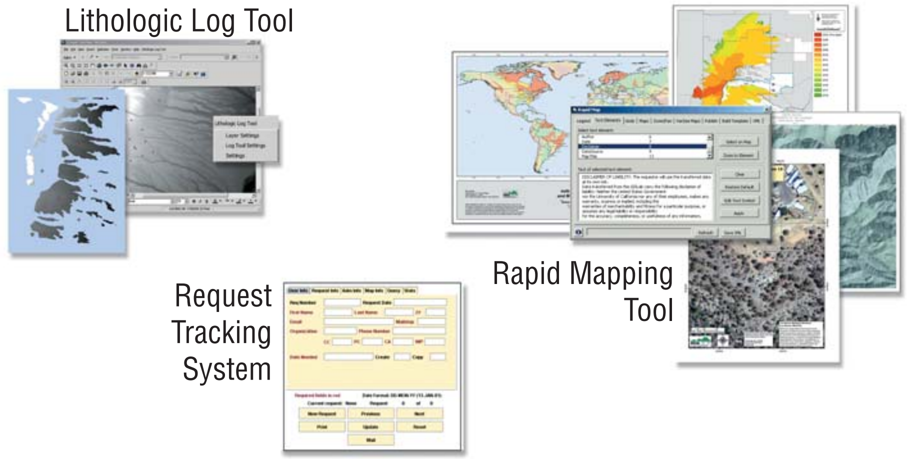

Fig. 2. Custom GIS tools enable rapid completion of complex tasks.

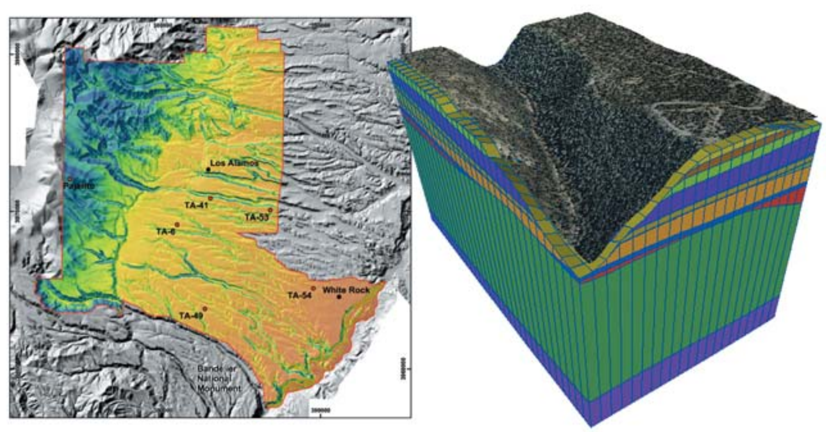

Fig. 3. GIS-based models of evapotranspiration (left) and subsurface geology (right).

Microhole Drilling and Instrumentation Technology

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EES-11, with the support of American industry and the DOE Natural Gas and Oil Recovery Partnership Program, has undertaken an integrated program of development to show that the cost of obtaining subsurface information can be substantially reduced through microhole technologies specifically developed to obtain that information. Collectively termed "Microhole Drilling and Instrumentation Technology," the program objectives include

- Drilling shallow microholes using currently available coiled-tubing technology.
- Evaluating the feasibility of drilling deep microholes.
- Miniaturization and testing of bottomhole drilling assemblies.
- Miniaturization of geophysical well-logging tools.
- Incorporating emerging miniature-sensor technologies into borehole seismic instrumentation packages.

Microhole technology development is based on the premise that because of the historic advances in electronics and sensors, conventional-diameter wells are no longer necessary for obtaining subsurface information. Thus, the combination of deep microholes having diameters at their terminal depth ranging from 1¼ to 2⅜ inches, and logging tools having a ⅞-inch diameter will comprise a very low-cost alternative to currently available technology for exploration and reservoir characterization. Microhole technology has the potential to revolutionize the economics of accessing the subsurface as well as improving the quality and quantity of subsurface information available for energy, environmental, and national security programs.

Fig. 1. Microhole coiled-tubing drilling rig (tan) capable of drilling 1¾- and 2⅜-inch microholes to 800 feet, and the flatbed-mounted mud-conditioning system (blue) supporting drilling operations at San Ysidro, NM.

Progress during the past year includes the following:

- Field trials and component tests continue to explore the extent to which current technology can be miniaturized to drill 5,000-ft. microholes. The result of this work has been integrated into a roadmap describing the current capabilities, technical challenges, and developments needed to drill and complete the 5,000 ft. microholes. With proper preparation we believe that the 5,000 ft. microhole is achievable by shrinking and adapting existing drilling equipment and well construction technology to operate in a smaller bore. It is believed that breakthrough technology will not be required. The roadmap is available on request.
- In collaboration with the logging industry, EES-11 has identified a suite of ⅞-inch state-of-the-art exploration logging tools that could be manufactured with existing engineering methods. These include gamma, density, porosity, acoustic, and high-frequency induction tools. We have built a wellbore-deviation survey tool and successfully tested it in a microhole at our San Ysidro test site.
- The performance of the coiled-tubing drilling system was improved by a redesign and overhaul of the mud-conditioning system. The previous system was doing a poor job of cleaning fines

from the mud, and, as a consequence, pump seals were washing out at unacceptably high rates. We increased our understanding of how to cement, rather than just to grout, PVC microhole casing.

- We continue to fabricate and test microhole seismic-instrumentation. Our industrial collaborators continue to make prototype microsensors available to us for comparative testing in microholes. We design and fabricate the electronics and environmental protection necessary for borehole deployment of these sensors. Then, through field testing, we compare the performance of the prototypes with conventional sensors and make these results available publicly. In the past several months, we have received from our collaborators an advanced miniature piezoelectric sensor and a hybrid microelectromechanical system device for testing. These sensors will be evaluated for use in our microgeophone tool as a potential replacement for the more expensive and complicated microgeophone that was originally demonstrated in the tool.

We investigated the feasibility of shallow oil production through microholes and of coal-bed methane production from microholes. Our investigations of coal-bed methane production resulted in a report and paper presented at the International Energy Agency's 22nd Annual Workshop and Symposium on Enhanced Oil Recovery, held September 9–12, 2001, in Vienna, Austria, and our work in shallow oil production through microholes resulted in a full demonstration proposal to DOE. We are preparing a related document, "Road Map for a 5,000-ft. Microborehole," for posting on the DOE National Transuranic Waste Program Office's Web site. ■

Subcritical Experiment Containment

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The Subcritical Program consists of dynamic zero-yield experimentation that supports the Stockpile Stewardship Program by assessing the effects of aging of nuclear weapons components and providing parameters to model the performance of weapons in our enduring stockpile. Components of the Subcritical Program necessarily involve the use of special nuclear materials (SNM) and their exposure to high explosives (HE) in the dynamic part of the experiment. As a result, the issue of safe containment of the SNM within the boundaries of the experiment is a problem of special concern.

Since 1995, Lawrence Livermore and Los Alamos national laboratories have used two basic underground experiment designs in their respective subcritical programs. The first designs involved mining a large alcove within the U1A complex, the tunnel complex at the Nevada Test Site (NTS) where subcritical tests are conducted. Within this alcove or room, the SNM and HE are placed in a subcritical assembly experiment package along with diagnostic equipment. These room experiments have a two- or three-vessel concept of containment. The first vessel barrier consists of a steel bulkhead and concrete keyway into walls of the drift. All cable and conduit penetrations into the working point side of the experiment must pass through the steel bulkhead. Features of the barrier include discrete gas blocks and gas-tight welding. It is the job of the containment scientist to model the predicted overpressures, assist in the design, and approve the as-built experiment before submission to the Containment Review Panel (CRP) to obtain detonation authority.

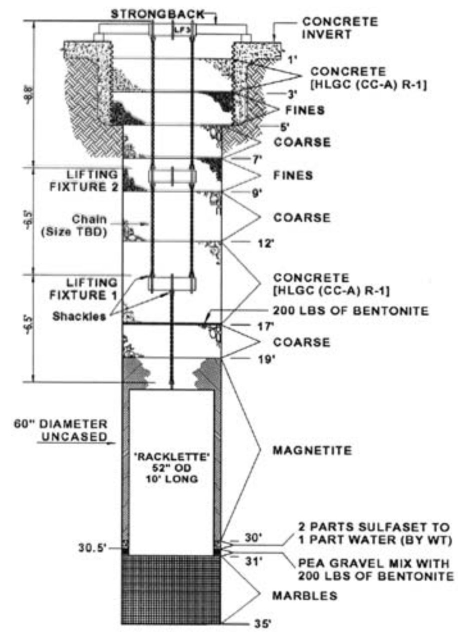

Fig. 1. (Above) A downgraded image of the racklette subcritical assembly. (Right) The stemming plan for the racklette below the invert of U1A (Mario and Rocco CRP).

A second experimental design by Los Alamos has proved to be very cost- and space-efficient. It involves a design reminiscent of full-scale nuclear testing. The experiment package and diagnostics are placed in a small-scale version of the original nuclear test racks (“racklettes”) and stemmed below the floor of U1A (see Fig. 1).

Again, as in the room experiments, the EES-11 Containment Team is responsible for designing and approving the stemming plan before presentation to the CRP.

The continuation of the Laboratory’s commitment to the containment of SNM in the subcritical experiments is now being exercised for larger-scale subcritical tests, some of which will be performed in full-scale nuclear emplacement holes at NTS. These full-scale subcritical tests require new stemming designs, as well as modeling and diagnostic capabilities never before employed.

Additionally, the containment program is playing a fundamental role in the United States’ posture for enhanced test readiness in the event that full-scale nuclear testing is resumed. Current US proposals are for a test readiness of less than 18 months should a national need arise. ■

Seismic Imaging

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Discerning the structure and properties of Earth's subsurface are the primary goals of seismic imaging. Because Earth's structure and properties are highly variable, seismic waves are bent and distorted as they travel between sources and receivers. Properly correcting for that bending and distortion to produce an accurate image can be extremely difficult, especially in 3-D. This project focuses on two topics in seismic imaging. The first is developing new methods for seismic reflection imaging, which is the most commonly used tool for oil and gas exploration. The second is developing new techniques for passive seismic imaging, which is a nontraditional approach to imaging that uses small earthquakes generated by fluid injections as seismic sources.

This work exploits expertise in seismology and seismic wave propagation to solve problems of particular relevance to finding and developing new fossil fuel resources. Results of the project can as well be used to solve problems related to homeland and national security. This work advances the Laboratory's mission of solving national problems in energy, environment, infrastructure, and health security. The project also supports the EES Division mission of using division capabilities in Earth and environmental sciences and engineering to provide solutions to complex problems of importance in the environment, energy, and national security. Although the new techniques are being developed for use by the oil industry, they are relevant to other fields such as nondestructive testing and medical imaging.

The two basic methods for seismic reflection imaging are called "ray-based" and "wave-based" methods. Ray-based methods rely on the simplifying assumption that seismic energy travels along individual rays, which are relatively simple to work with. Wave-based methods assume that seismic energy travels as waves that can undergo complex interactions and interference from other waves. Ray-based imaging methods are conceptually simple and computationally fast, and are routinely used by the oil industry. Wave-based methods are more complicated and require much more computing, but can provide more accurate images from geologically complicated areas. Accurate images are critically important because they play a key role in deciding where to drill wells that may cost tens of millions of dollars each. Laboratory researchers are developing new wave-based and ray-based techniques for seismic reflection imaging.

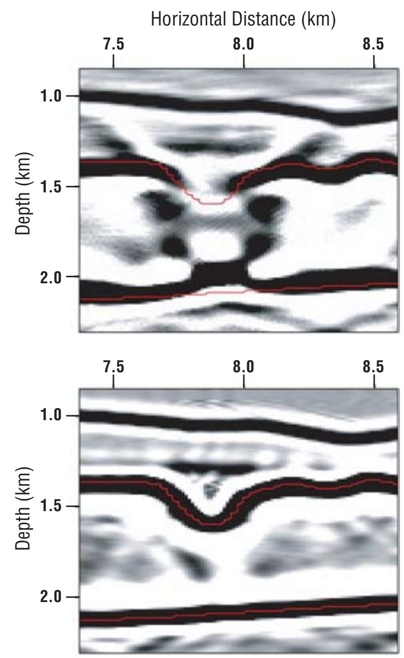

Fig. 1. Seismic images from a conventional ray-based imaging method (Fig. 1A, top), and from a new wave-based imaging method (Fig. 1B, bottom). These images are from an artificial test data set, thus the true structure is known. Thin red lines indicate the correct positions of two boundaries in the model.

We have also developed a new wave-based imaging method that is about as fast as ray-based imaging methods but produces more accurate subsurface images. Figure 1B shows an image from the new wave-based method. The thin red line shows the actual position of two boundaries in the test structure. These correspond to the top and bottom of a salt body and are difficult to image properly because of the large difference in seismic velocities between the salt and adjacent sediments. Note that the image derived from the wave-based imaging method accurately shows the shapes and positions of the two boundaries. In comparison, the image from a conventional ray-based imaging method shows the top boundary as having a gap rather than being continuous, and introduces imaging artifacts in the form of two dark lobes just below and on each side of the gap. It further distorts the bottom boundary, showing it as bending upward just below the gap.

Ray-based imaging methods are commonly used by industry because they are fast. Recognizing the limitations of the conventional ray-based imaging methods (Fig. 1A), the project is developing new ray-based imaging methods that should be able to produce images similar to the high-quality images from wave-based methods such as appear in Fig. 1B. The ray-based methods that the oil industry routinely uses include only the first-arriving seismic energy, which is sometimes very small in size. Our new ray-based imaging method takes advantage of multiple seismic arrivals to increase the accuracy of the image as well as to better image small structures. In addition, the method optimizes the contributions made by each arrival to form the final image. This optimization results in better continuity of individual geological features in the final image and helps reduce artifacts caused by seismic energy that is not properly imaged.

The second topic of this project, passive seismic imaging, uses the small earthquakes that accompany fluid injections as seismic sources to obtain images of the subsurface near the injection borehole. The most time-consuming step in imaging using these earthquakes is picking arrival times for them. This selection is tedious, yet it is crucial for the accuracy of the resulting images. By developing new analysis techniques that are fast, precise, highly automated, and require a minimum of experienced judgment, the techniques can be used routinely. We applied our new method for passive seismic imaging to earthquakes induced by fluid injection into a gas reservoir. The method provided a fourfold improvement in locational precision when compared to locations obtained with a conventional method.

The references listed are representative of the research on seismic imaging methods developed by this project. ■

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Nonlinear Elastic Waves in Geomaterials

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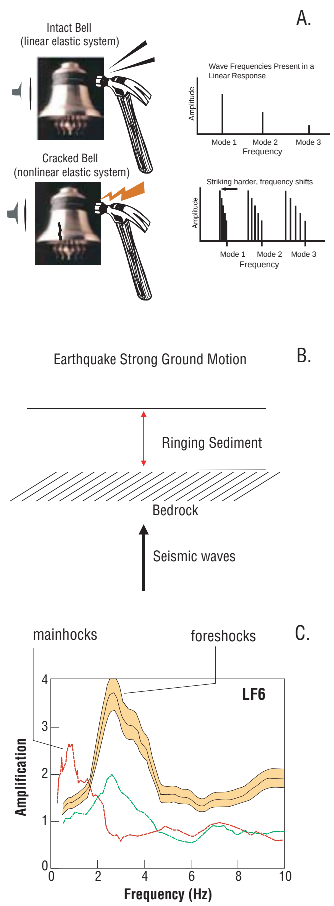
Increasingly rapid progress is being made in the field of dynamic nonlinear elasticity of earth materials. Approximately 15 years ago, three groups of scientists (at Los Alamos, the Institute of Applied Physics in Russia, and the Institute of Physics of the Earth in Russia) independently initiated this research field. Today, dynamic nonlinear elasticity of earth materials is well recognized in the domains of geophysics, materials science, and strong ground motion, and ever-increasing numbers of researchers are working in this area.

Rocks display unique elastic behavior. They are extremely nonlinear, hysteretic, possess discrete memory, and have slow dynamics (a long-term memory of strain). Although some of these types of nonlinearities may exist in other materials (for example, powdered metals), it is in rocks that these characteristics were first observed and are easiest to observe. It is now clear that rocks are part of a larger class of materials all of which exhibit the same type of nonlinear behavior. The class of materials includes rock, damaged solids, and



Seismic Wave Spectra from the 1994 Northridge California Earthquake

Fig. 1. Strike a bell and it rings at its modes. A, at top right, represents the frequencies of the modes that are ringing (known as a frequency spectrum). Strike the bell harder and it rings louder—that is all. But if the bell is cracked (bottom left of A), something very different happens. Strike the bell softly and it rings at its modes as usual. But striking it progressively harder, we find that the frequency shifts downward for all of the modes, as seen in the frequency spectrum at the bottom right.

A sediment layer at the Earth's surface can ring like a bell when seismic waves from an earthquake strike it. In B, the first mode of the layer is shown in the spectral plot for several small earthquakes ("foreshocks") that took place before the main earthquake in 1994 in Northridge, CA.

The main shock frequency shifts downward, just like the cracked bell, as shown in C. This is a nonlinear effect. If a building constructed on this layer has the same mode as the large earthquake, it could lead to catastrophic failure of the structure. On the other hand, if we predict the layer-ringing modes and the shift, we can construct a building that rings safely outside the modes of the layer. This same concept of following a downshift in frequency can be used to infer whether an automotive or weaponry part is damaged.

compressed or powdered metals like those used for the brakes on an automobile. We are finding other members of this class as we study additional materials. Furthermore, nonlinear behavior is beginning to play a central role in developing new methods with which to characterize material properties. Some of these new approaches include learning the elastic microstructure of rock, determining if a material is damaged, or monitoring progressive damage. Moreover, nonlinear attributes of rock have important consequences for processes in the Earth such as earthquake strong ground motion, stimulation of fluid flow in porous media (for example, enhanced oil production), seismic wave propagation and attenuation, stress fatigue damage of weapons and industrial components, hydraulic fracturing, and others.

Our work involves developing a comprehensive theoretical and experimental framework that (1) employs static and dynamic laboratory investigation of materials to provide a macroscopic and microscopic description of the elastic state, and (2) provides for turning the microscopic description into a prescription for material properties that can be used to predict change in stress states either static or dynamic.

This work has direct application to the Laboratory's mission in nuclear weapons and stockpile stewardship and also contributes to world-class basic science. This work is related to the EES Division's capabilities in geomaterials, geophysics, and national security science and technology.

We have made significant progress in our applications to the Nuclear Weapons Stockpile Stewardship Program. In addition, our work has progressed significantly toward developing nonlinear imaging as well as toward industrial applications. Furthermore, industrial applications for testing samples during the manufacturing process are underway in Europe. Two small companies, one based in Europe and one in the US, are marketing different aspects of this technology that were developed by Los Alamos and collaborators. In addition to publications, a patent was awarded (P.A. Johnson, K. Van Den Abeele, J. TenCate, and R. Guyer, *Resonant Nonlinear Ultrasound Spectroscopy,* US Patent no. 6,330,827, Dec. 18, 2001). We have published more than 10 peer-reviewed publications. ■

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Regional Location Calibration in Asia

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Los Alamos geophysicists and their colleagues are currently engaged in an effort to improve seismic-event location across the Asian continent. In this report we discuss a selection of issues that bear on the achievement of our goal. Recent developments are presented in the establishment of ground truth by satellite synthetic aperture radar (SAR), and the building and application of unified velocity models. We describe work on newly available Makanchi seismic detector array (MKAR) data as an example. Our location calibration research supports EES Division capabilities in the areas of computation science, geomaterials, geophysics and seismology, national security technology, and more.

Interferometric synthetic aperture radar (InSAR) holds the potential to provide ground truth in seismic areas that are difficult to reach. Limitations include the cost of event satellite image pairs, and the sparse distribution of download stations. In designing the analyses, we may compile theoretical elastic displacement amplitudes for different fault types and depths. We can then undertake to predict detectable earthquakes suitable for InSAR. Some sample processing is illustrated in Fig. 1.

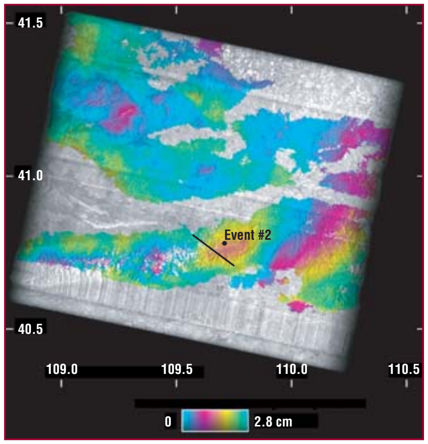

Fig. 1. Three earthquakes were selected with magnitudes lying roughly between M_b5 and M_b6. We retrieved image pairs for each. Problems with decorrelation affected several analyses, but the example shown here represents a success.

Computational models serve several functions in our calibration effort. Most importantly, we can use them to predict travel-time residuals in aseismic regions. They also offer validation of residual surfaces through forward simulation. Components of our program include literature searches for previous studies; the writing of code that pulls together unified representations from a variety of information types; forward modeling of 1-, 2-, and 3-D geophysical models using ray theory, global search, and finite difference algorithms; building kriged travel-time corrections on top of the best-fitting models for different regions; and, ultimately, seismic event relocation. We have developed Litho3D as a code for building 3-D velocity models. Litho3D assumes hard surfaces between which a series of layers is interpolated that conforms to the bounding hard materials. Velocity models of any dimension are then read in and interpolated to form a single unified crustal structure. We have also developed several codes for calculating and visualizing travel times. All function in spherical or Cartesian coordinates.

Data from the primary international monitoring station MKAR have recently become reliable and available. To perform a calibration for this set of sensors, we undertook a literature search of existing velocity models for regional distances from the array. Approximately 30 models were gathered and tested against data for different geophysical provinces. In addition to travel-time calibration, we will also consider calibrating MKAR for azimuth and slowness. To that end, we have created a pseudo-FK algorithm, a frequency domain beamformer with interpolation between beams and with precise estimates of azimuth and slowness errors based on fitting an ellipse to the half-maximum contour. ■

Evaluation of Monitoring Technologies for Nuclear Testing

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With an extensive background in monitoring and verification of nuclear weapons treaties, DOE and its laboratories look to the future of potential, unilateral, bilateral, and multilateral agreements and treaties concerning site-specific monitoring of nuclear tests (called nuclear testing limitations within DOE/NA-241). In order to make this monitoring and verification experience useful for future application, it is necessary to critically assess monitoring technologies from the standpoint of their designed capabilities and relevance to specific objectives of potential applications. Accordingly, we have taken stock of these technologies and considered their basic characteristics, historical applications, and strengths and weaknesses in order to make a useful evaluation. The approach we use for this evaluation consists of a matrix that compares technologies on the basis of a number of criteria known to be important in treaty negotiations.

Monitoring technologies are many and varied, but among these technologies is a subset that has both a direct application to nuclear testing and a precedent. Four general groups of monitoring technologies have played a role in nuclear test-site monitoring (TSM) treaties and agreements involving the DOE. They are (1) geophysical, (2) ground-based visual, (3) overflight, and (4) radiological.

Fig. 1. Aerial view of the U1A test facility at the Nevada Test Site. An evaluation of surface visual technologies notes a low detection sensitivity (unlikely to see features produced by a underground, low-yield, or subcritical test) and a very high discrimination threshold (difficult to discriminate significance of signals if monitored). Whereas surface visual technologies are given a low priority, subsurface technologies are highly desirable for monitoring this test environment.

Geophysical technologies involve the use of sensors designed to detect signals associated with the detonation of explosives and to provide data to identify and characterize residual phenomenological signatures of explosions.

Ground-based visual technologies primarily involve mapping to graphically document spatial data concerning location, dimensions, and characteristics of visible geological, cultural, and environmental features. Mapping also provides a basis for determining geophysical and radiological sensor emplacement, and data acquisition and interpretation.

Overflight technologies involve site-specific aerial observations and imaging, Open Skies Treaty overflights, and commercial satellite imagery.

Radiological technologies involve direct measurements and sample analysis to detect and characterize nuclear events. Samples may be acquired by collection of material transported in the atmosphere and by environmental sampling.

In summary, these technologies can monitor a very wide range of phenomena associated with activities at nuclear test sites. Some of these signals can be definitive on their own, but others are important to a synergistic analysis of an ensemble of different signals.

Monitoring technologies have strengths and weaknesses related to the monitoring objectives and the circumstance under which they are implemented (Fig. 1). Accordingly, we developed evaluation criteria that we based upon an extensive review of issues that have received specific attention during implementation considerations and treaty-related negotiations, and, thus, have precedence. We considered a large number of viable evaluation criteria. The chosen criteria are intended to capture the critical concerns in determining the desirability of a potential monitoring technology.

Although the future will bring new technologies that bear upon nuclear test monitoring, we wish to apply our experience from past nuclear explosion monitoring efforts to define the general technologies and equipment used for nuclear test monitoring. In doing so, we now have a distillation of our experience that reflects not only our point of view regarding relevance, feasibility, and applicability, but also what we have learned from the opinions expressed by experts from other countries.

Following the completion of the initial report that describes the technology evaluation process and includes an example scenario, reports will be prepared for a number of additional scenarios. Table-top and field exercises will be employed to further refine the process and provide insights useful in technology evaluations. ■

Plutonium-239 in Synthetic Brines After Equilibration with Magnesium Oxide Backfill

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The EES-12 Group is currently engaged in an effort to better understand the role of backfill materials in geologic repositories of radioactive waste. A significant criterion in evaluating disposal strategies for radioactive waste is the assessment of the isolation capacity for the most radiotoxic radionuclides, the actinides.

For some radioactive waste destined for disposal in geological salt deposits, MgO is being used as a reactive backfill material. This material is ideal for buffering the pH of the repository to between 8.5 and 10, and for sorbing carbon dioxide and water, conditions that are favorable for stabilizing plutonium in the repository. Plutonium can exist in more oxidation states in the environment than any other element. The oxidation state, which can be thought of as the excess charge on the central atom, for plutonium can be III, IV, V, or VI under many conditions in nature. Generally, the higher the oxidation state, the more mobile the element.

We conducted equilibration experiments at MgO-to-water ratios of 1:0.15, 1:0.25, and 1:10. We determined the release of plutonium from plutonium-loaded MgO agglomerates in the presence and absence of hypochlorite (OCl^-) under agitated and nonagitated conditions. After the Pu(VI)-brines were equilibrated with MgO backfill for 68 days, the solution pH and alkalinity changed dramatically, while approximately 99%–100% of the introduced Pu(VI) was removed from the brines. Under agitated conditions, the release rate of plutonium from the plutonium-loaded MgO agglomerates followed the order of MgO-Brine G > MgO-Brine E > MgO-NaCl > MgO-$MgCl_2 \cdot 6H_2O$. Under nonagitated conditions, a small amount of plutonium was released from the plutonium-loaded MgO-Brine G agglomerates after 110 days, but there was no plutonium released from the plutonium-loaded MgO-Brine E agglomerates (Fig. 1).

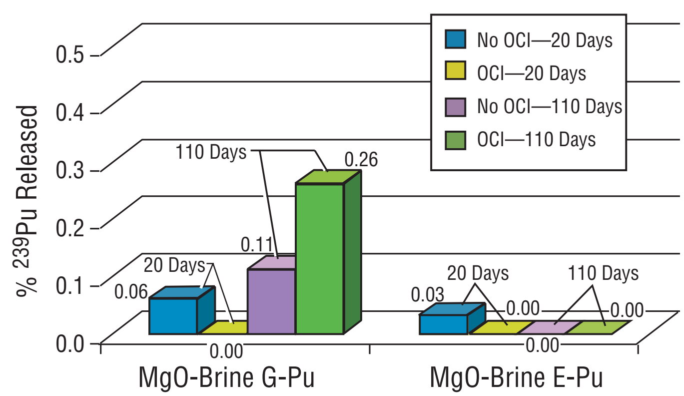

Fig. 1. Desorption of plutonium-239 from plutonium-loaded MgO Brine E and Brine G agglomerates under nonagitated conditions.

X-ray absorption spectroscopy (XAS) results for the plutonium-loaded MgO-agglomerates indicated that plutonium was incorporated by precipitation, and the oxidation state of plutonium was primarily Pu(IV). Separate experiments in these brines with pH adjustment without MgO indicated that pH change alone could not account for the removal of plutonium from Brine G solutions, but pH change alone could account for the removal of plutonium from Brine E solutions.

Therefore, in NaCl brines, the buffering capability of the MgO backfill alone may be adequate to completely retard plutonium migration, but in MgCl brines, the backfill is performing a sorptive function in addition to simple pH buffering that enhances its ability to retard plutonium migration. ■

Irradiation of $MgCl_2 \cdot 6H_2O$ Applying Beam-Line Experiments

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Los Alamos geochemists are currently engaged in an effort to better understand the disposal of radioactive waste in deep geologic repositories, and, in particular, the effects of radiation from the waste on the brines in bedded salt formations used to dispose of transuranic waste. In the event of inundation of a nuclear waste repository located in a deep geological salt formation, chloride brines could contact waste and be exposed to radiation from the waste. Ionizing radiation affects the chemistry of aqueous solutions through the generation of free radical, ionic, and molecular products such as hypochlorite (OCl^-) and hypochlorous acid (HOCl), which are similar to the constituents of chlorine that are effective in backyard pools. In the absence of reductants, hypochlorite could cause a high redox potential in the brine, which may accelerate the dissolution of waste forms and oxidize actinides to their more mobile forms. Therefore, the effects of radiolysis on high-saline-content brine are of particular interest because the presence of oxochlorides could influence the stability of plutonium waste forms.

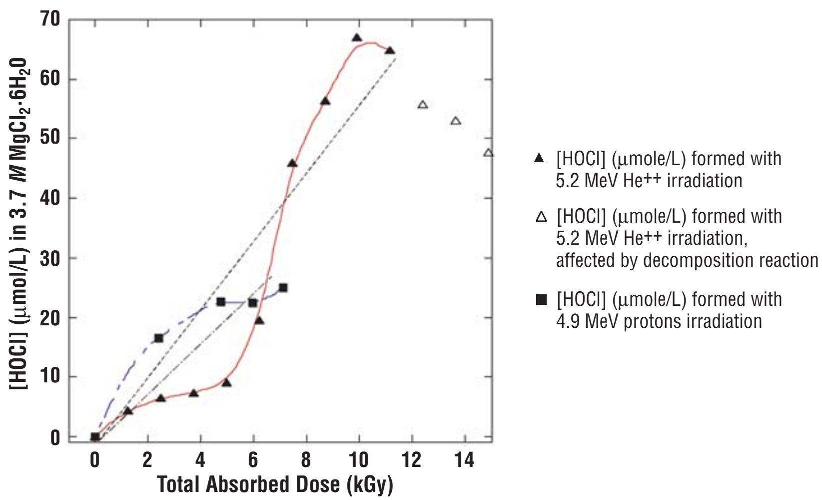

Fig. 1. Proton- and helium-ion irradiation-induced hypochlorous acid formation as a function of total dose absorbed while irradiating 20 mL of 3.7 M $MgCl_2 \cdot 6H_2O$ with 4.9-MeV proton ions or 5.2-MeV He^{++} ions. The straight lines represent linear regressions (straight-line averages) of the data.

We are using a novel approach to quantify the generation of these radiolysis byproducts by irradiating brine solution with a 4.9-MeV proton source. The vastly increased dose rates available in such a procedure allow exposure to high doses in a convenient time scale, and, therefore, the investigation of the radiation-induced formation rates of α-radiolysis byproducts as a first step in assessing long-term, steady-state repository conditions. As an example, the measured G (Generation) values for HOCl formation in 3.7 *M* $MgCl_2 \cdot 6H_2O$, pH 4.42, irradiated by 5-MeV helium ions is determined to be 0.0536 ± 0.0049.

To simulate the effects of plutonium self-irradiation on repository-related chloride solutions, we irradiated 3.7 *M* $MgCl_2 \cdot 6H_2O$ solution with 5.2-MeV He^{++} ions in incremental steps of 1.2 kGy to reach a final absorbed irradiation dose of 14.87 kGy. Irradiation of liquid targets used an accelerated beam of He^{++} ions passing through a 10-µm-thick window of Havar® foil and a 8-µm window of Kapton® foil within a small sample chamber that was isolated from the main vacuum chamber of the ion beam by means of the foil windows. To monitor the formation of HOCl, we took a UV-Vis absorption spectrum after each irradiation step. We observed at 256 nm the formation of ClO_2^- as an intermediate species for both irradiation sources—4.9-MeV protons and 5.2-MeV He^{++} ions. The concentration of chlorite ion was in the micromolar concentration range.

After we introduced 4 kGy with 5.2-MeV He^{++} ion source, the chlorite species disappeared in favor of HOCl formation. This was evidenced by a peak spectrum at 232 nm, which we confirmed in parallel experiments by adding hypochlorous acid to a 3.7 *M* $MgCl_2 \cdot 6H_2O$ solution. The buildup of HOCl was not directly proportional to the dose (Fig. 1) but shows an alternation overlying an overall linear growth. The highest HOCl concentration formed after we introduced a 9.91 kGy dose in a 3.7 *M* $MgCl_2 \cdot 6H_2O$ solution with 5.2-MeV helium ions was 67.4-µmol HOCl, based on a molar extinction coefficient of 13044 $Lmol^{-1}cm^{-1}$ at 232 nm. ■

Synchrotron X-Ray Absorption Spectroscopy Applications in Actinide Molecular Environmental Science

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The EES-12 Group is investigating the effects of iron and other metals contained in radioactive waste on the chemistry of plutonium and other constituents in geologic repositories in salt formations. In order to characterize the speciation, structure, and spatial distribution of these constituents in solid and liquid phases, we are using synchrotron-based characterization methods that have been applied increasingly over the past several years to study fundamental issues in actinide science. Our study concerns the reduction of pertechnetate by metallic iron, and the reduction of Pu(VI) by metallic iron and aluminum in the presence of NaClO in brines. These examples give insight into the reaction mechanisms between radionuclides and metallic iron and aluminum. Our results demonstrate the capabilities and opportunities that x-ray absorption fine-structure (XAFS) spectroscopy provides for the investigation of chemical speciation and structure of actinides in real environmental systems down to the molecular level.

XAFS spectroscopy is one of the most incisive means for determining element-specific local structure and chemical speciation in both pure and complicated samples. XAFS uses the high-intensity, polychromatic x-ray beam available at synchrotron light sources. By scanning through and beyond an absorption edge of the target element, XAFS can identify an element's valence and the average types of, numbers of, and distances to, the shells of neighbor atoms, with an accuracy of Z±2–4, N±15–30%, and R±0.01–0.04 Å. The sensitivity to changes in these values is significantly better. These parameters define the chemical speciation of the element, which, in turn, controls the solubility, reactivity, and other characteristics that are critical to understanding and predicting the degree of hazard and the environmental impact. Plutonium spectra can be measured even down to the 1 ppm level without special sample preparation.

We have used XAFS to characterize the plutonium speciation in solids precipitated from WIPP brines by the

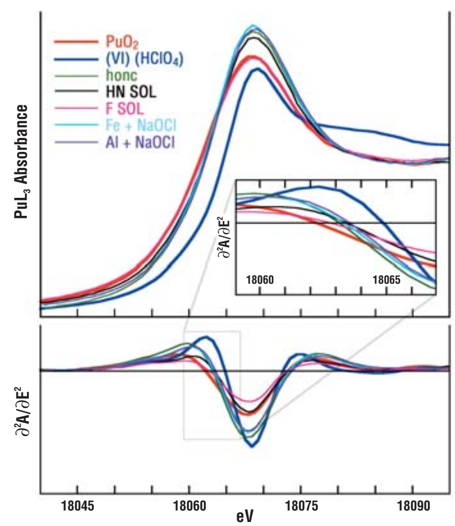

Fig. 1. X-ray absorption near-edge spectroscopy of Pu(IV) oxyhydroxide compounds (top, normalized absorbance; bottom, second derivative; inset, expanded zeros of second derivative). Honc, HN Sol, and F Sol were prepared by hydrolysis, the last two by reduction of Pu(VI) with iron and aluminum metals in WIPP brines, indicating that reduction of plutonium can occur in the repository.

heterogeneous reduction of Pu(VI) with iron and aluminum in the presence and absence of hypochlorite, a redox-active radiolysis product (Fig. 1). The plutonium in these materials displays several similarities to oxyhydroxides prepared by more conventional methods. It is predominantly Pu(IV); there are several distinct O shells with Pu-O distances ranging from 1.8–3.6 Å; the plutonium is found in only a single, disordered shell with a Pu-Pu distance very close to that of PuO_2; and there are often very short Pu-O distances that are consistent with a fraction of the plutonium being present as Pu(V). There are, however, also differences from other colloids. The number of plutonium atoms is often significantly reduced, and the primary O shell centered around the crystallographic Pu-O distance of 2.32 Å is broader and more diffuse. In addition, reduction with aluminum may result in reduced numbers of plutonium atoms, and the presence of hypochlorite may reduce the fraction of Pu(V). This structural heterogeneity in the Pu(IV)-oxyhydroxide system is likely to be the origin of the variability in the formation constants and their changes in time. It is, therefore, necessary both to understand this structural disorder and to develop the correlations of the microstructure with the macroscopic properties that affect the performance of the WIPP site. ■

An Apatite II Permeable Reactive Barrier to Remediate Lead, Zinc, and Cadmium in Acid Mine Drainage

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Los Alamos geochemists and their colleagues at PIMS NW, Inc., have developed a new technology to remediate metals and radionuclides from contaminated ground water and soil. We are using phosphate-induced metal stabilization (PIMS) that employs the reactive media, Apatite II, in a subsurface permeable reactive barrier (PRB), for the purpose of treating ground water containing elevated levels of zinc, lead, cadmium, sulfate, and nitrate at the Success tailings and waste rock pile. The impacted groundwater is treated in situ before it enters the East Fork of Ninemile Creek, a tributary to the Coeur d'Alene River in northern Idaho.

Laboratory feasibility studies demonstrated the greater effectiveness and lower cost of Apatite II relative to eight other reactive media. As a result, Apatite II was selected for use in a voluntary non-time-critical Comprehensive Environmental Response, Compensation and Liability Act removal action completed by the Silver Valley Natural Resource Trustees at the Success Mine and Mill site. The emplaced PRB has been operating successfully since January 2001, and has reduced the concentrations of cadmium and lead generally to below detection (2 µg/L or ppb), zinc levels to near background (about 100 µg/L or ppb), and sulfate and nitrate to below detection (50 µg/L or ppb). The PRB is filled with 100 tons of Apatite II at $350 per ton. It has been in operation for over two years and has removed over 6,000 lb of zinc, both sorbed onto the Apatite II and as ZnS; over 100 lb of lead as pyromorphite; and over 50 lb of cadmium.

Fig. 1. Success Mine tailings pile. The armored East Fork of Ninemile Creek channel is in the foreground and the subsurface PRB filled with Apatite II is to the right.

We hope that projects of this kind will demonstrate the ease and cost-effectiveness of using inexpensive reactive media to treat sources of metal loading that are difficult or costly to remove, such as very large sources for which no landfill space is available, sources located beneath infrastructures, sources that would require significant disruption of communities, industries or services, and tailings piles and access tunnel discharges located in remote areas with limited access. ■

Phosphate-Induced Metal Stabilization Remediation of Lead-Contaminated Soil at Camp Stanley

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The Carlsbad Field Office together with PIMS NW, Inc., has implemented a new technology to remediate metals and radionuclides from contaminated soil. We have successfully implemented the phosphate-induced metal stabilization (PIMS) method by using Apatite II to remediate particulate lead contamination at an open burn and detonation site, Solid Waste Management Unit (SWMU) B-20, at Camp Stanley Storage Activity (CSSA) in Boerne, TX.

Three thousand cubic yards of lead-contaminated soil were previously sieved to remove uranium oxides and metal particulates greater in size than ¾ inch. The sieved soils were left at SWMU B-20 in six 500-cubic-yard lead-contaminated soil piles. After sieving, lead concentrations in the soils ranged from 200–100,000 mg/kg (ppm), an average of about 3,000 mg/kg. The toxicity characteristic leaching procedure (TCLP) results showed that leachable lead in the soils ranged from 1.07–3.22 mg/L (ppm).

Our field objectives included the following: (1) to demonstrate the use of PIMS with Apatite II for stabilizing and remediating particulate lead in situ; (2) to determine actual field implementation costs; (3) to determine the degree of regulatory acceptance; (4) to remediate the lead-contaminated soils at SWMU B-20; and (5) to provide the base with an acceptable in situ alternative to off-site disposal or to reduce off-site disposal cost through treatment of soil to a lesser waste classification.

Fig. 1. Mixing of Apatite II into lead-contaminated soil at Camp Stanley before spreading at the site. This technology uses simple earth-moving equipment.

The demonstration remediated all six lead-contaminated soil piles in place at SWMU B-20 by using a backhoe to mix 5% Apatite II by the dry weight of the soil into the lead-contaminated soils (Fig. 1), then covering the mixture with 6 inches of clean soil and monitoring the leachate.

To date, leachates collected and monitored show the following results: 0.004 mg/L, 0.003 mg/L, 0.002 mg/ L, 0.007 mg/L, 0.006 mg/L and 0.002 mg/L, all consistently below the maximum concentration level (MCL) of 0.015 mg/L for lead in drinking water. Our first and fourth objectives are now complete. Regarding the second objective, the full field-scale effort was determined to cost $24 per treated ton of contaminated soil. The third and fifth objectives require our showing that the PIMS method for remediating firing ranges and open burn and open detonation sites leaves makes them safe for human beings and the environment. TCLP on the PIMS-treated soils gave results between 0.05–1.23 mg/L Pb, which classifies the treated soils as Class 2 Nonhazardous Waste according to the State of Texas' Waste Classification Criterion of less than 1.5 mg/L. This classification would enable a decrease in disposal cost from $120 per ton to $18 per ton, if disposal were the objective. However, the best method to obtain approval to leave the treated soils in place (fulfilling the third and fifth objectives) is to show beyond doubt that the lead in the soils is not leaching into ground water or impacting the environment. Over the last year, shallow lysimeter wells emplaced below the treated soil revealed a leachate concentration averaging 3 ppb, well below MCL of 15 ppb. This indicates that lead is not leaching from the treated soil. By contrast, shallow lysimeters below the untreated soil showed lead concentrations of more than 390 ppb.

When regulatory approval is obtained, SWMU B-20 can be officially upgraded from a field demonstration to an Interim Measure/Corrective Action, our fourth objective. CSSA will be an acceptable in situ alternative to off-site disposal options for other contaminated soil sites—our fifth objective. Parsons Engineering, the on-site contractor, showed that PIMS technology averages $23 per cubic yard total costs for remediation. Other technologies that they have used on this site were grout and disposal ($104 per cubic yard), electrokinetics ($473 per cubic yard plus disposal costs of the resulting concentrate), phytoremediation ($175 per cubic yard plus future necessary operation and maintenance costs), or simply digging it up and disposing of it elsewhere without treatment ($58 per cubic yard). As a result of our fieldwork, PIMS is now being applied at three other military ranges in California and New Jersey. ■

Emerging Astrophysical Phenomena

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The astrophysics focus fosters theoretical, observational, and instrumentation research. Of particular interest are multidisciplinary projects at the boundaries between astrophysics and nuclear physics, particle physics, condensed matter physics, plasma physics, and general relativity. Recent research supported under this focus includes projects in gamma-ray astrophysics, space instrumentation, stellar dynamics, neutron star physics, cosmic rays, solar neutrinos, primordial black holes, intergalactic magnetic fields, active galactic nuclei, and the cosmic microwave background. Besides these topics, we studied aspects of the supernovae, the energetics of supermassive black holes, physics of accretion disks, dynamics of radio pulsars, and the dynamics of the interactions between superfluids and normal matter. Use of Laboratory facilities, for example, exploitation of the Milagro gamma-ray observatory, is highly desirable.

Two exciting topics of modern astrophysics are the evolution of stellar systems and the generation of observable radiation by stars. We researched the x-ray and gamma-ray emission from neutron stars and other compact objects. With the development of new x-ray and gamma-ray satellite-based observing systems, the astrophysics community has, for the first time, the ability to observe stellar objects over broad spectral bands and with fine time resolution.

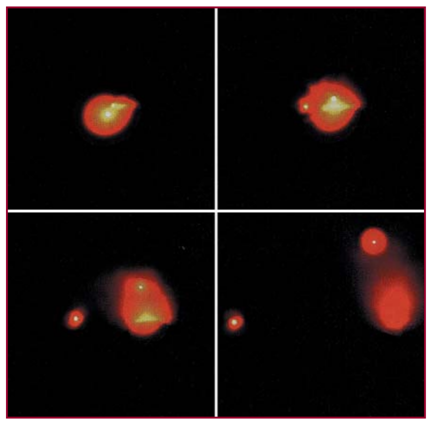

Fig. 1. High-speed encounter between a 2-solar-mass red giant and a 16-solar-mass black hole. The velocity at infinity is 550 km/s. The color scale is logarithmic in the density of the gas. The four images represent slices in the plane of the encounter at different times. (Upper left) The collision just after the impactor has penetrated the giant's envelope. The impactor exerts a strong gravitational force on the giant's core; (upper right) the core's trajectory has been notably deflected towards the top of the figure. (Lower left) The impactor has exited the giant's envelope with material (about 0.02 Msolar) that is now bound to it. The core, with only a small fraction of the envelope, continues its motion toward the top of the figure. (Lower right) The core (with its bound fluid), leaving behind the remains of the envelope. The latter, which constitutes almost all of the envelope, will disperse on a few sound-crossing times (a sound-crossing time is the time it takes for a sound wave to cross the object).

In our theoretical work, we modeled and computed the variable spectra from neutron star surfaces and gamma-ray bursts. Neutron stars are born as rapidly rotating objects that later slow down as a result of interactions with their environments. Our objective was to acquire optical data on neutron stars from ground-based facilities in order to measure the periodic fluctuations from stellar rotation and to deduce the initial rotation rates and the subsequent deceleration.

In addition, we researched high-energy astrophysics involving gamma rays from compact stars. More than eight groups throughout the world have reported these emissions, but their exact nature and even their existence is still in question. We have launched an extensive search for these gamma rays, using the most advanced scintillator array and Cherenkov detectors. Of all the groups worldwide, we are in the best position to resolve the perplexing issues of discrete gamma-ray celestial sources.

Recent observations of long-term precession-like behavior in several pulsars have created a crisis in the understanding of the interiors of neutron stars. Earlier observations showed that most, if not all, neutron stars exhibited glitches. Glitches are events in which the surface of the star suddenly spins more rapidly, by as much as several ppm. After decades of research, the consensus is that glitches are the result of the transfer of angular momentum from a more rapidly spinning neutron superfluid in the interior of the neutron star. The physical mechanism that allows the neutron superfluid to spin more rapidly than the crust is "vortex pinning," in which the superfluid vortex lines (which determine the superfluid spin rate) are trapping the crust of the neutron star. As the crust of the neutron star slows through magnetic braking, vortex pinning prevents the superfluid from slowing as rapidly as the crust.

Our theoretical work has shown that nearly perfect, or even just very strong, vortex pinning suppresses the free precession of a neutron star very effectively. However, free precession is the plausible explanation of the observed long (hundreds to thousands of days) time-scale variations of the pulsar spin. Our continuing and future work is devoted to reconcile these apparently contradictory ideas. ■

Table 1. Research Projects by Principal Investigator (PI)

Los Alamos PI	Group	University PI	University	Research Project
Chris Fryer	T-6	David Arnett	Univ. of Arizona	Nucleosynthesis in Asymmetric Core-Collapse Supernovae.
Gus Sinns	P-23	David Williams	Univ. of California, Santa Cruz	Improvement of Background Rejection Algorithms in Milagro.
Hui Li	X-1	Richard Lovelace	Rice Univ.	The Origin of Magnetic Fields in Galaxy Clusters.
Thomas Vestrand	NIS-2	France Cordova	Univ. of California, Santa Barbara	Using XMM-Newton to Probe the Properties of Isolated Pulsars.
Richard Epstein	NIS-2	Ira Wasserman	Cornell Univ.	Precessing Neutron Stars.
Hui Li	X-1	Douglas Lin	Univ. of California, Santa Cruz	Migration of Proto-Planets in Gaseous Disks.

Dynamic Science of Earth Processes

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Through support of collaborative research with Los Alamos staff, university faculty, and graduate students, this project seeks to enhance our basic understanding of the Earth and planets, from the physical, chemical, and rheological nature of Earth at the atomistic scale to the complex interactions of the system as a whole at the scale of the entire planet. Our tasks cover a broad range of approaches, including observation, field, laboratory, modeling, and theory. The focus of these tasks is on fundamental scientific questions in Earth and planetary sciences, but the long-term impact is a better understanding of the processes that control natural resources, hazards, and environments. Although the focus of this project is the solid Earth, an effort is made to link with related studies of the hydrosphere, biosphere, atmosphere, and magnetosphere.

Viewed in relation to DOE's threat-reduction mission, this project provides technological benefit to monitoring and verifying the Comprehensive Test Ban Treaty, more efficient remediation of contaminated sites, integrity of nuclear and nonnuclear geologic waste disposal sites, and nuclear nonproliferation. The experimental and computational techniques we have developed for geological and geophysical applications can be applied in other applications, such as environmental restoration, after they have matured. The results of this project, which are clearly demonstrated by the extensive publication list, including seven *Nature* articles, also contribute to DOE's basic science mission.

The work described is sponsored by IGPP and funded by Los Alamos' Laboratory-Directed Research and Development. A table of the principal investigators and their institutions is included (Table 1). Investigations of the Middle Awash, northwest Ethiopia geology indicate early hominids moved into more open savannah settings after 4.4 million years. We investigated clay minerals formed in situ in an active fault so that we may understand seismic risk in populated areas. Some of the first time-of-flight neutron diffraction measurements at the new Los Alamos Neutron Science Center's (LANSCE) high-pressure preferred orientation (HIPPO) diffractometer facility illuminated textural changes in minerals during thermally induced phase changes. It was confirmed that free oscillations of Earth related to atmospheric and ocean dynamics are associated with seasonal variations in modal amplitudes. Resonant ultrasound spectroscopy on Berea sandstone has shown that the hysteretic elastic tensor softens as temperature is lowered. In addition, we have made progress in developing and integrating a model description of hysteresis in rocks that includes liquid saturation. We also have made progress in our efforts to develop a conceptual model in which spatial variations in fault-zone architecture are articulated in the form of spatial variations in permeability structure. We have shown that optically stimulated luminescence is well suited to determining the age of sediments in river tie channels and that it provides constraints on evolution of tie-channel systems.

An experimental study investigated the discrepancy of silicate dissolution rates between those derived from field sites and laboratory measurements. Modeling of electromagnetic induction indicates a potential for developing methods to detect mantle plumes using ground-based geomagnetic data. Models of subducting slabs have shown that volumetric reductions caused by equilibrium-phase transformations cause high-shear stress in the mantle transition zone. This stress is the result of variable viscosity inside the subducting slab. The main influence of complex mineralogical composition is through viscosity. Application of numerical adjoint methods to mantle convection models indicates that we can infer mantle flow back in time for at least 100 million years.

Some projects involve research into other planets in our solar system. Modeling of convection in the lunar mantle indicates that a pulse of core heating accompanying early thermochemical overturn, as evidenced by the eruption of maria basalts, may explain the existence of a lunar dynamo and magnetic field. (A maria is any of the large, dark areas on the moon, Mars, or other planets.) Work is progressing on coupling a dynamo model for the deep liquid interior of Jupiter and Saturn with a modified version of an atmospheric global climate model for the shallow gaseous atmospheres of Jupiter and Saturn. ■

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Los Alamos PI	Group	University PI	University	Research Project
Mike Murrell	CST-11	Craig Lundstrom	Univ. of Illinois	Time Scales of Crustal Level Differentiation: U-series Measurements and Geophysical Monitoring at Arenal Volcano, Costa Rica.
Cathy Wilson	EES- 2	William Dietrich	Univ. of California, Berkeley	Analysis of the Evolution of Floodplain (“tie”) Channels Using Optically Stimulated Luminescence Dating: Links to Land Use and Global Environmental Change.
Douglas ReVelle	EES- 2	Toshiro Tanimoto	Univ. of California, Santa Barbara	Continuous Free Oscillations and Its Application to Planetary Seismology.
Carl Gable	EES- 6	Barbara Dutrow	Louisiana State Univ.	Coupled Fluid Flow and Chemical Transport Implications for Mineral Chemistry, Permeability Evolution and Thermal-Chemical Feedback Effects.
Carl Gable	EES- 6	Gerald Schubert	Univ. of California, Los Angeles	Deformation, Stresses, and Earthquakes in Descending Slabs.
Carl Gable	EES- 6	Mark Person	Univ. of Minnesota	Three-Dimensional Physical and Numerical Models of Groundwater Flow and Solute Mass Transport Through Naturally Heterogeneous Porous Media at the Basin Scale: A Critical Test for Geostatistical Methods and Solute Transport Algorithms.
Dave Bish	EES- 6	J. Casey Moore	Univ. of California, Santa Cruz	Weak Faulting and Smectite Concentration Across the San Gregorio Fault Zone.
David Bish	EES- 6	Dennis Bird	Stanford Univ.	Nearest-Neighbor Atomic Environment and Thermodynamic Properties of Zeolitic Water in Ca-, Na-, K-, and Sr- Exchanged Heulandites.
George Guthrie	EES- 6	Chen Zhu	Univ. of Pittsburgh	Silicate Reaction Kinetics in a Major Aquifer in New Mexico.
Scott Baldridge	EES- 6	James Ni	New Mexico State Univ.	Colorado Plateau/Rio Grande Rift/Great Plains Seismic Transect.
Claudia Lewis	EES- 9	Laura Goodwin	New Mexico Tech	Characteristics of Faults in Non-Welded Tuffs from the Pajarito Plateau and Implications for Fluid Flow.
Claudia Aprea	EES-11	Fumilo Tajima	Univ. of California, Berkeley	High-Performance Computer Simulations for Modeling Electrical Conductivity.
James Ten Cate	EES-11	Koen Van Den Abeele	Katholieke Universiteit, Leuven	Nonlinear Elastic Micro-Macro (NLEM3) for Ultrasonic Research of Micro-Inhomogeneous Media at Low Saturations.
Paul Johnson	EES-11	Katherine McCall	Univ. of Nevada, Reno	Ultrasonic Determination of Moduli in Earth Materials.
Paul Johnson	EES-11	Koen Van Den Abeele	Catholic Univ., Leuven	Resonance Template Matched Filtering (RTMF) and the Mechanism of Nonlinear Response in Earth Materials.
Scott Baldridge	EES-11	Robert Coe	Univ. of California, Santa Cruz	Paleointensity and Large Igneous Provinces—Are They Plume-Driven?
Juergen Eckert	LANSCE-12	Katherine McCall	Univ. of Nevada, Reno	Neutron Spectroscopy of Earth Materials.
Carlos Tomé	MST-8	H. Rudy Wenk	Univ. of California, Berkeley	Development of Anisotropy in Deformed and Recrystallized Rocks.
John Baumgardner	T-3	Mark Richards	Univ. of California, Berkeley	Global Models of Plate Motions and Mantle Mixing.
Carl Hagelberg	X-4	Hans-Peter Bunge	Princeton Univ.	Variational Assimilation in Mantle Convection Models.
Jim Kao	X-4	Gary Glatzmaier Peter Olson	Univ. of California, Santa Cruz Johns Hopkins Univ.	Studies of Giant Planets with a Coupled Atmospheric-Interior Model.

Complex Dynamical Systems

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To simulate climate or any other complex integrated system, one must understand not only its individual compartments (for example, atmosphere, ocean, and biosphere) but also the dynamics of interactions between compartments on a variety of temporal and spatial scales. This project focuses on several key pieces of the climate puzzle. These pieces include optimal combinations of models and data sets to enhance the understanding of the nonlinearities governing critical climate-system processes, time scales, and uncertainties; the behavior of the West Antarctic ice sheet and its effects on the oceanic thermohaline circulation; regional processes influencing interannual variability of water cycles; the use of terrestrial and oceanic cores to reconstruct climate history; and the use of satellite observations of lightning to track its influence on both short-time weather and climatic variations.

The overall goal of this project is to extend the understanding of dynamical aspects of the atmosphere and ocean system, based on collaborations between Los Alamos and external scientists. Specific project objectives focus on furthering our understanding of physical, chemical, and biological processes in the atmosphere and ocean. We also are focusing on building interdisciplinary models based on, for example, coupling the atmosphere to the ocean and coupling the atmosphere to the terrestrial biosphere, and then by applying the science to specific scientific issues associated with pressing societal issues such as wildfires and climate change.

We are emphasizing heavily the physics and chemistry governing the effects of momentum, energy, and scalar transport (including moisture, salinity, temperature, and trace chemical compounds); turbulence on the behavior of water and trace gases in the atmosphere; and and trace species and biomass involved in the ocean. Models that can be applied to climate change through, for example, oceanic thermohaline circulation and atmospheric monsoonal dynamics, will be direct applications that are central to our project goals.

To foster and encourage collaborations, we are carrying out basic research on topics that are relevant to ongoing Laboratory interests such as modeling of oceans and atmospheres, biogeochemistry, and the carbon cycle. Our tasks include furthering our understanding of geophysical fluid dynamics and refining biogeochemical theory, numerics relevant to model system performance, models for multiphase behavior of water, and the introduction of biological and chemical dynamics into physical systems. Efforts extend from local and regional scales to studies of global climate change.

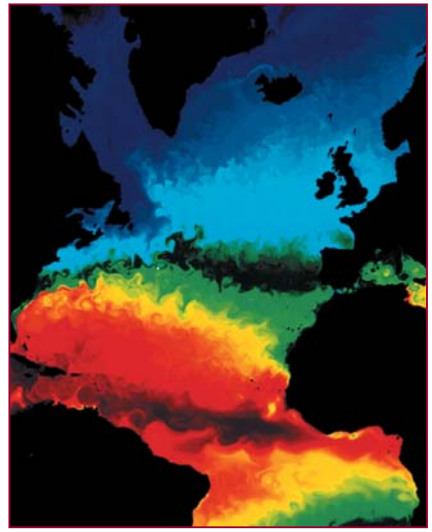

Fig. 1. A snapshot of the simulated sea-surface temperature in the Atlantic Ocean in midautumn from a model run with the Los Alamos Parallel Ocean Program (POP). The resolution of the model grid is 0.1 degrees in latitude and longitude with 40 depth levels. This is sufficiently refined to resolve the size-spectrum of oceanic mesoscale eddies, as evidenced by quantitative comparison of satellite-measured and model-simulated sea-surface-height variability. Red (blue and purple) colors indicate warm (cold) temperatures. Eddies are evident almost everywhere in the ocean.

Our research into complex dynamical systems includes the following highlights:

Our study of deep-sea corals led to an improved calibration of the Mg/Ca paleothermometer using the deep-sea coral *Primnoa resedaeformis.* We used that calibration to reconstruct temperature variations in the mixing zone between the Labrador current and the Gulf Stream.

Research suggests that we may be able to use the FORTE satellite instrument, and, by implication, its follow-on instruments, to monitor and perhaps to predict convective storms, which in turn represent a regional manifestation of global change

We showed that the extended Kalman filtering approach to data assimilation helps resolve and describe the scales and mechanisms that govern surface evaporation—an atmosphere-ocean coupling process that is critical to climate.

We showed that removing the parts of the West Antarctic ice sheet influences not only the oceanic circulation surrounding Antarctica but also oceanic currents and subduction rates throughout the southern oceans.

Coupled atmospheric and oceanic modeling reveals realistic frontal dynamics of boundary currents and El Niño/Southern Oscillation dynamics (Fig. 1). ■

Table 1. Research Project by Principal Investigator (PI)

Los Alamos PI	Group	University PI	University	Research Project
Jeff Heikoop	EES-6	R. Scott Anderson	Northern Arizona Univ.	Sensitivity of Global Thermohaline Ocean Circulation to Disintegration of West Antarctic Ice Shelves.
Elizabeth Hunke	T-3	Slawek Tulaczyk	Univ. of California, Santa Cruz	Sensitivity of Global Thermohaline Ocean Circulation to Disintegration of West Antarctic Ice Shelves.
Alan Hurd	LANSCE-12	Edwin Waddington	Univ. of Washington	In Situ Neutron Scattering Deformation Apparatus for Fine-Grained Ice IH and Hydrates.

Space Weather Foundations

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The space environment of the Earth is populated with electrically charged particles (plasma) whose motions are controlled by the geomagnetic field and driven by energy extracted from the solar wind, the supersonically expanding solar atmosphere. Although their densities are extremely low, the populations of charged particles in the Earth's geospace environment form a medium in which stormlike disturbances occur, driving powerful electrical currents into the ionosphere and accelerating charged particles to extremely high energies. These disturbances can affect communications, navigation, and radar systems. Such disturbances are triggered by storms on the sun and hence are known as geomagnetic storms. They represent an extreme form of "space weather."

The majority of our satellites operate in the regions affected by these storms and can therefore be exposed to intense fluxes of extremely energetic particles. Characterizing the dynamics of these regions and understanding the underlying physics are, thus, not only matters for basic research, but also essential to spacecraft operations, spacecraft safety, and mission planning.

The objectives of our comprehensive efforts are to characterize and understand the mechanisms that govern space weather, including the propagation of solar disturbances and their interaction with the terrestrial magnetosphere, ionosphere, and atmosphere. The mechanisms of concern also include "magnetospheric substorms," sudden releases of solar wind energy inside the magnetosphere. Specific processes include acceleration, transport, and variability of electrons and ions.

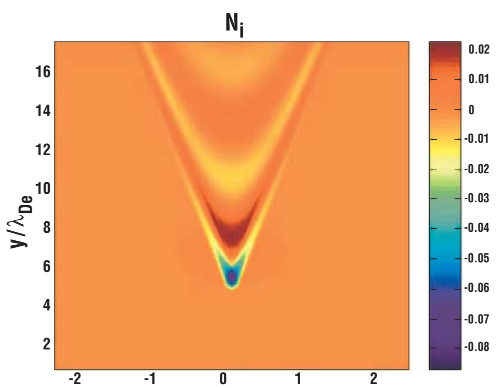

Fig.1. Example of a trail left behind by a small object such as a meteor falling in the atmosphere, as obtained from a plasma simulation.

Integral elements of our program are the analysis of satellite and ground data to improve our understanding of the characteristic processes, and the development and application of models that incorporate the improved physical understanding of the geospace environment.

New accomplishments are made possible by three major advances: (1) multispacecraft experiments that describe spatial gradients of physical quantities and the full separation between temporal and spatial effects; (2) remote-sensing satellites that provide unprecedented regional and global views of the magnetosphere; and (3) computer simulations describing 3-D, time-dependent processes, even on typical particle scales. These advances collectively provide unprecedented possibilities to reveal the physics that govern space weather from microscale to global scale, and also governs the cross-coupling between the different scales.

Studies of solar wind-magnetosphere coupling have clarified how this interaction takes place—for example, which waves, instabilities, and particle and field processes are involved and how plasma and energy penetrate the boundaries. In addition, we have investigated the characteristic properties of how plasmas and fields influence each other on different spatial and temporal scales. Flux transfer events (FTEs) at the magnetopause (the interface between terrestrial and interplanetary magnetic fields) play an important role in the coupling. Current scientific understanding holds FTEs to be based on magnetic flux tubes connecting the two regions. Using a combination of 2-D and 3-D hybrid codes, we have addressed the magnetic and plasma signatures of FTEs, explained a number of observed characteristics, and made predictions to test by experiment.

A particularly difficult region for spacecraft to study is the region from 1000 km to 4 Earth radii, where many communication relay satellites reside. Using a new technique, magnetospheric seismology, we began monitoring this region from the ground by studying the propagation of magnetic pulsations and sudden impulses.

The physics of finite size charged particles ("dusty plasmas") is an area of growing interest in plasma physics. Meteor trails in geospace, which exhibit characteristic plasma wave and wave-particle interaction phenomena, provide an application of this research topic. As illustrated by Fig. 1, we have simulated these processes and studied the instabilities involved as well as the physics of heating and the ablation of meteoric particles. ■

Table 1. Research Projects by Principal Investigator (PI)

Los Alamos PI	Group	University PI	University	Research Project
Richard Elphic	NIS-1	Margaret Kvelson	Univ. of California, Los Angeles	Multispacecraft Studies of the Structure and Dynamics of the Magnetotail Current Sheet.
Joachim Birn	NIS-1	Joachim Raeder	Univ. of California, Los Angeles	Simulations of Magnetotail Equilibria and Dynamics.
Michelle Thomsen	NIS-1	Christopher Russel	Univ. of California, Los Angeles	Magnetospheric Seismology: A Pilot Study.
Giovanni Lapenta	T-15	Marlene Rosenberg	Univ. of California, San Diego	Interaction of Small Bodies with the Atmosphere.
Jeremiah Brackbill	T-3	Homayoun Karimabadi	Univ. of California, San Diego	Three-Dimensional Kinetic Simulations of the Magnetosphere II.
Michelle Thomsen	NIS-1	Mark Moldwin	Univ. of California, Los Angeles	Quantifying IMAGE EUV Plasmaspheric Images Using the In-Situ LANL Geosynchronous Orbit Plasma Measurements.

Turbulent Transport and Surface Fluxes of Momentum, Heat, and Mass for Inhomogeneous and Nonstationary Conditions

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Fluxes of momentum, heat, gases, and particles (including bacteria and viruses) are modeled by application of Monin-Obukhov Similarity (MOS) theory. In its presently used form, MOS theory requires that assumptions of horizontal homogeneity and stationarity of all relevant state variables must be valid. Unfortunately, in most domains of present day interest such as in urban canopies and coastal zones, substantial horizontal inhomogeneity exists, thus implying that the assumptions are systematically and routinely violated. Model predictions using MOS theory on issues such as biochem warfare, offshore wind power resources, or even modeling of ocean wave phenomena in coastal zones are, therefore, strongly limited by limitations of MOS theory. Limitations of the theory in such domains as risk assessments in heterogeneous urban canopies are anticipated to introduce an order of 50% uncertainty in predictions, thus decreasing public confidence in model output.

The primary goal of this project is to extend MOS theory where the assumptions of heterogeneity and nonstationarity are allowed.

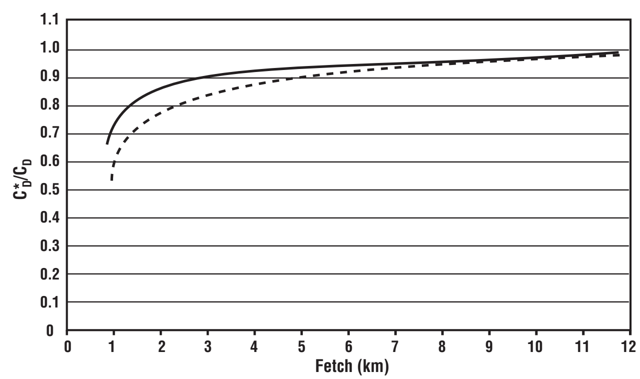

Fig. 1. Calculations of the ratio of CD/CD in which the drag coefficient computed for horizontally homogeneous conditions (CD*) is normalized by the drag coefficient for horizontally inhomogeneous conditions (CD). These are illustrated with wind speeds of 5.4 ms-1 and 7.5 ms-1.*

A secondary goal is to demonstrate improved model performance with a more general form of MOS theory on scientific issues related to such issues as local-scale meteorology, homeland defense, fisheries, offshore energy, and regional scale modeling.

In order to extend MOS theory for quasi-inhomogeneous conditions, the principal investigator has derived a more general form of similarity theory by allowing flux divergence to be caused by horizontal gradients of roughness, stratification, wind speed, and thermal wind (Geernaert, 2002). To continue this work, the general form of MOS will be used to address a number of issues facing the community. Objectives are to answer the following questions: Is the wind-drag coefficient dependent on wave state or vertical-flux divergence? Do offshore windmills need to be optimized in regions where horizontal wind-speed gradients are systematic—for example, for winds blowing offshore? Do vertical fluxes of bacteria and viruses in urban canopies, specifically for inhomogeneous conditions, affect the along-wind transport of such species? ■

Reference

Geernaert, G.L., "On Extending the Flux Profile Similarity Theory to Include Quasi-Homogeneous Conditions in the Marine Atmospheric Surface Layer," *Bound. Layer Met.* **105**, 433 (2002).