Lawrence Livermore
National Laboratory

Earth and Environmental Sciences

1998 Annual Report

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National Security

Treaty Verification

Accomplishments

Developed and applied innovative statistical techniques to characterize seismic location and identification capabilities

Characterized seismic location capabilities in large parts of the Mid-East and North Africa

Provided containment measures for subcritical experiments at the U.S. Nevada Test Site

Seismic, hydroacoustic, and on-site inspection models, databases, and methods supporting Comprehensive Nuclear-Test-Ban Treaty monitoring

and

Atmospheric Release Hazards

Prepared forecasts of gas- and material-dispersal patterns following the Indian and Pakistani nuclear tests

Supported the Goodwill Games, the State of the Union Address, and urban-terrorism exercises involving surrogate chemical and biological weapons

Models, personnel, and an operational center to assess and mitigate the effects of atmospheric releases

Earth and Environmental Sciences at Lawrence Livermore National Laboratory

Our Roles and Accomplishments

Accomplishments

Received LLNL Strategic Initiative award to develop and apply models of the physical, mineralogical, and chemical evolution of the Yucca Mountain repository

Constrained computer models with experiments to explain reactive flow and transport and saturation imaging phenomena

Science and technology projects complementary to programmatic funding

Received LLNL Strategic Initiative award to develop and apply terascale-computer climate models to anthropogenic climate change and natural climate variability

Developed and refined biomedical applications of accelerator mass spectrometry

Nuclear Materials

Options for storage, immobilization, and sequestration of radioactive materials

Accomplishments

Defined the thermal-hydrologic performance of the potential Yucca Mountain nuclear repository for the total system performance assessment

Directed a multilaboratory effort to design and characterize ceramic wasteforms for sequestering nuclear weapons materials

Climate, Carbon, and Energy

Models and impact assessments of current and future climatic conditions

Completed a sequence of climate model intercomparison and diagnosis, changing the way climate models are evaluated and improved

Identified processes that affect the role of the southern oceans in uptake and sequestration of carbon dioxide

Environmental Risk Reduction

Characterized and cleaned up a Superfund site contaminated with pole-treating compounds using hydrous pyrolysis/oxidation technologies

Assessed radiological conditions and developed mitigation measures for resettlement of the Marshall Islands

Systems to characterize and remediate environmental hazards

Earth and Environmental Sciences at Lawrence Livermore National Laboratory

Lee W. Younker

Lawrence Livermore National Laboratory (LLNL) provides broad-based, integrated scientific and engineering capabilities to address some of the nation's top national security and environmental priorities. National security priorities are to ensure the safety and reliability of the U.S. nuclear weapons stockpile and to counter the spread of weapons of mass destruction; environmental priorities are to keep our environment healthy for the long term and to assess the consequences of environmental change.

The Earth and Environmental Sciences (E&ES) Directorate at LLNL pursues applied and basic research across many disciplines to advance the technologies needed to address these national concerns. Our current work (*see foldout illustration*) focuses on

- Storage and ultimate disposition of U.S. spent reactor fuel and other nuclear materials (*top right*).
- Assessment of the current global climate and simulation of future changes caused by humans or nature (*center right*).
- Development of broadly applicable technologies for environmental remediation and risk reduction (*lower right*).
- Tools to support U.S. goals for verifying the international Comprehensive Nuclear-Test-Ban Treaty; subcritical tests for stockpile stewardship (*top left*).
- Real-time assessments of the health and environmental consequences of atmospheric releases of radioactive or other hazardous materials (*lower left*).
- Basic science research that investigates fundamental physical and chemical properties of interest to these applied research programs (*bottom*).

For each of these areas we present an overview in this report, followed by an article featuring one project in that area. Then we delineate E&ES's resources, including workforce, facilities, and funding. Finally, we list the publications by and the awards and patents received by E&ES personnel during 1998.

LLNL is a facility of the U.S. Department of Energy (DOE) operated by the University of California (UC).

Dedicated to the memory of

Dr. Ivan Proctor

E&ES Deputy Associate Director for Operations and
Deputy Director of the Center for Accelerator Mass Spectrometry
from October 16, 1972 to October 17, 1998

Nuclear Materials and the Environment Overview

Henry Shaw

The Department of Energy and its predecessors have been the primary U.S. agencies involved with the development and implementation of nuclear technologies, both civilian and military. As a result, DOE is responsible for a wide variety of nuclear materials (such as spent fuel from reactors) and numerous defense-related wastes (such as tanks of high-level waste and surplus fissile materials). DOE is also responsible for the management and cleanup of the billions of cubic meters of contaminated soil and groundwater that are the legacy of 50 years of production and testing of nuclear materials under environmental controls that do not meet modern standards.

Because of its historic focus on the use of nuclear technology, particularly in national security applications, LLNL has developed extensive capabilities and expertise relevant to DOE's role as nuclear steward for the nation. In fact, the roots of most of the disciplinary expertise in the earth and environmental sciences in E&ES extend back to support provided to early programs for testing and for the peaceful uses of nuclear explosions. These roots have given rise to a set of diverse programs addressing the behavior and consequences of environmental releases of radionuclides. Some examples of our recent work in these areas are highlighted below.

The Disposal of Spent Nuclear Fuel and High-Level Waste

LLNL's involvement in the nation's nuclear waste disposal programs began in the late 1970s. Since then, attention has been focused on a single candidate repository site at Yucca Mountain, Nevada, where we have the responsibility for the design and assessment of the Engineered Barrier System (EBS). This system comprises the waste

container, wasteform, and other man-made materials. We are also responsible for defining the environment that the EBS will experience over time. The recent adoption of a repository design based largely on the results of our modeling of the thermohydraulic evolution of the repository underscores the significance and importance of our work.

Initiation of the Drift-Scale Heater Test, for which LLNL was the main driver, was a recent major milestone for the Yucca Mountain Project. This large test is being conducted in a 47-meter-long section of a 5-mile tunnel beneath Yucca Mountain (the Exploratory Studies Facility) that provides access to the potential repository rock. Approximately 10,000 cubic meters of rock will be heated to 100°C. Overall, 200,000 cubic meters of nearby rock will be affected by the heat. The heat will be generated by 9 electrical floor heaters and by 50 electrical side heaters. Video and infrared cameras will monitor the test during the approximately 4-year heat-up period and comparable cool-down phase. Sensors installed in boreholes surrounding the drift will measure the thermal, mechanical, hydrological, and chemical changes in the rock. These data will be used to refine computer models of the long-term effects of heat generation at Yucca Mountain.

Predicting the Fate of Atmospheric Releases of Radioactive Materials

The Atmospheric Release Advisory Capability (ARAC) is an emergency response operation that evaluates the effects of releases of hazardous materials into the atmosphere. Although its primary mission is to provide DOE and the Department of Defense with assessments of radiological releases, ARAC has also assisted local, state, federal, and international agencies in responding to both

natural and anthropogenic releases. Since 1979, ARAC has responded to more than 100 incidents involving radiological and chemical releases, smoke from fires, and plumes from volcanic eruptions.

ARAC recently exercised its capabilities by estimating the timing and magnitude of an accidental atmospheric release of radioactive cesium-137 in Spain (Figure 1). In June 1998, the Spanish government announced that a medical radiotherapy source of cesium-137 had been melted in a steel mill's scrap-metal furnace near Algeciras on the southern tip of Spain. Some of the cesium had been released into the atmosphere. Initially, the time and the amount of the release were unknown, though the release was thought to have occurred sometime during the last week of May 1998. When ARAC staff heard of the incident, they began accessing meteorological data for the area and acquiring measurements of cesium air concentration from colleagues in Europe and Russia. Although the radiation levels were well below those that would cause a health concern, ARAC scientists used the incident as an exercise to recreate a source term from measurement data, similar to the way they had responded to the Chernobyl accident. ARAC determined the path taken by the plume through the atmosphere, and by fitting calculations to measurements, estimated that the release was about 50 curies. This compared favorably with the estimate of 8–80 curies later provided by the Spanish government. ARAC's calculations were considered the definitive results at a September 1998 meeting of the European Union's Joint Research Center. This analysis proved to be a valuable exercise of ARAC's capabilities and again demonstrated its ability to quantify the effects of an incident from sparse information.

Supporting Nonproliferation: Disposition of Surplus Plutonium

Disarmament and the termination of weapons production accompanying the end of the cold war have resulted in a surplus of plutonium (and other fissile material) in both the United States and Russia. Disposition of these materials has to meet

both environmental and national security constraints. Therefore, as part of a nonproliferation initiative, both countries are studying ways to dispose of surplus plutonium, such as burning mixed-oxide fuels in power reactors or immobilizing the plutonium in a matrix suitable for geologic disposal. LLNL has been given the lead responsibility in the U.S. for the development of the technology needed for the immobilization option. Our partners in this work include the Savannah River Plant, Argonne and Pacific Northwest National Laboratories, several U.S. universities and companies, and research institutions in Australia and Russia. In this approach, the plutonium would be incorporated into a ceramic wasteform that would ultimately be emplaced in a geologic repository for permanent disposal.

The Nonproliferation, Arms Control, and International Security Directorate at LLNL manages the Plutonium Immobilization Project. The E&ES Directorate provides disciplinary expertise to the project in the

Figure 1. Computed atmospheric plume from an accidental release of cesium-137 in southern Spain on May 30, 1998. Colors show the predicted concentrations of cesium-137 in air averaged over the 7 days ending June 5, 1998 (red indicates highest concentration).

areas of mineralogy, geochemistry, and high-temperature phase equilibria. Our experience with testing and modeling nuclear wasteforms for the Yucca Mountain Project makes us the natural choice to lead the work needed to characterize the performance of the ceramic wasteform and determine if it is acceptable for disposal in a deep geologic repository. Currently, we are conducting dissolution tests of the chemical phases present in the ceramic to establish the mechanisms that limit the rate of dissolution. Data from these tests will be incorporated into a model that will be used to assess the ceramic's performance in the candidate repository at Yucca Mountain.

Marshall Islands Program

The mission of the Marshall Islands Program is to provide measurements and assessments of current radiological conditions in areas of the Marshall Islands exposed to fallout during the U.S. atmospheric testing in the Pacific, in order to minimize exposure of South Pacific islanders who desire to return. We characterize radionuclide concentrations in food crops, vegetation, water, and soil at contaminated sites; identify radionuclide transport mechanisms in the atoll ecosystem; evaluate exposure pathways; estimate doses to populations; and identify and evaluate remedial measures for reducing radionuclide uptake by locally grown crops. LLNL has had a program in the Marshall Islands since 1972. During this time, approximately 85,000 environmental samples have been collected and analyzed.

Last year, we continued characterization and monitoring experiments on Rongelap, Bikini, and Enewetak Atolls. These experiments provided data for calculating dose estimates useful in deciding among various resettlement options. Cesium and potassium cycling and transport experiments were also conducted at Bikini Atoll. Rainfall, temperature, and related meteorological data were incorporated into new databases, and a sample inventory and tracking database was established for the environmental samples taken throughout the program's history. We continued to provide expert assistance in

support of resettlement activities, including assistance with the development of a Memorandum of Understanding outlining DOE's role in assisting resettlement of Rongelap Atoll.

Assessing the Legacy of Testing: The Underground Test Area

The Underground Test Area (UGTA) Subproject is investigating the contamination of the groundwater at the Nevada Test Site resulting from years of underground nuclear testing. The goal is to provide data and models to help DOE and the Nevada Department of Environmental Protection develop risk-based regulations. UGTA is a multi-contractor project, with IT Corporation as the prime contractor. LLNL is responsible for quantifying radioactive materials present in the subsurface due to nuclear tests and determining their transport and attenuation in the groundwater system.

As an example of LLNL's capabilities, personnel from the E&ES and Chemistry and Material Science Directorates have used data from the site of the Cambric nuclear test in Frenchman Flat to develop a framework for evaluating the nature and extent of radionuclide contamination in groundwater near underground tests. Reactive-transport modeling provided details on important geochemical processes in this porous alluvial environment. Sensitivity analyses addressed the effects of melt glass and reactive mineral surface area, as well as the total abundance and spatial distribution of reactive minerals in the alluvium. On the basis of our studies to date, we have concluded that the cavity, chimney, and melt-glass regions all act as distinct long-term sources of radionuclides and that the quantity and distribution of reactive minerals can significantly affect the transport of radionuclides. The surface areas of the melt glass and the reactive minerals are also important factors and their effects need to be determined by further work. Current efforts use classified data to develop a more detailed and complete source term for Frenchman Flat.

21st-Century Tools for Modeling Reactive Transport in Dynamic Geologic Systems of Economic and Environmental Significance

Reactive-transport modeling of dynamic geologic environments provides a unique tool for predicting the consequences of natural or engineered perturbations to these highly complex systems. Perturbations such as magmatic intrusion or fluid withdrawal impose disequilibrium within these environments, which is dissipated through a set of interdependent processes that redistribute mass and energy. Understanding and modeling this redistribution is important because many of these systems have crucial economic or environmental—often strategic—significance; examples include groundwater environments, petroleum reservoirs, confined aquifers, geothermal fields, and hydrothermal ore deposits. In systems of economic interest, our goals at LLNL focus on developing optimized exploration and production techniques for valuable reserves (water, energy, metals). In systems of environmental concern, our focus shifts to developing optimized containment and remediation strategies for toxic materials (industrial pollutants, agricultural runoff, high-level nuclear waste).

A common thread binds all of these applications: critical dependence on our ability to accurately predict the integrated system evolution that results from imposing alternative perturbations. For virtually all of the relevant environments, such predictions must span spatial, temporal, and complexity scales whose extent precludes the development of direct analytical or experimental analogs. Reactive-transport modeling provides the *only* viable means for quantifying and visualizing predictions of this kind.

Development and application of advanced reactive-transport simulators requires explicit integration of multifaceted geoscience technology (experimental/theoretical hydrology, geochemistry, geomechanics) and broad-based mathematical and computational expertise (numerical methods, software engineering, visualization, parallel architectures, relational databases). Very few institutions can match LLNL's personnel, experimental

facilities, and computational resources in these areas; fewer still can compete with the inventory of widely used reactive-transport simulators, geochemical software, and supporting thermodynamic/kinetic databases developed here.

Modeling Concepts, Capabilities, and Validation

Reactive-transport simulation of dynamic geologic systems is based on explicit mathematical models of the integrated thermal, hydrologic, geochemical, and mechanical processes catalyzed by perturbing events (Figure 1). Translation of these theoretical

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Figure 1. Integrated processes in dynamic geologic systems of the earth's crust and upper mantle. When an initial, intermittent, or continuous perturbation imposes gradients in temperature, pressure, or fluid density, it catalyzes fluid flow in permeable media. Porosity and permeability are the fundamental variables that link hydrologic (blue), geochemical (green), and mechanical (yellow) processes. (Modified from Norton [1984], *Annual Review of Earth and Planetary Sciences* **12**, 155–177).

frameworks into advanced reactive-transport simulators requires robust numerical methods that approximate and discretize the models, efficient software that encodes these numerical representations, and advanced computer architectures that permit software execution and visualization of results. Application of such simulators to any specific system further requires sufficiently complete and accurate hydrologic, compositional, thermodynamic, kinetic, and structural data to permit specification of initial and boundary conditions and facilitate modeling system evolution.

The global-implicit method is the most rigorous (and computationally expensive) mathematical approach to reactive-transport modeling. However, the relative insignificance of specific processes for certain systems warrants use of less expensive methodologies such as the streamline approach. Hence, it is highly advantageous to develop a *suite* of simulators; this has been our development strategy. Using the appropriate simulator, iterative reactive-transport modeling of a given geologic environment yields the integrated system evolution catalyzed by alternative imposed perturbations, from which optimal exploration, production, containment, or remediation strategies can be identified. Typically, these predicted results cannot be corroborated analytically or experimentally; hence, our confidence in such predictions is necessarily built upon accurate simulation of well-constrained laboratory/field experiments and systems.

Opportunities for such model validation studies include plug-flow reactors, subsurface contaminant migration, and magma-hydrothermal systems. Laboratory experiments are most valuable because system parameters, boundary conditions, and data collection are tightly constrained. Field data from disturbed systems provide spatial scale-up, but also introduce uncertainties associated with system heterogeneity and indirect sampling. Active magma-hydrothermal systems yield a wealth of data, but only a vanishingly small space-time fraction of the system is observable; their fossil counterparts typically reveal an expanded spatial profile, but only time-integrated effects can be sampled. Despite these difficulties, each forum can be used to validate certain aspects of simulator performance, and we are exploiting each.

During 1998, we completed many significant projects in the emerging research area of reactive-transport modeling. The most important results from four of these studies are described below.

An Advanced Reactive-Transport Simulator for Yucca Mountain

Accurate modeling of alternative emplacement/response scenarios at the potential Yucca Mountain nuclear repository demands an advanced reactive-transport simulator. To develop this capability, we are incorporating all requisite geochemical models into the existing framework of our state-of-the-art thermal-hydrologic simulator, NUFT. Concomitantly, we are optimizing the new simulator (NUFT-THC, which implements the global-implicit method) for execution on massively parallel architectures (LLNL's ASCI Blue), interfacing a comprehensive thermodynamic/kinetic database (GEMBOCHS), customizing advanced visualization software (Vis5D), developing an extensive suite of validation problems, and modeling simplified Yucca Mountain scenarios.

Our initial NUFT-THC simulations have provided new insights into potential evolution of the repository environment. One critical concern at Yucca Mountain is the degree of mineral dissolution/precipitation and dependent porosity/permeability modification catalyzed by the emplacement of high-level waste packages. There are two fundamental questions: "Will post-emplacement evolution seal these packages from potential fluid infiltration, or expose them to it?" and "Can their emplacement be designed to minimize the likelihood of such exposure?"

Results from a preliminary NUFT-THC simulation that addressed these issues are illustrated in Figure 2. This simulation integrates unsaturated flow, boiling, and kinetically controlled reactions within the context of dual-permeability transport through heterogeneous porous media for the chemical system silica-water ($\text{SiO}_2\text{-H}_2\text{O}$). Coupling thermal-hydrologic and geochemical processes revealed the potential formation of a relatively impermeable, cap-like region directly above the emplacement tunnels; local distribution of this region is strongly dependent on that of

“hot” and “cold” packages (Figure 2). This preliminary simulation portends future, iterative use of NUFT-THC to elucidate an optimal emplacement strategy (precise spacing of drifts, separation of packages within drifts, and distribution of hot and cold packages) that will minimize the risk of fluid infiltration.

Reactive-Transport Modeling of Plug-Flow Reactor Experiments

Successful reactive-transport modeling of well-constrained dissolution experiments validates the modeling approach and is an effective means of evaluating and estimating thermodynamic and kinetic data. In this study, a plug-flow reactor, scanning electron microscopy, and the reactive-transport simulator GIMRT were used to determine and model steady-state effluent concentrations and dissolution/precipitation features associated with quartz and tuff dissolution at 240°C. Because the relevant thermodynamic data are well established for these systems, the simulations were used to obtain and place constraints on kinetic parameters.

For quartz dissolution, we obtained model interdependence of the specific surface area and

reaction rate constant (using a linear rate law) by fitting the product of these two important kinetic parameters to the experimental steady-state effluent concentration. This model interdependence agreed closely with that obtained from an analytical solution to the relevant reaction-transport equation, validating model behavior. Independently determined surface areas and rate constants were shown to be internally consistent with respect to this model interdependence, validating use of the linear rate law. These results suggest that for monomineralic dissolution, this integrated experimental/modeling approach provides a rigorous framework for assessing the internal consistency of independent surface-area and rate-constant data, predicting rate constants from existing surface-area data (which are significantly less uncertain), and rapidly evaluating alternative rate laws.

For tuff dissolution, modeling results defined minimum supersaturation thresholds for secondary nucleation of primary minerals and yielded non-unique estimates of the relative precipitation rates of alteration minerals. Reactive-transport simulators provide the only practical means of estimating and constraining these kinetic parameters for such multicomponent, multiphase

Figure 2. NUFT-THC simulation of the time-integrated evolution of porosity 3000 years after emplacement of high-level nuclear waste packages within subterranean tunnels at Yucca Mountain. (left) Cross section through “hot” waste packages (pink objects; maximum temperature 190°C) within two parallel tunnels. (right) Lengthwise cross section of a single tunnel, showing the distribution of “hot” and “cold” (blue objects; maximum temperature 140°C) waste packages. Silica precipitation has formed relatively impermeable cap-like regions overlying the tunnels; local configuration of these impermeable zones correlates with that of “hot” and “cold” waste packages.

experiments. In the best-fit simulation, model and experimental effluent sodium, aluminum, and potassium concentrations agreed to within 3%; the agreement for silicon and calcium was within 15%.

Close agreement between experimental and simulation results for both quartz and tuff dissolution provides an important measure of confidence for extending the modeling approach to address increasingly complex systems.

Streamline-Based Modeling of Radionuclide Migration at the Nevada Test Site

We have developed a three-dimensional (3-D) streamline-based reactive-transport model and—using unclassified data—applied it to analyze local subsurface migration of radionuclides away from an underground nuclear-test cavity at the Nevada Test Site. This model accounts for kinetically controlled

release of radionuclides into groundwater as it flows through melt-glass debris and contaminated rubble, downstream migration of the radionuclide solutes, and their chemical interaction with reactive minerals.

We used our hydrologic simulator ParFlow to model a 3-D flow field of sufficiently fine resolution to represent heterogeneous permeability and dependent non-uniformity of flow rates. Approximately 800 streamlines were extracted from this model and used to forecast the migration of more than 30 radionuclides and other solutes (Figure 3). Chemical evolution along each of these 800 migration pathways was simulated individually, using a customized 1-D version of the reactive-transport model GIMRT. When recombined, these simulations yielded a chronologic, 3-D map of downstream aqueous solute concentrations (Figure 4).

The streamline approach provides an efficient technique for studying subsurface radionuclide transport because it facilitates decomposition of a complex 3-D reactive-transport problem into a tractable number of independent 1-D problems, whose results can be obtained rapidly in parallel and later recombined into an approximate 3-D solution.

Experimental Observation of Reactive Flow in Single Fractures

Many critical questions regarding the fundamental process of reactive flow along single fractures can only be addressed experimentally, using digital imaging

Figure 3. 3-D view of the nuclear test cavity and near-field environment, showing selected groundwater streamlines that move through the collapsed cavity (18 meters in radius). Maximum concentrations of plutonium and certain other radionuclides occur in the melt-glass volume, which is found at the base of the cavity. The direction of flow is from upper left to lower right. Streamline age is travel time along the streamlines; the variegated character of the near-field environment reflects its heterogeneous permeability.

techniques and highly resolved profilometer measurements of pre- and post-flow fracture surfaces. In this study, experimental reactive flow of a dilute carbonic acid solution along a single fracture through Carrara marble, together with non-reactive flow simulations for measured aperture topographies, led to several important discoveries relevant to simulator development.

Of greatest significance was the discovery that mineral dissolution along fracture surfaces caused a *decrease* in mean fracture aperture and permeability. This finding, initially counterintuitive, is attributable to the fixed-stress boundary condition of the experiment, which becomes increasingly relevant with depth. Here, as opposed to the fixed-displacement boundary condition (characteristic of shallow environments), the mean aperture decrease from mineral dissolution at fracture contacts predominates local aperture increase from dissolution along disconnected fracture surfaces. This observation has enormous ramifications for reactive-transport models; it suggests that without explicit account of stress-field effects, the (implicit) fixed-displacement boundary condition for fracture flow may lead to predictions of reaction-dependent porosity/permeability evolution that directly oppose reality in deep geologic systems.

Another important result of this study involves the scale dependency of flow evolution, which was revealed by comparing

flow simulations executed for the measured initial and final aperture topographies. These simulations, based on Reynolds approximation to the Navier–Stokes equation, illustrate that on a fine (micron-to-millimeter) scale, dissolution decreases the mean tortuosity of flowpaths, in effect smoothing the background flow pattern. In contrast, at the coarse system (40–80-millimeter) scale, maximum dissolution and flow are localized within a broad central channel, distinctly superimposed on the relatively uniform fine-scale flow pattern. These observations underscore the potential significance of multiscale flow within both fractures and bounding matrix blocks.

A Suite of Numerical Laboratories for the 21st Century

Advanced reactive-transport simulators represent an invaluable resource for addressing many critical issues; these include subsurface contaminant migration, geologic carbon sequestration, and fundamental challenges in the petroleum, geothermal, and mining industries. LLNL has established a significant and growing presence in this emerging research area. As our simulators mature, this suite of numerical laboratories will play an increasingly central role in diverse exploration, production, containment, and remediation activities.

Figure 4. 3-D perspective of predicted total aqueous plutonium concentrations in the downstream near-field environment 600 years after detonation of the nuclear test. Concentrations increase from purple to green to gold (M = molarity). Flow proceeds from left to right. Maximum plutonium concentrations emanate from the melt glass at the bottom of the cavity.

Climate, Carbon, and Energy Overview

William Dannevik

The balance of evidence suggests a discernible human influence on global climate.” This now-famous conclusion in the 1995 Assessment Report by the Intergovernmental Panel on Climate Change (IPCC) has ignited a global debate about the likelihood of significant climate change induced by human activities, and what should or should not be done about it (see Figure 1). This controversy, coupled with the increasing use of fossil fuels, is shifting the center of gravity in energy policy formulation from the question, “Will there be enough affordable energy?” to “How clean will energy have to be, and will the clean energy still be affordable?”

If there is any agreement among the stakeholders in the contentious energy–climate policy debate, it is that the scientific basis of the debate is not adequate. In part, this inadequacy exists because we cannot perform controlled experiments on the climate system that will allow us to correlate the magnitude and timing of climate changes with changes in atmospheric chemical composition. Instead, we must depend largely on imperfect computer simulations. The reliability of these simulations must be greatly improved in just a few years if policy decisions in this area are to be timely, effective, and affordable. Informed decisions will require a systems approach that links the results of the simulations with analyses of the feasibility and costs of various “carbon management” strategies.

The national laboratories, and LLNL in particular, are poised to enhance the scientific basis of the climate–energy policy debate. LLNL has much of the requisite disciplinary expertise in-house, and is a leader in development and application of the powerful high-performance (“terascale”) computing systems required for problems such as climate prediction, combustion simulation, and related modeling challenges.

The E&ES Directorate plays a vital role in LLNL’s efforts to address these challenges. Our role comprises three interrelated elements: (1) development, evaluation, and application of advanced climate system models; (2) research into the biogeochemical linkages between greenhouse-gas emissions and the behavior of the climate system, including the management and sequestration of carbon; and (3) investigations of the feasibility of alternative energy sources having lower carbon intensity. Some highlights of recent work are given below.

Advanced Climate System Models

The Program for Climate Model Diagnosis and Intercomparison (PCMDI) has developed an advanced method for diagnosing the forcing and feedback functions in climate-change experiments that avoids the expensive, multiple simulations required by traditional approaches. The method uses a highly idealized radiation code and readily available mean-monthly model outputs to calculate the sensitivity of climate to changes in greenhouse gases and aerosols and variations in water vapor, clouds, snow cover, and sea ice. It includes fluxes of infrared and solar radiation, temperatures, and cloud fraction. In a test case the new method has been found to be accurate to within about 10%. It can therefore be routinely used to analyze forcing, feedbacks, and response in climate-change experiments, since the computational resources required are insignificant. The method is particularly useful for decade-to-century-long climate model simulations.

Initial applications of the method have already yielded results. Simulations of the last glacial maximum (~20,000 years ago)

explain the similarities in sensitivities demonstrated by different models subjected to the same changes in surface boundary conditions (for example, changes in ice coverage). An extension of this method is being developed to analyze coupled climate model experiments. The method's computational advantages for this application will reduce by several fold the number of experiments that will be needed.

Climate Variability

The Climate System Modeling Group has compared observations of climate variability with the variability exhibited in 17 model simulations. The comparisons have yielded two significant results. (1) Temperature variations observed in simulations that used "flux adjustments" (computational adjustments made to conserve momentum, energy and mass over a yearly cycle) were similar to those seen in simulations that did not. Thus, the evidence does not support the hypothesis that flux adjustments suppress temperature variability in climate models. (2) Almost all simulations underestimated air-temperature variability over oceans and overestimated the variability over land. These are significant, systematic, and previously unrecognized errors. This work soon will be extended to include a prototype of the next-generation climate model as part of the new DOE Accelerated Climate Prediction Initiative.

Carbon Dioxide in the Oceans

We have developed additional insights into the likely fate of anthropogenic carbon dioxide (CO_2) absorbed into the southern ocean. Comparisons of simulations with measurements of ocean carbon made in collaboration with the LLNL Center for Accelerator Mass Spectrometry (CAMS) and other institutions suggest that the southern ocean is an important locus of CO_2 uptake but not of storage. Most of the CO_2 appears to end up in the Antarctic convergence. This

may have important implications for the role of the southern ocean in future CO_2 uptake if, as predicted, the surface waters warm and the extent of seasonal sea ice diminishes.

El Niño Analyses

The distribution of radiocarbon in the ocean is a powerful tracer of ocean circulation dynamics and related atmospheric climate variability. CAMS scientists have used carbon-14 time series determined from Galapagos Island coral to investigate the apparent shift in the frequency and intensity of the El Niño/Southern Oscillation (ENSO) that occurred in the mid-1970s. We have found that the amplitude of the seasonal variation of carbon-14 increased markedly from the middle 1950s to the middle 1970s, and then declined abruptly after 1976. The latter change appears to be correlated with the change in ENSO frequency and magnitude. This analysis will be extended to the period from 1978 to the present, and to the period 1890–1910, which was a time of frequent El Niño events.

Figure 1. The Northern Hemisphere has been warmer in the 20th century than in any other century of the last thousand years, according to this reconstruction of the hemispheric temperature record by scientists at the University of Massachusetts and the University of Arizona. The sharp upward jump of the last 100 years was recorded by thermometers at and near the earth's surface. Earlier fluctuations were reconstructed from "proxy" evidence of climatic change contained in tree rings, lake and ocean sediments, ancient ice, and coral reefs. (From M.E. Mann et al. [1998], "Global-Scale Temperature Patterns and Climate Forcing over the Past Six Centuries," *Nature* **392**, 778–787.)

Fundamental Physics of Hydrates

Using a synthesis technique pioneered at LLNL, we are continuing measurements of the fundamental physical properties of methane hydrates and other hydrates, including strength, elastic, and thermal properties; species diffusivity; and dissociation kinetics. We now know that methane hydrate is far stronger than normal water ice, the material to which it is often compared. We will be expanding these measurements to include hydrates of natural gas and of carbon dioxide, and will be studying mixtures of hydrates, sediments, and sea water that more closely match the settings for hydrates existing in nature. The studies have important implications for energy reserves, climate, and the stability of the ground in some regions.

Geothermal Energy

We are “mining” LLNL technologies developed in other program areas to apply and extend them to problems in geothermal energy exploration and production. For example, we are evaluating the applicability of multispectral imaging to detect plant stress induced by upflow from geothermal fault zones and monitoring hydrogen sulfide at geothermal power plants using cross-dispersion infrared spectroscopy. In addition we have identified possible electrical signals from fluid-transport mechanisms associated with boiling in super-permeability zones. In the future, we will apply rock mechanics and fluid-flow modeling, along with capabilities for measuring deformation such as InSAR (synthetic aperture radar), in a new DOE effort to enhance geothermal production systems.

New Initiatives and Opportunities

The DOE is launching several new initiatives in the climate-carbon-energy cycle area. The Accelerated Climate Prediction Initiative (ACPI) is a major element of the FY00 Scientific Simulation Initiative, and LLNL climate scientists and managers are playing crucial roles in the ACPI program design and implementation planning process. The new LLNL strategic initiative in Multiscale Climate Prediction will align our expertise with and develop tools for a significant role in the execution of ACPI. We will partner with other U.S. Global Change Research Program participants in this effort. In collaboration with the National Science Foundation’s National Center for Atmospheric Research (NCAR) and the National Aeronautics and Space Administration (NASA) Data Assimilation Office, we have already started a project to parallelize and evaluate the performance of an advanced climate-model dynamics algorithm for a new-generation Climate System Model.

We have proposed that DOE fund the “National Center for Research on Ocean Carbon Sequestration,” as part of the DOE Climate Change Technology Initiative. This Center would be operated jointly with Lawrence Berkeley National Laboratory (LBNL) and several academic collaborators. In partnership with LBNL and NCAR, PCMDI has proposed a pilot project to apply distributed database and next-generation Internet technologies for management of large climate-model and observational databases that will be typical of the ACPI analyses. Collaborations in these and other projects with other LLNL components such as the Computations and Energy Directorates, and with other DOE laboratories, universities, and private industry, will allow us to build an integrated, multidisciplinary approach to manage a large-scale system that will become increasingly important to the nation’s interests in the next century.

Global Atmospheric Temperature Change: Estimating the Observational Uncertainties

Over the past 100 years, atmospheric temperatures within a few meters of the earth's surface have been monitored by thermometers at thousands of locations worldwide. The record of atmospheric temperature changes well above the earth's surface is much shorter. Since the late 1940s, weather balloons (radiosondes) have made direct measurements of tropospheric (from the earth's surface to 10–20 kilometers high) and lower-stratospheric (from the troposphere to about 30 km) temperatures at several hundred stations. However, the radiosonde and surface thermometer networks both have large gaps in space and time, which introduce errors in estimates of global-scale temperature changes. These observational uncertainties make it difficult to evaluate how well computer models simulate present-day climate and project future climate changes. Accuracy is important because the projections may influence significant national decisions about actions to be taken to mitigate human-induced climate change.

Discrepancies in the Temperature Records

Since 1979 polar-orbiting satellites have provided the capability to monitor atmospheric temperatures on a truly global scale. Typically, satellite temperature measurements are vertically weighted averages over a considerable depth of the atmosphere. They are not the same physical quantity as the near-surface temperatures monitored by surface thermometers. Recently, scientists have also used numerical weather prediction (NWP) models to study global-scale atmospheric temperature changes. Such “reanalyses” typically combine an NWP model with radiosonde, satellite, and surface-based observations to extrapolate information to data-poor regions.

Since the Second Assessment Report of the Intergovernmental Panel on Climate Change in 1996, scientific and popular attention has focused on the interpretation of discrepancies that exist among the temperatures estimated from these different measurement systems. Some have suggested that, over the last 20 years, there is a significant discrepancy between the surface warming of roughly 0.2–0.3°C/decade recorded by thermometers and the slight cooling of the lower troposphere inferred from radiosondes and satellites. Even though the latter actually show a slight warming when data for 1998 are included, this apparent discrepancy over the short period of the satellite record has been used to cast doubt on the reliability of the much longer surface thermometer record, which shows warming of roughly 0.5°C over the last century. Others have claimed that the differential temperature changes at and above the earth's surface are partly related to inhomogeneities in the satellite data. A variant of the latter interpretation proposes that this discrepancy is not wholly due to data-quality problems in the satellite and/or surface data, but may in part arise from real physical processes that cause different temperature effects at the surface and in the lower troposphere.

Why are these issues important? Recent studies that consider whether human activities have affected global climate rely heavily on observed records of temperature change, both at the earth's surface and in the free atmosphere. If these records are seriously flawed, then the studies that use them may have reached incorrect conclusions. Furthermore, without knowing the size and structure of observational uncertainties in atmospheric temperature, it is difficult to evaluate how well current models simulate present-day climate. It is even more difficult to assess

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the uncertainties inherent in model projections of climate changes over the next century. Given the importance of these studies in national decisions about the mitigation of human impacts on climate change, it is imperative to:

1. Quantify the observational uncertainties that currently exist in the individual estimates of atmospheric temperature change obtained from satellites, radiosondes, reanalyses, and the surface thermometer network.
2. Identify the issues that impact comparisons of temperatures estimated from different measurement systems (for example, differences in spatial coverage and in the atmospheric layers monitored).
3. Better understand the physical processes that might contribute to different temperature changes in different atmospheric layers.
4. Determine whether statistically significant differences exist between observed atmospheric temperature changes and those predicted by climate models.

Comparison of Datasets

Our recent research, in collaboration with scientists at the National Center for Atmospheric Research, the Hadley Centre for Climate Prediction and Research, and the National Oceanic and Atmospheric Administration's (NOAA) Air Resources Laboratory, has primarily addressed the first two issues. We used the following datasets:

- Temperatures from the satellite-based Microwave Sounding Unit (MSU), which uses the upwelling microwave radiation from oxygen molecules to monitor the vertically weighted temperature of the lower stratosphere, the mid troposphere, and the lower troposphere.
- Actual temperatures at specific pressure levels from two radiosonde datasets, each with a different spatial coverage.

- A third radiosonde dataset comprising so-called "virtual" temperatures computed from the height differences between specific pressure levels.
- Actual temperatures at specific pressure levels from reanalysis projects performed by the National Center for Environmental Prediction (NCEP) and the European Centre for Medium-Range Weather Forecasts (ERA).

We wanted to compare these disparate datasets in a way that isolated their true temperature differences—in other words, in a way that accounted for any differences in spatial coverage and for any differences in the vertical extent of the atmospheric layers that they sampled. We therefore computed "equivalent" MSU temperatures from the NCEP and ERA reanalyses and the Hadley Centre radiosonde data. This was done in two ways: first using vertically weighted averages of simple global-mean profiles (one profile for each of the three MSU layers), and then with a more complex radiative transfer code, which more closely approximates the processing steps involved in computing the actual MSU temperatures. To look at the effect of differences in dataset coverage, we imposed the incomplete coverage of the sparsest radiosonde dataset on the globally complete MSU and reanalysis datasets.

These tests allowed us to estimate the temperature-change uncertainties arising from differences in measurement systems (radiosondes versus satellites versus reanalyses), versions of the MSU and radiosonde data, spatial coverage, and methods used to compute an equivalent MSU temperature.

Model Sources of Discrepancy

One of our first findings was that there are serious problems with certain aspects of the layer-average atmospheric temperatures in the two reanalyses. This is particularly evident in the case of NCEP's lower stratospheric temperatures, which are quite different from radiosonde temperatures

prior to 1979 (Figure 1). This offset is related to the assimilation of satellite data in the NCEP reanalysis. Satellite data became available toward the end of 1978 in the northern hemisphere and a few years earlier in the southern hemisphere. When the satellite temperature retrievals are assimilated by NCEP's NWP model, they have two effects: they markedly improve certain aspects of the model's simulation of the lower stratosphere, but they also introduce a large bias in the tropics. The net effect is to introduce large, spurious changes in the global-mean temperature of the lower stratosphere toward the end of the 1970s. Any climate-change detection study that relies on these data will yield erroneous results.

The “linear trend” is one statistical metric that is frequently used to characterize temperature changes over some specified period or to compare changes in different datasets. Previous comparisons of lower-tropospheric temperature changes during 1979–1996 have claimed that the small cooling trends in MSU and radiosonde data are in close agreement. This agreement is often interpreted as evidence supporting the reliability of trends estimated from MSU.

Such comparisons typically neglect differences in data coverage. However, these differences can have an important effect on levels of trend agreement. For example, we found that two versions of essentially the same raw radiosonde data had very different lower-troposphere trends over 1979–1996 ($+0.040^{\circ}\text{C}$ and $-0.037^{\circ}\text{C}/\text{decade}$, respectively), primarily due to large differences in their spatial coverage. We also found that the choice of the statistical method to fit a linear trend to the data affects the trend agreement between MSU and radiosondes. Other uncertainties arise from residual inhomogeneities in the radiosonde data.

All of these sources of uncertainty make it very difficult to use trend comparisons between MSU and radiosondes to draw

inferences about the reliability of short (20 years or less), relatively small trends in the temperature of the lower troposphere.

One hitherto puzzling aspect of the MSU data is that in some versions, the mid troposphere warms relative to the lower troposphere. The converse is the case in all of the radiosonde and reanalysis datasets we examined. Accounting for the orbital decay of the satellites carrying the microwave sensor resolves this discrepancy.

In the lower troposphere, the overall temperature changes over the past 20 years have been relatively small compared with the much larger year-to-year changes associated with phenomena such as El Niño. One consequence of this is that adding or excluding a year of data can in some cases change the sign of the trend. So-called “confidence intervals” are a way of expressing the purely statistical uncertainties inherent in trend estimates—they say nothing about how well we might know the

Figure 1. Temperature changes in the lower stratosphere for 1958–1997, estimated using different measurement systems: weather balloons, satellites, and weather-prediction models. All results are expressed as seasonal anomalies relative to long-term seasonal averages over 1979–1993.

cause of the trend, or the likelihood that it will continue in the future. There are various ways of estimating confidence intervals, and the most appropriate involve accounting for persistence of the data from year to year or from season to season. When this is done, we find that the 95% confidence intervals on recent lower-tropospheric trends span a wide range of positive and negative values (Figure 2). This range encompasses both “zero trend” and the positive trends of around 0.08–0.03°C/decade predicted in

climate model experiments attempting to simulate historical changes in carbon dioxide, aerosols, and stratospheric ozone. Thus our present research does not support claims that the temperature trend in the lower troposphere over the last 20 years is known to within a few hundredths of a degree Celsius per decade. Nor does it support the contention that observed lower-tropospheric temperature trends over the last 20 years differ significantly from the trends predicted from climate model experiments.

Figure 2. Lower-tropospheric temperature trends and estimated 95% confidence intervals in various satellite, weather balloon, and reanalysis model (NCEP, ERA) datasets. Trends (shown by circles and diamonds) and their associated confidence intervals were calculated with both seasonal-mean and annual-mean anomaly data over 1979–1993. Linear trends are standard least-squares estimates; the 95% confidence intervals are adjusted for the persistence in the data. Notes: ^aComputed with a complex radiative transfer code; ^bComputed with a simple weighting function; ^cSampled with incomplete coverage in one weather-balloon dataset.

Real Sources of Discrepancy

The large statistical uncertainties for estimates of linear trends, when combined with other sources of uncertainty (such as those arising from coverage differences), make it difficult to determine whether there is a real discrepancy between recent temperature changes at the surface and in the lower troposphere, and if so, what its likely cause or causes might be.

Possible sources of any discrepancy are remaining errors in the surface data and/or the MSU and radiosonde data themselves. However, even if the surface and lower-tropospheric temperature data are perfect, the temperature changes at and above the earth's surface are unlikely to be identical on timescales of one or two decades. Our work and that of others have shown that there are regions in which temperatures at the surface and aloft do not vary in concert (Figure 3). Natural modes of climate variability, such as El Niño and the North Atlantic Oscillation, have different temperature effects at different locations, on different timescales, and at different heights above the earth's surface. Other physical processes can also lead to localized "decoupling" of near-surface and tropospheric temperatures. These include formation of temperature inversions and low-level marine stratus clouds, and the transport of warm air masses over relatively cool ocean regions. Human-induced climate forcings, such as stratospheric ozone depletion, may also have different temperature signatures at the surface and aloft.

Our research to improve our understanding of these issues will continue through analyses of observational data and climate model simulations.

Figure 3. (top) Correlation between temperature changes close to the earth's surface and in the lower troposphere. Correlations were computed using monthly-mean temperature data from the NCEP reanalysis. Temperature data spanned the period 1979–1993 and were in the form of anomalies relative to the average monthly means over this period. Red denotes areas where the time series in the two atmospheric layers vary in a similar way. (bottom) The time series at a point where there is relatively low correlation between the average temperature–time series in the two layers.

Environmental Risk Reduction Overview

Dave Layton

Man-made and natural hazards ranging from groundwater contamination to earthquakes pose a variety of health and environmental threats. Moreover, as shown in Figure 1, such hazards have widely varying spatial and temporal scales, which further complicates efforts to assess the nature and magnitude of the hazards' impacts and devise prevention or mitigation measures. Although no single research organization has the capabilities for dealing with the full range of environmental risks and disasters, the E&ES Directorate has the multidisciplinary expertise, science base, and operational experience to address a very large subset of them. Historically, our scientists have conducted research that addresses the key elements of the environmental risk reduction process: (1) the development of experimental

and computer-simulation techniques for characterizing hazards and their risks, and (2) the development and application of technologies for risk mitigation. Summaries of selected projects and initiatives in E&ES pertaining to the reduction of environmental risks follow.

Reducing Risks through Improved Predictive Capabilities

Our participation in NASA's Global Modeling Initiative (GMI) is a good example of the use of advanced simulation capabilities to address important environmental issues. The basic purpose of this multi-investigator assessment project is to predict the effect of emissions from future high-speed civil transport aircraft on the distribution of important atmospheric chemical species. Since these aircraft fly in the stratosphere, the depletion of stratospheric ozone caused by emissions of nitrogen oxides is of special concern. Our role in this effort was to create a three-dimensional assessment model capable of running on parallel processors to simulate the dynamic chemical and physical processes controlling the distribution of ozone in the stratosphere. The resulting model, which utilizes algorithms and data derived from GMI scientists, has been used to examine the consequences of a proposed fleet of 500 stratospheric aircraft. Figure 2, for example, shows the predicted percentage increase in nitrogen oxide concentrations resulting from aircraft emissions and the resulting percentage decrease in stratospheric ozone. These results are part of a major NASA report currently undergoing international review. Current efforts to add more chemistry and physics will allow us to assess the impact of subsonic commercial aircraft.

Figure 1. The E&ES science base, with its multidisciplinary expertise and operational experience, provides capabilities for addressing a wide range of man-made and natural hazards (E&ES projects are shown in red).

Another example, the National Wildfire Prediction Program (NWPP), is a unique new collaborative effort involving the Atmospheric Release Advisory Capability (ARAC) at LLNL and the Wildfire Modeling Team at Los Alamos National Laboratory (LANL). The basic goals of this program are to provide a resource for around-the-clock assistance to firefighting across the U.S. and to prepare special predictions and simulations that can be used for guiding controlled burns to manage fuels (dry biomass), managing forests, and training firefighters. The NWPP would utilize ARAC's emergency response infrastructure and LANL's wildfire models to predict the behavior of wildfires in order to help fire managers decide on the most effective firefighting strategies. The information would be available nationally to all required levels of firefighting management via interactive Internet access. Given the enormous costs of fires nationwide (in 1998 wildfires in Florida alone caused over \$400 million worth of damage), such a program would represent a national technical resource that could save lives, optimize limited firefighting assets, and reduce fire damage.

Two other efforts that the directorate supports in the area of environmental risk reduction are the Hazards Mitigation Center, which was formed in 1998 as a multi-directorate initiative, and the Center for Fuels Assessment, which is a joint program-development effort with LLNL's Energy Directorate. The underlying goal of the Hazards Mitigation Center is to be "an important contributor to the nation's ability to understand, plan for, mitigate, and respond to natural and man-made hazards." A special capability of the Center is its collection of analytical tools for predicting the ground motion caused by a seismic event and the response of structures to that motion. For example, sophisticated models are available for completing three-dimensional simulations of earthquake scenarios (for example, a magnitude 7.1 earthquake on the Hayward fault) and the nonlinear transient responses of suspension bridges to earthquakes. By combining predictive capabilities for both

ground motion and structures, Center staff are able to evaluate the response of alternative structural designs to realistic earthquake ground motion. The resulting designs will reduce earthquake-induced damage to life and property without introducing unnecessary construction or retrofit costs.

The Center for Fuels Assessment, also initiated last year, uses our multidisciplinary expertise in the earth and environmental sciences to scientifically assess the health and environmental risks of new or modified transportation fuels prior to their introduction. The need for such assessments has been underscored by the current concerns about groundwater contamination resulting from the subsurface storage of reformulated

Figure 2. Predicted changes in nitrogen oxide levels in the stratosphere due to aircraft emissions (*top*) and the associated changes in ozone (*bottom*).

gasoline containing the oxygenate methyl tertiary butyl ether (MTBE). We are now developing a methodology for predicting the impacts of diesel fuel additives designed to reduce particulate emissions. The reduction of these emissions is one of the key challenges facing this engine technology, and we believe that a Center for Fuels Assessment can provide the studies needed by the Department of Energy and oil companies to select environmentally sound additives.

Reducing Risks through Improved Measurement and Treatment Technologies

Technologies for risk reduction can be broadly grouped into two categories: those that provide critical data needed to assess a given hazard and those that mitigate it. In the first category, the Center for Accelerator Mass Spectrometry provides E&ES scientists with a unique capability to measure extremely low levels of several long-lived isotopes. Of particular interest is carbon-14, which can be incorporated into organic compounds in very small amounts so that their disposition (for example, their distribution and metabolism) can be evaluated at levels appropriate for environmentally relevant exposures to the substances. In contrast, the detection limits of standard scintillation techniques for measuring carbon-14 are orders of magnitude higher; consequently, toxicokinetic studies using this technique necessarily involve rather large extrapolations to environmentally relevant exposures. Using directorate Laboratory-Directed Research and Development funding, we are also developing accelerator mass spectrometry and related chemical preparation techniques for measuring plutonium-239 at levels likely to be found in environmental and biological samples. Initial results from this project are very encouraging, and if we are successful, we will achieve our goal of

detecting as few as 1 million atoms per sample. Sensitivities of this order will allow us to conduct a variety of new health and environmental studies involving this long-lived nuclide.

Our most notable technology for risk mitigation involves thermal degradation of organic contaminants in soil and groundwater. In this process, destruction of subsurface contaminants occurs through hydrous pyrolysis/oxidation (HPO) reactions, which have proven to be very effective in treating substances difficult to remove using conventional pump-and-treat methods. Demonstration of the HPO process at the Visalia Pole Yard in southern California has been an unqualified success. The Visalia cleanup is now in the final stage, cleaning the "floor" on the bottom of the site. More than 115,000 gallons of creosote have been removed from a volume of approximately 600,000 cubic yards. This is almost three times the initial estimate of 40,000 gallons. Some free product is still being recovered.

The project has attracted national attention, and the EPA has formed a standing working group composed of experts and providers of thermal remediation services; two E&ES personnel are members. This group will aid other EPA-led sites in designing thermal cleanups. Designs are under way for two Superfund pole-treatment sites in Washington and California. In addition, two privately controlled sites are being addressed in Washington; our licensees are performing this work. On the solvent cleanup side of the problem (our initial DOE interest), trichloroethylene cleanup at the Portsmouth, Ohio, diffusion plant is under way, and a project for the Savannah River site is scheduled to begin this fall. A demonstration at Cape Canaveral, in parallel with six-phase electrical heating and permanganate oxidation, will begin next year.

Biological Applications of Accelerator Mass Spectrometry

The first application of accelerator mass spectrometry (AMS) in biomedical research was published nine years ago by a group of LLNL scientists. This initial work led to successes in assessing the dosimetry of chemical carcinogens, determining the pathways and bioavailability of such compounds, developing supporting technologies, and applying these tools with collaborators from a wide variety of academic and professional disciplines. Of the four full-time AMS facilities in the United States, only the LLNL Center for Accelerator Mass Spectrometry (CAMS) has demonstrated a serious interest in applying the technology to biomedical problems. CAMS is now recognized as the world leader in a technology that can address fundamental issues of environmental and biomedical science, improve risk assessment, and change research and clinical practices. This technology development and dissemination, coupled to the needs of scientific users, is an appropriate mission for LLNL and is of particular value to UC. The Office of the President of UC has described CAMS as the most successful Campus-Laboratory collaboration.

In parallel with this core scientific research, CAMS scientists have led the technological advances necessary to make AMS a more effective, dependable, and economic tool for the biomedical, pharmaceutical, chemical, and clinical communities. These successes were a major factor in establishing AMS as a routine biomedical research tool whose operation does not require the presence of a large and expensive staff of physicists and technicians.

New Applications and Techniques

AMS was originally applied to life sciences by LLNL scientists to attain the detection sensitivity needed to study the molecular damage caused by chronic low-dose exposure to environmental carcinogens and pollutants. AMS is now being used to establish the relevance of animal models through the direct study of natural product and xenobiotic metabolism in humans. The use of radiocarbon-labeled molecules and AMS provides 100 million times greater sensitivity than stable-isotope labeling techniques and 1 million times greater sensitivity than decay counting of radioisotopes. Initial studies using agents labeled with carbon-14 (^{14}C) show that radioactivities as low as a few nanocuries (nCi) per person can be used to assess metabolism, and activities as low as 100 nCi/person can be used to address macromolecular binding in the study of candidate drugs or toxicants. This level of radioactivity is less than that from a single day's exposure to background ionizing radiation or from a single chest x-ray. Thus, AMS opens the door to many studies of molecules of biological significance that can now be conducted safely and with great sensitivity and precision at very low dosages in humans.

As we conducted these and other studies at CAMS, we developed and refined the AMS technology for biological applications. Our accomplishments include

- Development and demonstration of the microchemistry protocols needed for routinely handling and preparing organic samples of 50 nanograms (ng, one-billionth of a gram) to 1 milligram (mg, one-thousandth of a gram) in weight. (These may vary over 6 orders of magnitude in isotope concentration.)

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- Routine use of sealed-tube graphitization techniques that allow simple and rapid production of hundreds of samples on a daily basis.
- Development and routine operation of very reliable, computer-controlled high-current spectrometer components.
- Measurements of separate molecular fractions isolated by analytical techniques such as high-performance liquid chromatography (HPLC).

Tracing Chemicals in Humans

Two recent research projects highlight the value of AMS as a method to trace the passage of chemicals through humans without disturbing normal metabolic processes. We applied this method to two different problems in the past year: assessing the dermal uptake, excretion, and metabolism of a herbicide; and determining the disposition of vitamins at physiological levels in individual humans.

Pesticide Excretion and Metabolism

Each year millions of pounds of pesticides and herbicides are used in the United States. Exposure to residues of these chemicals in food and drinking water is monitored and generally considered to be safe. However, occupational exposures to agricultural and chemical production workers can be considerably higher than exposures to the general population. Workers' families can also receive high exposures if work clothes are worn home and washed with general family laundry.

An ideal exposure assessment assay would use samples obtained non-invasively (urine or saliva, for example) and be sensitive to environmental doses. It would identify the specific metabolite or class of metabolites

most dominant within the time frame of the target exposure and sampling window. (An assay that identifies a class of compounds is often more desirable than one that identifies a specific one. Variations in metabolism among individuals are less problematic when an analyst can detect a class of compounds and address a wider range of conditions, such as dose and time after dose.)

The value of this sensitive assessment technique was demonstrated in a 1998 pesticide study. Researchers at UC-San Francisco, UC-Davis, and Novartis Crop Protection conducted a 24-hour human dermal exposure trial using ^{14}C -labeled atrazine, a common herbicide. The aims of this study were to determine the major metabolites in urine and ultimately develop an occupational exposure assay. Unfortunately, the subjects in the trial absorbed less atrazine than expected and the radioactivity of the urine was often too low to count efficiently using liquid scintillation counting (LSC). Hopes of separating and determining the dominant metabolites waned and the samples were stored in a freezer.

The levels of ^{14}C -labeled atrazine metabolites in the collected urine samples, although too low for quantitation by LSC, were ideal for AMS. Excretion rates for atrazine equivalents (parent compound and all metabolites) were determined and time points for the analysis of metabolites were selected (Figure 1). Samples from a subject in this study were chromatographically separated by HPLC to observe differences in metabolite profiles during exposure, a day after exposure, and several days after exposure. The quantity of ^{14}C in each fraction was measured by AMS (Figure 2). Co-elution with known standards allowed tentative identification of the metabolites. The AMS application showed that chromatographic separation of metabolites mated with AMS sensitivity is an effective

method for determining the important metabolic biomarkers needed for developing a field assay for occupational exposure.

Carotene from Spinach Traces Retinoids in Humans

A nutrition study with UC–Davis scientists demonstrated the value of single-bolus administration of ^{14}C -labeled compounds to find the detailed metabolic pools through which vitamins pass throughout their long life in the body. Vitamin A (retinol) is required for the continual reproduction of our epithelial system—the “latex glove” of our respiratory, esophageal, and excretory systems that protects us from infections by sloughing off the infected outermost layer for disposal. Retinol is available from red meats, but the primary source is dark and colored vegetables that contain beta-carotene, which is metabolized to retinol.

A single dose of beta-carotene (0.98 mg, 200 nCi) from spinach grown in a ^{14}C -labeled atmosphere was given to a human subject. Blood, urine, and feces were collected for 3 months after the dose. Figure 3 shows the plasma concentration of ^{14}C -labeled carotene and/or retinoids over that time period. Three primary pools are easily seen: the first Gaussian peak is due to carotene metabolism to retinol in the intestine. This component moves freely in and out of the gut and is quickly excreted. The primary plasma pool maximizes during the day after dosing, but is drawn into a deeper pool, perhaps the muscular tissue, over the next 5–10 days. This pool is slowly metabolized back to a circulating form with a 38-day half-life. The absorption of the primary circulating pool into the “tissue” is confirmed by the integral of the concentration curves, showing that the

Figure 1. Uptake and elimination of ^{14}C -labeled atrazine following dermal exposure in a human volunteer. Carbon-14 excreted in urine and quantified by AMS was used to determine the half life of elimination of this herbicide.

Figure 2. The resolution of ^{14}C -labeled atrazine metabolites by HPLC, 24–48 hours after dermal exposure. Major metabolites (at retention times of approximately 20, 28, and 40 minutes) correspond to known mercapturates; the peak at 11 minutes is an unidentified metabolite.

Figure 3. Three identifiable pools of circulation are apparent in the plasma concentrations of ^{14}C -labeled carotene and its metabolites. A Gaussian curve fits the first peak and Bateman functions describe the second and third pools. The total amount of carotene derivatives in the last pool equals that in the peak circulation.

delayed metabolite curve is equal in area to the plasma uptake curve.

This type of experiment was only possible with AMS. No other molecular label can be followed for 3 months within a large unlabeled pool. The existence and equivalence of the slowly changing pool that starts 9 days after dosing would be undetectable without AMS.

Significance to Biomedical Fields

These studies strengthen our belief that AMS tracing will have an expanding future in nutrition, pharmacology, toxicology, physiology, and related biomedical fields. Initially supported by the UC Campus-Laboratory Collaboration Program, they have resulted in proposals and successful grants for more research.

The overall significance of these accomplishments is that we have developed and applied unique measurement techniques to provide quantitative data on the disposition of chemicals at exposure concentrations relevant to humans. These advances allow us to quantitatively compare the applicability of animal models to the human situation. We have demonstrated the ability to measure uptake pathways and the chemical effects of the active agent on the target molecule.

With protocols, techniques, and accuracy that are appropriate for the researchers who pose the problems and interpret the results, we continue to lead

the emerging field of BioAMS. Similar applications can be envisioned in other disciplines, such as exercise physiology, agriculture, gerontology, cardiology, and neonatology. BioAMS can have a significant impact in all these areas by providing increases in sensitivity and accuracy at low concentrations, thereby reducing the isotope exposure of individuals, reducing the need for high-specific-activity probes, and providing unique diagnostic data.

Dedicated BioAMS ^{14}C -Spectrometer

Expanded research can only come with an expansion of AMS capabilities within CAMS. In 1994, the clear conclusion of a DOE-sponsored workshop on the use of AMS in the life sciences was that, while the technology had great potential, smaller, less expensive, bio-dedicated instruments were needed to make significant scientific advances. In addition, simple methods for sample preparation are required, along with tight coupling of the technology development to biomedical research needs. With funds from the Office of Health and Environmental Research at DOE, the UC-Directed Research and Development program, and the LLNL Laboratory-Directed Research and Development program, we have purchased the components of a small ^{14}C -spectrometer (Figure 4). This small spectrometer, currently undergoing installation,

is the core component of a pending Research Resource grant that has undergone favorable review by the National Institutes of Health. This instrument will provide high throughput for biological samples and will serve as a test bed for advanced sample preparation and

delivery technologies. Use of the new instrument for these applications will allow other CAMS programs to proceed more effectively by affording them more measurement time on the large (10-million-volt) research AMS machine.

Figure 4. Diagram of the 1-million-volt ^{14}C -spectrometer currently being assembled at the Center for Accelerator Mass Spectrometry. This spectrometer will provide the foundation for an expanded BioAMS program at LLNL.

National Security Overview

Norman Burkhard

National security work at LLNL focuses on two national priorities: ensuring the safety, security, and reliability of the U.S. nuclear stockpile, and preventing the proliferation of weapons of mass destruction (chemical and biological as well as nuclear). The E&ES Directorate addresses these priorities through programs that we manage directly and discipline support that we provide to the Defense and Nuclear Technology and the Nonproliferation, Arms Control, and International Security Directorates.

Our current national security efforts are direct outgrowths of our combination of discipline strengths in the earth and environmental sciences and our historical involvement in the nuclear testing, peaceful nuclear explosion, and test-ban-monitoring programs. For example, our

- Expertise in atmospheric sciences and experience gained from tracking and monitoring atmospheric releases from nuclear tests and reactors provide the basis for programs addressing the transport and fate of chemical and biological releases into the atmosphere (Chem-Bio Program).
- Experience in conducting technical field programs at the Nevada Test Site (NTS) provides the background for our design and operation of the Remote Sensor Test Range, used to support the development of systems for spectroscopic analysis of weapons-signature materials in the air.
- Support of the nuclear test program and test-ban-treaty monitoring programs for many years has created disciplines and knowledge bases that are the basis for the support that we provide to the DOE Comprehensive Nuclear-Test-Ban Treaty Program and the Defense and Nuclear Technologies subcritical experiments program at NTS (Containment Program).

Many projects in E&ES support national security programs at LLNL. A few are highlighted below.

Preventing and Countering the Proliferation of Weapons of Mass Destruction

Assessing and Mitigating Accidental and Deliberate Atmospheric Releases

We research and develop techniques for real-time tracking of atmospheric releases of hazardous material, and manage and staff a facility for doing so, the National Atmospheric Release Advisory Center (ARAC). ARAC provided information about the Three-Mile Island and Chernobyl reactor releases, continues to support DOE and Department of Defense efforts, and is part of a broad effort to develop effective responses to chemical and biological threats.

ARAC is a national emergency-response service for real-time assessment of incidents involving nuclear, chemical, biological, or natural hazardous material. When a hazardous material is released into the atmosphere, ARAC can quickly map the probable spread of contamination and the resulting exposure, providing the information to the emergency manager.

The Center's primary function is to support DOE and the Department of Defense for radiological releases. It can also assist several other federal agencies. During the past year, ARAC responded to numerous alerts and emergencies and conducted several major exercises working with hypothetical problems in the field. For example, we

- Prepared forecasts for the dispersal of gases and particulates following the Indian nuclear weapons tests in May 1998. An initial 2-day simulation using meteorological observations on a 1600-kilometer grid was extended to 5 days using the U.S. Navy's forecast model.

- Supported the Nassau County Police Department, which was responsible for security at the Goodwill Games. ARAC deployed three assessment meteorologists, each for one week, to the county command center. They demonstrated our real-time dispersion modeling for nuclear, biological, and chemical threats using a portable ARAC workstation. Each day they posted hypothetical real-time calculations as well as “what-if” calculations for the next day based on 24-hour model forecasts.

In a related effort, E&ES supports the DOE Chemical and Biological Nonproliferation Program, which is developing the capability to predict the fate of chem-bio releases both outdoors and indoors. Our focus is the prediction of airflow and dispersion in an urban environment; the extremely heterogeneous surface features within typical population centers make this a challenging problem. We are developing computational fluid-dynamics models to simulate the flow and dispersion of releases around multi-building complexes (Figure 1). Eventually, computer models like those used to produce the figure will be used to assess the transport and fate of urban releases of hazardous agents and to support emergency-response activities.

more than 100 hours of gas-plume time; as many as six different chemicals were released each day. Figure 2 shows the RSTR stack used to release the chemicals in the desired concentrations while maintaining compliance

Figure 1. Model of flow and dispersion of an atmospheric release around a hypothetical building complex. The surface concentration pattern from two line sources of aerosols is shown 240 seconds after the release (orange indicates highest concentration). Such models will be used to assess releases of hazardous agents within urban areas and to support emergency-response activities.

Remote Sensing of Airborne Materials for Weapons Signatures

The Remote Sensor Test Range (RSTR) provides DOE with a facility to field-test remote-sensing techniques. It allows realistic remote-sensor evaluation by creating reliable, controlled test-gas plumes of chemical mixtures at NTS. The RSTR's controlled releases with known concentrations are often used as surrogates for the effluents from nuclear weapons production facilities. These releases are essential to remote-sensor development at several DOE laboratories.

The RSTR project successfully completed the “Mountain Lion” test series this year, supporting simultaneously four aerial and two ground-based remote-sensing collection activities. The test series included 21 test days during which there were 108 releases totaling

Figure 2. The Remote Sensor Test Range provides DOE with a facility to field-test techniques for remote sensing. It allows realistic remote-sensor evaluation by creating reliable, controlled test-gas plumes of chemical mixtures at the Nevada Test Site.

with environmental and safety rules. The stack can be used for scenario simulations involving chemical concentrations from 1 to 1000 parts per million by volume for up to four chemicals simultaneously. No testing days were lost due to malfunctions of the RSTR facility, and the schedule was dynamically modified to maximize user results and balance the needs of the aerial and ground-based systems. The evaluations emphasized the user's ability to detect and characterize potential scenarios that could be indicative of real industrial operations.

Monitoring the Comprehensive Nuclear-Test-Ban Treaty

LLNL is part of a four-laboratory DOE effort to provide the U.S. government with the research and development it needs to meet its Comprehensive Nuclear-Test-Ban Treaty (CTBT) monitoring goals. The goals are to provide a monitoring capability able to detect explosions of a few kilotons, tested evasively; locate them within a region of 1000 square kilometers or less; and distinguish them from other events with high confidence. Our primary customer, the U.S. National Data Center at Patrick Air Force Base, has the mission to carry out U.S. CTBT monitoring.

Our CTBT Program focuses on seismic monitoring for the Middle East and North Africa, hydroacoustic monitoring, and on-site inspections (OSI). Our primary product for the National Data Center is a "Knowledge Base" that will provide region-specific corrections to the seismic-event location and identification algorithms in the data-processing pipeline at the Center. LLNL led the DOE-wide team to develop a mathematical technique, the modified kriging algorithm, that will be the heart of the operation of the Knowledge Base.

Kriging is an interpolation algorithm that we modified to have special properties. The lack of data in some regions requires the use of global averages; if discontinuities exist between regions with data and those without, large errors are introduced into the location and identification algorithms used to identify events. Our modification improves the mechanisms that kriging algorithms use to handle such discontinuities.

Our treatment of non-stationary error is the most significant improvement. Since the accuracy of correction information varies across a region, the uncertainty information must be accurately propagated through the algorithms so that they not only calculate the event location or identification accurately, but also characterize the uncertainty that exists.

In 1998 our first test of the Knowledge Base with real data proved that the concept will be able to meet the U.S. monitoring goals. Using data from published reports for an earthquake-aftershock sequence in the Caucasus Mountains, we showed that our event-location corrections removed approximately 40 kilometers of location bias and reduced the uncertainty of the locations to less than 1000 square kilometers.

In the OSI area, an E&ES member is the U.S. point of contact for issues at the CTBT Preparatory Commission in Vienna, helping prepare and coordinate OSI policy in the U.S. government and then representing these positions internationally. This last year he led the international development of the OSI concept of operations, which cleared the way for work on the operational manual required by the time the treaty is implemented. Several of our personnel are members of other committees and subgroups.

Ensuring the Safety, Security, and Reliability of the U.S. Nuclear Stockpile

Subcritical experiments provide data on the properties of plutonium for use by the Stockpile Stewardship Program of the Defense and Nuclear Technologies Directorate. The Containment Program in E&ES is responsible for developing containment plans for subcritical experiments at NTS so that these experiments can be conducted safely. During the past year, the Containment Program successfully supported the Bagpipe and Clarinet subcritical experiments at NTS. We also worked to develop a new experiment-fielding method that will provide faster experiment turnaround, will be cheaper to field, and will provide a higher level of containment assurance.

Calibrating to Enhance International Monitoring for Clandestine Nuclear Explosions

The Comprehensive Nuclear-Test-Ban Treaty (CTBT), which the United States signed in 1996 but has not ratified, prohibits “any nuclear weapon test explosion or any other explosion” and creates an international monitoring system (IMS) to permit effective international verification of the treaty by searching for evidence of clandestine nuclear explosions. As specified in the treaty, the IMS will consist of 170 seismic stations to record underground elastic waves, 60 infrasound stations to record low-frequency sound waves in the air, 11 hydroacoustic stations to record underwater sound waves, and 80 radionuclide stations to record airborne radionuclide gases and particles. The International Data Center, located in Vienna, receives the data from the IMS system and uses them to detect and locate the sources of any signals that are observed. Applying standard criteria, it also screens the detected events in order to characterize and highlight those events considered to be consistent with natural phenomena or non-nuclear man-made phenomena. The National Data Center for each country may undertake additional verification activities by integrating IMS data with information from its own national sources and applying its own processing techniques and value system to identify events as natural events, man-made but non-nuclear events, or nuclear tests.

The U.S. National Data Center (USNDC) is responsible for U.S. CTBT monitoring. In order to carry out its responsibilities, it is developing an automated process, or “pipeline,” to detect, locate, and identify events. Following the application of this automated process, trained analysts refine the description of the events and communicate the technical analyses to the U.S. national authorities.

At LLNL, we aid the USNDC in its pipeline and analyst-review processes by calibrating IMS seismic stations and networks located in the Middle East, North Africa, and portions of the former Soviet Union. Our primary mission is to enhance the USNDC’s ability to accurately detect, locate, and identify nuclear explosions that may occur underground or in the oceans. Through the DOE CTBT R&D program, in coordination with Los Alamos National Laboratory, Sandia National Laboratory, and Pacific Northwest National Laboratory, we are developing a comprehensive framework of data, models, and algorithms to achieve this goal. A key element of the framework is the Livermore end-to-end statistical model that propagates the primary errors through the automated analysis and accurately quantifies the technical uncertainties in location and identification for the decision maker.

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The Challenge: Regional Variability in Seismic Monitoring Capabilities

Regional variations in the properties of seismic waves are the largest source of uncertainty for seismic monitoring of the CTBT (Figure 1). Unlike the Threshold Test Ban Treaty, which banned nuclear explosions larger than 150 kilotons, the CTBT bans all nuclear explosions. Thus the emphasis has shifted from estimating the yields of large, easily identified nuclear explosions using data recorded at numerous stations throughout the world to detecting, locating, and identifying even the smallest nuclear explosions using data recorded at a few stations located at regional distances (less than about 2000 kilometers) from the explosions. The CTBT monitoring challenge is further complicated by the many earthquakes and mining explosions that generate tens of thousands of seismic signals annually, some very similar to the signals generated by nuclear explosions.

Detection, location, and identification of small seismic events all require a region-specific understanding of the effects of the path between the sources and the recording stations, because the heterogeneity of the earth's crust and upper mantle have significant effects on seismic signals. Thus, we are developing a DOE Knowledge Base (KB) of regional seismic properties as our primary product for the USNDC. This KB will characterize regional variations in the travel times, amplitudes, and frequency content of the seismic waves generated by

small, shallow sources. In addition, we are developing new methods that use this information to discriminate between nuclear and non-nuclear sources.

Location and Identification Efforts

To characterize variations in regional structure, we are developing a comprehensive framework that accounts for dramatic variations in travel times and amplitudes that occur over relatively short distances in the crust—variations that can lead to significant errors in event location and identification. Figure 2 gives a general overview of how we estimate these errors. Calibration events play a critical role in this process.

We begin by cataloging data from historic earthquakes and explosions that are well constrained in space, time, and source characteristics in the DOE KB. We map the variations in amplitude and travel time as a function of geographic coordinate and use this information to refine our models of the earth's velocity structure. These refined models can then be used to predict the travel-time and amplitude variations that will occur along the paths from different source locations to the recording stations. As more events occur over time, we use the additional information to refine the velocity models and improve our ability to account for crustal effects. However, one quickly realizes that the model will never be perfect—since it is determined by limited observational data, it gives only an average estimate of the true earth structure.

Figure 1. Seismic signals such as those from the large nuclear tests of interest prior to the CTBT usually propagate through the simple structure of the deep earth and can be recorded by many distant stations (*left*). Seismograms associated with these events are relatively simple. Under the CTBT, a country may detonate a small nuclear test to attempt to evade the treaty. In such cases, the explosion may be recorded seismically at only a sparse set of nearby stations. The paths for these events are quite complex, as they travel predominantly through the structures of the crust and upper mantle (*right*). We are working to calibrate the CTBT seismic monitoring network for these complexities.

We have developed a set of innovative statistical techniques and algorithms based on a nonstationary Bayesian kriging technique to provide an accurate characterization of the travel times and amplitudes and the uncertainties associated with them. This technique accounts for the nonstationarities in the correction surface (see Figure 2) that exist between geophysically distinct regions, and allows for the introduction of tomographic models. In addition, this technique allows for interpolation and extrapolation and provides robust error estimates for the predictions. Using this technique, we have demonstrated that estimates for a new event co-located with a historic event in the region have minimal error. In the case that the new event is not co-located, but instead is located near a set of historic events, we can provide a robust prediction based on interpolation or extrapolation from the nearby events.

We have demonstrated the benefit of this calibration framework using accurately located aftershock sequences and well-constrained explosions at former nuclear test sites (Figures 3 and 4). Using what we have learned from these focused studies, we have been applying this capability to broad areas of North Africa, the Middle East, and the former Soviet Union. More specifically, we have developed and refined a procedure that involves a number of specific steps, including: (1) collecting all available seismic data; (2) defining geophysical boundaries where propagation characteristics change abruptly; (3) using collected seismic data to develop refined three-dimensional tomographic models of the earth's crustal

and upper mantle structure; (4) calibrating the magnitude scale; (5) applying magnitude and distance corrections; (6) determining detection capability for each seismic phase; (7) evaluating and optimizing seismic location and identification measures; and (8) establishing independent source information to avoid circularity in testing location and identification performance. Although each step in this calibration procedure requires much effort, once all are done, we integrate all the information into a station-correction surface using a modified

Figure 2. Bias uncertainties can cause locations to be in error and can cause overlap in the earthquake and explosion populations used to discriminate an event. To correct for these travel-time and amplitude biases, we utilize this statistical framework. Ground truth events are cataloged in our database and then used to refine earth models that can be used to predict travel-time and amplitude anomalies for seismic phases. We account for model errors by adding correction surfaces using a nonstationary Bayesian kriging technique, which robustly interpolates and extrapolates corrections spatially and can provide an accurate representation of the error in prediction.

Figure 3. Our comprehensive framework to improve the location of clandestine nuclear tests using the IMS: optimal two-dimensional (2-D) velocity models for all stations (left); 2-D and 3-D tomography of the crust and upper mantle to further refine our models (right).

form of kriging to interpolate and extrapolate corrections to a new event of interest. To date, all comparison studies at LLNL and Los Alamos National Laboratory have shown that the model combined with nonstationary Bayesian kriging outperforms other conventional approaches.

Calibration Opportunities and a Planning Tool

The DOE effort is entering a new phase in which field calibration projects are becoming more critical to its CTBT mission.

As discussed above, we have already collected the majority of easily available over-the-Internet historic data from the Middle East, North Africa, and the former Soviet Union and are incorporating many of them into our current calibrations. As this work is completed, the primary improvements to seismic monitoring will come from the installation of stations and from dedicated calibration experiments. Station installations may include new IMS stations coming on line and other supporting stations that may further enhance the IMS network.

Calibration experiments can take various forms. Controlled explosions

Figure 4. The Indian nuclear test on May 11, 1998, is an example of how regional seismic discrimination correction surfaces might work. The seismogram of the nearest earthquake is compared with the possible explosion (*top right*). Note the significant difference in the relative amplitudes of the seismic phases Pn and Lg. We use the Pn/Lg ratio as a discriminant. Measuring this ratio for all regional earthquakes recorded at station NIL, we form a correction surface using kriging (*left*). This correction surface makes the appropriate path corrections so that events in different areas can be compared. When the Indian event occurred we used its geographic location to make the appropriate corrections to the Pn/Lg discriminant and compare the event with other events south of NIL (*lower right*). Note the separation (discrimination) of this explosion compared with the earthquakes; it should extend to much lower magnitudes if future testing occurs.

provide well-defined locations, origin times, and source characteristics. Careful monitoring of known mining areas or the deployment of stations can better constrain the crustal structure in a region. Given such a broad variety of calibration opportunities and a limited level of funding, it is essential that we provide an objective tool to plan and prioritize future station installation and calibration experiments on the basis of their combined benefit and cost.

In response to this need, we have utilized the combined statistical/KB framework described above to develop a planning tool. This tool draws on the entire CTBT KB, including our current state-of-the-art techniques, algorithms, and calibrations. We evaluate our location capability by

synthetically generating the travel times for seismic events spanning a given region. We use our best estimates of observational and model uncertainties in the process. We then relocate these events and estimate the location uncertainty across the entire region as shown in Figure 5. In the identification case, we evaluate capability by mapping the number of suspicious events that need to be reported under assumptions of a specific magnitude threshold and missed-violation confidence. As an added benefit, this tool allows us to objectively measure and report progress to our sponsor as we proceed.

With these tools in hand and our efforts to develop new innovative techniques in location and identification, we are well poised to meet our mission goals in the year 2000 and beyond.

Figure 5. Our planning tool to aid future calibration efforts in location: a kriged correction surface is generated for each station (*left*) and used to account for the inaccuracies in our model; then, utilizing kriging, we propagate uncertainties in the seismic location (*right*). This framework allows us to estimate the actual location performance across a given region.

Basic Science Research Overview

Susan Carroll

The vitality of a large research organization depends upon its ability to recruit and retain top-level employees and maintain and expand its staff's scientific credentials. Collaborations with universities, presentations at national and international conferences and workshops, and peer-reviewed publications all help maintain vitality, and the Directorate encourages and supports these activities. The Directorate also supports principal-investigator (PI)-driven responses to wide calls for proposals. The resulting proposals go through peer-review processes at LLNL, at DOE, or at other organizations. They offer the staff an opportunity to pursue research in areas outside of current programmatic funding; generate internal and external interactions in areas complementary to, but unconstrained by, the immediate goals of LLNL's existing programs; and provide external incentives for maintaining and improving the quality of our efforts.

During 1998, the Directorate had more than 60 PI-driven, peer-reviewed projects, making up \$11.7 million (about 18%) of the Directorate's budget. About 30% of these projects were funded by Laboratory-Directed Research and Development (LDRD). LDRD is a funding source internal to LLNL based on a 6% tax on the labwide budget. This pool of money is divided into three categories: large new scientific directions at Livermore (LDRD-SI) and exploratory research within a directorate (LDRD-ER); institutes designed to stimulate university collaborations

(LDRD-ERI); and science and engineering projects across the Laboratory (LDRD-LW). Projects funded by LDRD reflect the range of science conducted in each division.

DOE's Office of Basic Energy Science, Office of Science, and the Environmental Management Science Program collectively fund about 40% of our PI-driven, peer-reviewed research projects. Our Office of Basic Energy Science portfolio comprises projects ranging from mantle petrophysics to crustal geochemistry. Awards from the Office of Science support research in climate modeling. The Environmental Management Science Program is relatively new, and targets basic research aimed at remediation of DOE lands. Research from this program is highlighted in the following article.

Our largest source of funds external to DOE is the National Aeronautics and Space Administration (NASA). It funds climate modeling and research in the properties of planetary materials. We also receive peer-reviewed external funds for health and ecological assessment from the National Institute of Health, the National Cancer Institute, the U.S. Air Force and Navy, the U.S. Geological Survey, and the Environmental Protection Agency.

The impact of these PI-driven, peer-reviewed research projects on the scientific staff is significant: about one-third of the scientists in E&ES are involved in such projects, many postdoctoral fellows are hired with these funds, and most projects involve external collaboration.

Environmental Management Science Program

The Department of Energy and its predecessors have protected national security through nuclear weapons work for more than 50 years. As a result of some of this work, many DOE sites now have badly contaminated soil and groundwater. The LLNL Environmental Management Science Program (EMSP) was established in 1996 to provide long-term, basic research in disciplines related to environmental cleanup. Its objective is to develop a scientific foundation for the advancement of cost-effective technologies and expertise that could reduce environmental hazards at existing sites. LLNL has six EMSP projects, five of which are in E&ES. All six projects use experimental data to improve the predictive capabilities of modeling codes. The payoff from these projects will apply to other DOE sites and to other government and private sites.

experiments ran for 48 hours in various soil minerals. As shown in Figure 1, temperature had no impact on sorption of strontium in goethite (an iron hydroxide) or in kaolinite (a clay mineral), but a pH above 7 did.

We are using x-ray absorption spectroscopy to study how strontium bonds with various soil minerals and how those bonds change over time. These studies indicate that sorption of carbonate may nucleate the precipitation of strontium carbonate in the pH range in which carbonate sorption on goethite is near a maximum. At higher pH (>8.6), carbonate sorption decreases as dissolved carbon dioxide decreases and hydrated surface complexes, rather than a precipitate, are observed.

Strontium's high mobility had been observed in the field, but these LLNL experiments were some of the first to confirm its mobility in the laboratory under a range of conditions. The goal is to develop a geochemical model that will predict the type

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The Geochemistry of Strontium Movement

Strontium-90, a highly mobile contaminant produced by the testing and production of nuclear weapons, is found in soil, sediment, and/or groundwater at more than 50% of DOE lands. Because it is significantly more mobile than other hazardous radioactive metals, it is important to determine and understand the chemical conditions and molecular mechanisms that control its reaction with soil- and rock-forming minerals.

We are examining these geochemical processes as a function of temperature, pH, and time. Our experiments on strontium sorption/precipitation and desorption/dissolution track changes in solution composition and identify the molecular structure of strontium at the mineral-water interface. For example, batch sorption experiments were run at 25, 50, and 80°C, with pH ranging from 4 to 10. The

Figure 1. Experiments in two different types of soil minerals show that pH has a much greater effect on sorption of strontium than does temperature.

of chemistry needed to mobilize or immobilize strontium. Our data provide some very fundamental information about strontium's behavior, but they are only a small piece of the puzzle.

Radionuclide Movement in Undisturbed Soil

This project is designed to fill two gaps in current knowledge about environmental management: how contaminant radionuclides move when they are far from the contaminant release point, and at what rate fluids move in unsaturated soils (a process known as moisture flux). The core of this study is trace-element studies of radionuclides released into the atmosphere during above-ground nuclear testing in the 1950s and 1960s. These radionuclides are present in shallow soils worldwide, including permafrost, in a quite uniform distribution.

The project combines field work, the development of sensitive measurement methods, and computer simulation. The field work took place at the Nevada Test Site, where we trenched along a fault to get soil samples from the shallow vadose (unsaturated) zone (Figure 2). In order to analyze for trace amounts of strontium-90, zirconium-93, technetium-99, chlorine-36, and iodine-129, the team developed or improved highly sensitive accelerator mass spectrometry techniques. Without these techniques, only relatively high concentrations of many radionuclides could be detected—levels higher than those of the radionuclides used in this study.

Analysis of the field data indicated that nuclear-test-related chlorine-36 is migrating faster than stable chlorine. This result casts doubt on the validity of using natural chlorine as an indicator of moisture flux.

We are combining measurements of all five radionuclides in the shallow vadose zone with NUFT, an LLNL flow-and-transport code, to develop a numerical model that simulates the radionuclides' movements in the deep vadose zone. This model will improve our understanding of radionuclide transport far from the contaminant release point and its implications for potential health risks. The results will have general applicability because the targeted radionuclides are common contaminants that show migration behavior representative of radionuclides and heavy metals. The models developed in this research will thus furnish a foundation for a variety of contaminant-migration assessments.

Contaminant Migration to the Water Table

Complex interactions among the atmosphere, groundwater, and the surrounding matrix take place in heterogeneous vadose zones, where fractures or other discontinuities contribute to permeability. These interactions affect the dispersal of liquid or dissolved contaminants driven by gravity and capillary action. Vapor phases may be present, depending upon the contaminant's volatility and their dispersal, and these must also be examined.

A Vadose Zone Observatory on the LLNL site permits monitoring of the migration of both liquid and gas phases of contaminants to the water table under controlled conditions. The observatory consists of a set of wells for introducing and extracting fluid and gas phases and for measuring changes in saturation in the vadose zone. The introduction of slightly saline solutions with dissolved gas tracers as a "contaminant" through a central well provides controlled sources. The resulting changes in the saturation of the vadose zone are determined from electrical resistance tomography (ERT) measurements made in

Figure 2. A trench at the Nevada Test Site provides samples for studying radionuclide and heavy-metal movement in undisturbed soil.

surrounding wells. Measurements made in other nearby wells determine various hydrologic variables, including gas-phase pressure and soil moisture content.

Before activation of the observatory, ERT measurements, lithologic logs, soil samples, and other data were collected to characterize the site. Then 6300 gallons of slightly saline water spiked with noble-gas tracers were introduced into the center well over a period of ten days. Figure 3 shows the changes in resistivity over time.

An initial conclusion that the contaminant infiltration occurred much faster than suggested by permeability measurements of soil samples is causing a reconsideration of how a site should be characterized. Ultimately, we hope to use these measurements to create a model to predict liquid- and gas-phase distributions and downward fluxes of contaminants in the vadose zone.

Imaging of Contaminants with Electromagnetic Tomography

Electromagnetic induction tomography (EMIT), a technique that uses magnetic fields to image the subsurface, was developed by the oil and gas industry to determine where reserves are located. Like the ERT method, EMIT maps changes in the resistance of the subsurface and allows the determination of soil properties such as saturation. However, EMIT uses magnetic fields rather than electric currents to do so. In principle, the technique is applicable to sites of interest to environmental cleanup. However, several challenges must be met before the method can be applied at the higher frequencies necessary to achieve the resolution needed for environmental cleanup.

An LLNL team is developing the code necessary to bring this powerful imaging tool to environmental management. EMIT is inherently a three-dimensional process, which makes the code for imaging the subsurface through magnetic fields more complicated. Unfortunately, the code used by the oil and gas industry is tailored to low frequencies and could not be used easily for the higher frequencies of environmental interest.

Consequently, we chose to start from scratch. Despite complications with the algorithms used to provide three-dimensional interpretations of the magnetic field data, our code is fully functional, and the EMIT imaging technique may soon be field-tested at a Superfund site in Visalia, California. Successful development of the code will provide a basis for applying a proven oil-and-gas technique to environmental monitoring and remediation.

Joint Inversion of Multiple Data Sets to Image the Vadose Zone

Various types of data—seismic, electrical, and electromagnetic properties—can be used to characterize the porosity and saturation of a site. The current state of the art in underground imaging is to look at each set of data individually. Used together, the different types of data should provide a more complete picture of the subsurface. The goal of this project is to combine multiple data in a joint-inversion process in order to take advantage of the interrelated information about the subsurface contained in each data set.

Before the joint-inversion algorithm can be completed, however, the geophysical properties of unconsolidated sediments, such as clay-rich sands, must be determined at the low pressures found in the near

Figure 3. Contaminant infiltration into the vadose (unsaturated) zone occurs faster than expected, as shown by electrical resistance tomography. Resistivity changes indicate changes in saturation (red indicates no resistivity change; blue indicates most negative resistivity change, or greater saturation).

surface and related to the hydrogeologic parameters—porosity, saturation, and permeability—that are most useful for environmental applications. Therefore, we conducted numerous laboratory experiments to study a range of unconsolidated sand-clay mixtures and other artificial soils. These measurements suggest that microstructure controls the geophysical properties. Studies of the microstructure assumptions used in empirical and theoretical methods may identify methods that will be most successful in relating geophysical properties measured in the field to porosity and saturation in the subsurface.

The necessary algorithms for the joint inversion for environmental site characterization are under development. Unlike the oil industry codes designed to address problems associated with consolidated rock at depths of a kilometer or more, these algorithms will be tailored to address environmental problems associated with depths of a few meters to a few hundred meters of mostly unconsolidated sediments.

Emission-Free Treatment

The DOE today is responsible for the disposal of a variety of wastes. Some of the waste left from weapons production, operation of nuclear power plants, and other sources can only be stored, but some

organic-based mixed and radioactive wastes can be treated thermally to reduce their volume or destroy them. DOE lists emission-free destruction of organic low-level and mixed low-level wastes as a primary science need. We are combining experimental studies and thermodynamic modeling in an examination of the vaporization of wastes containing uranium, plutonium, and other actinide elements at the high-temperature conditions of thermal treatment. Using conditions comparable to those found in various treatment processes, we are making transpiration measurements, conducting thermal-gradient-transport experiments, and determining key thermodynamic parameters for gaseous actinide species. At LLNL we are performing work on plutonium and neptunium (and americium, if time permits), while a small team at UC-Berkeley is doing work on uranium. In parallel with the experimental effort, a complete thermodynamic database for expected gaseous actinide species is being developed from the literature, proposed measurements, and data predictions using bond-energy correlation and statistical thermodynamic estimation methods.

Out of this work will come an understanding of the thermodynamics of actinide vaporization and partitioning/speciation behavior under conditions that exist during thermal treatment. This should help in predicting the behavior of radioactive and volatile metals during treatment.

Geospeedometry: Application of Cosmic-Ray-Exposure Dating to Active Tectonics in Central Asia

The Indo–Asian continental collision formed the Himalaya–Tibetan Plateau, the Tien Shan mountain range, and the marginal basins along the east coast of Asia (South China and Andaman Seas).

Associated deformation extends as far north as Siberia. The ongoing collision has driven the original southern boundary of Asia as much as 2000 kilometers (km) north and represents a geologic event that is probably unique in the last billion years of earth history. Uplift of the plateau has been linked to the modification of ocean chemistry, global atmospheric circulation patterns, climate, and floral and faunal distributions within Asia.

Considerable effort has been devoted to understanding the tectonic evolution of Asia. However, the manner in which various deformation mechanisms have contributed to the accommodation of Indo–Asian convergence remains controversial. The controversy centers on some basic issues: How do continents deform? Do they respond as a continuum, or as rigid blocks where strain is localized along the boundaries? This controversy endures,

partly because of poor constraints on the primary input to kinematic models—the rates of movement along major active fault zones.

Determining Slip Rates on Active Faults

We have used a combination of remote sensing, field mapping, cosmic-ray surface exposure, and radiocarbon dating to determine slip rates on the major active strike-slip and thrust faults associated with the Indo–Asian collision. Here we present recent results on the Kunlun Fault, which, along with the Altyn Tagh and Haiyuan strike-slip faults, bounds the northeast quarter of the Tibetan Plateau (Figure 1). Their great lateral extent and spatial relationship to large, active, northwest–southeast-trending thrust faults and growing mountain ranges suggest that these faults play a major role in accommodating current Indo–Asian convergence as well as in the long-term growth of the Tibetan plateau.

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Figure 1. Tectonic map of the Kunlun Fault, showing its segmentation and our sampling sites (numbers). The inset map shows the location of the fault in northeastern Tibet.

Some of the largest earthquakes recorded this century in northern Tibet ruptured segments of these large faults or the associated thrusts. Slip rates on these features may define discontinuities that extend through the entire continental lithosphere (the upper 100 km of the crust and upper mantle) as well as the crust.

The Kunlun Fault is composed of twelve principal segments that can be clearly identified on Landsat and SPOT satellite images (Figure 1). To better quantify slip rates and earthquake recurrence intervals on the fault, we studied surface landforms

along much of its length, using SPOT satellite imagery to identify prominent cumulative offsets along several segments. Three segments of the fault, the Xidatan–Dongdatan, the Dongxi, and the Maqen, could be reached in the field and were analyzed in greater detail. At each site terrace risers or morainal ridges are offset along the fault trace (Figure 2). Cosmic-ray dating of quartz-rich pebbles and radiocarbon dating were performed at LLNL's Center for Accelerator Mass Spectrometry and used to determine the terrace surface ages. Together with the cumulative slip, these dates yield the time-integrated slip rate on the fault.

The morphology of terrace surfaces is similar at each of the Xidatan–Dongdatan sites, as illustrated by the features at Site 1 (Figure 3). Using the underlying terrace to constrain the time since a riser became a passive offset marker (the time of terrace abandonment by humans), we obtained a slip rate of 12.1 ± 2.6 millimeters per year (mm/yr) for this site.

At two locations on the Dongxi–Anyemaqen segment of the fault, we observed terrace risers offset by as much as 400 meters (m)

Figure 2. Photograph of a morainal ridge offset by 180 meters near Maqen. The view is to the southeast from north of the fault trace.

intersecting the fault trace at high angles. Unlike the sites within the Xidatan–Dongdatan trough, the terrace surfaces that constrain these offsets did not contain quartz-rich material sufficient for cosmic-ray exposure dating. Instead, we used radiocarbon dating of charcoal collected beneath the surfaces of a number of terraces to constrain the age, and found slip rates comparable to those from the Xidatan–Dongdatan valley.

At the eastern extremity of the Maqen segment of the fault, the Huang He river is offset left-laterally about 85 km. About 40 km east of Maqen, the western lateral moraine of one extinct glacier is offset 180 ± 20 m by the main strand of the fault (Figure 2). A charcoal sample collected from a terrace that constrains the minimum age of this offset yielded an age of $11,156 \pm 157$ years before present (BP). The moraine, whose shape is well preserved north and south of the fault, originated during the last glacial maximum. Taking the last glacial maximum in the Anyemaqen region to be coeval with that elsewhere at comparable latitude ($\sim 20,000$ BP), the moraine must have been abandoned between 20,000 and 11,000 BP, yielding a slip rate of 12.5 ± 3.5 mm/yr.

The Utility of Cosmic-Ray Dating

The observed offsets and the terrace ages determined in this study of 600 km of the fault are consistent with a constant slip rate of 12 ± 2 mm/yr over a time interval of 40,000 yr. This rate is consistent with those used in recent kinematic models in which more than 90% of current Indo–Asian convergence is localized on active strike-slip and thrust faults, as opposed to being treated as distributed deformation. The agreement between the rates based on cosmic-ray dating and those based on radiocarbon dating supports the utility of cosmic-ray dating in active tectonics. Perturbation of cosmogenic nuclide systematics by post-depositional disturbance and inheritance appears to be negligible in this particular setting.

The large Holocene slip rate we determined confirms that slip on the Kunlun Fault accommodates a large fraction of the eastward component of the motion of Tibet relative to the Gobi. In addition, the minimum geomorphic offsets inferred from field and SPOT image observations along this 600-km section of the fault are 9–12 m. Coupled with

Figure 3. Site 1 in the Xidatan–Dongdatan valley. (far left) Enlargement of satellite image of site area. White arrows show offsets of two principal terrace risers. The active stream floodplain entrenches one side of the site, and abandoned terraces rise sequentially to the east. The trace of the fault is clearly defined by a series of pressure ridges. (center) Schematic interpretation of satellite image. Alluvial surfaces are numbered as a function of increasing height and age (inset), starting in T0 (the active stream floodplain). Riser offsets were measured in the field and on air photos and satellite images; the fault offsets the T1/T2 and T2/T3 risers by 24 m and 33 m, respectively. Fist-size quartz pebbles (circles) were sampled on top of main alluvial surfaces south and north of the fault trace. (right) Plot of sample ages for each terrace, in relative position from west to east. For each terrace level, samples were grouped and a mean age was calculated. Surface-exposure ages for samples from each terrace form clusters with ages of ~ 1800 , ~ 2900 , and ~ 5100 years. Light and dark arrows indicate data points attributable to other sources.

this slip rate, these offsets imply that great earthquakes (magnitude ≈ 8) rupture this section of the Kunlun Fault with a recurrence time of 800–1000 years. The calculated ages of morphologic features support the idea that much of the surface geomorphic imprint is tightly linked with climate change and, in particular, with the drastic changes between glacial periods and interglacials or stadials.

We believe that this is the first time that the slip rate on a single fault has been

determined for spatial and temporal baselines of these lengths. That the Kunlun Fault currently exhibits a constant slip rate is indicative of the termination of propagation and associated shortening at its terminus. This pattern leads to the counterintuitive conclusion that the northern part of the Tibetan plateau grew by the accretion and uplift of fault-bounded basins associated with strike-slip fault propagation, rather than by the coalescence of mountain belts.

Resources

The E&ES Directorate operates programs and pursues basic and applied research to support LLNL major program areas. To achieve these goals, the management team for E&ES strives to

- Staff with talented and diverse scientists, engineers, and administrative personnel.
- Provide high-performance scientific computational capabilities, such as the powerful parallel computing platforms and computer codes needed for large-scale simulations that address generic environmental and national security challenges.
- Execute good business practices and continually review financial systems.
- Operate, maintain, and enhance high-quality facilities with an emphasis on maintaining an excellent safety record.

Workforce

Our directorate currently employs 274 people in 27 job series, reflecting a wide range of employment categories. Of this total population, 73% are scientists, engineers, and post-doctoral research staff members. A strength of the directorate is its diverse workforce with the skills and flexibility required to meet administrative and programmatic objectives. Approximately 78% of the workforce have advanced degrees reflecting a wide range of skills, knowledge, and abilities (Table 1). Personnel from other Livermore organizations, such as Engineering and Computation, who are assigned to support the directorate's programs complement this workforce. The total number of people working with and within E&ES makes it one of the largest environmental research organizations in the nation. The workforce breakdown by function and other categories is shown in Figure 1.

Table 1. Skills, knowledge, and abilities within the Earth and Environmental Sciences Directorate.

Discipline	Skills, knowledge, and abilities
Physics	Accelerator applications; astrophysics; atomic, computational, solid state, and theoretical physics; materials; biophysics; and geophysics. Staff includes specialists in meteorology, atmospheric science, seismology, hydrology, geology, physical properties of rocks, climatology, and oceanography.
Chemistry	Geochemistry and biochemistry; nuclear, physical, and organic chemistry; isotope and theoretical chemistry. Staff includes specialists in marine, agricultural, and soil chemistry; environmental analytical chemistry, and accelerator mass spectrometry for analysis of cosmogenic radionuclides.
Life sciences	Environmental science; agronomy; biology; genetics; plant science; radiobiology; toxicology; ecology; water resources; marine biology; and zoology. Staff includes an environmental lawyer, a geographer, and an economist.
Engineering	Mechanical, electrical, civil, geotechnical, environmental, marine, nuclear, geological, and chemical engineers. Staff includes specialists in mining, applied science, and aeronautical, industrial, and cybernetics systems.
Administrative and Technical support	Accounting; arts; biology; business administration; carpentry; commercial administration; education; geology; history; labor and industrial relations; organizational psychology; psychology; social sciences; and zoology.

Total workforce, by function **Scientists and engineers, by discipline** **Gender** **Ethnicity** **Augmented workforce, by function** **Appointment type** **Degree** **Years of service**

Figure 1. Workforce breakdown for E&ES by function, discipline (scientists and engineers), function (augmented workforce), appointment type, gender, ethnicity, educational degree, and years of service.

Funding

The E&ES Directorate provides scientific leadership, technical support, and management expertise to a diverse set of programs and projects (Figure 2). In fiscal year (FY) 1998 the total funding for E&ES programs from all sources was \$64.7 million,

including a \$3.5-million allocation from Laboratory-Directed Research and Development. DOE directly funded E&ES programs in Defense Programs, Office of Science, Environmental Restoration and Waste Management (ERWM), Environmental Safety and Health, and others (International

Affairs and Nuclear Reactors). The Environmental Waste Management program shows a decrease from the FY97 funding level; this is primarily due to the downscaling and completion of the Molten Salt Demonstration Project in FY99. The E&ES Directorate also received \$8.2 million for projects in support of Work for Others. This included work from DOE field offices and integrated contractors; from other federal agencies, such as U.S. Navy, Air Force, Department of Defense, and the National Aeronautics and Space Administration (NASA); and from private industry and universities, such as California State University.

Finally, in FY98, our directorate received \$28.9 million of funds through other LLNL directorates. This represents programs for which our personnel provided scientific and program leadership and expertise. The dollar amount rose from \$25.7 million in FY97, primarily due to a growth in the Chem-Bio areas that are funded through the Nonproliferation and National Security programs. Continuing programs include the

Comprehensive Test Ban Treaty Program, the proposed repository at Yucca Mountain, and others.

The directorate is a composite of environmental sciences, geophysics, atmospheric physics, and other geoscience disciplines. Listing the funding sources does not describe the diverse nature of our research. A representation of the funding sources in Figure 3 shows the breakdown of funding by project or program.

Figure 3. Breakdown of 1998 funding by major projects and programs. Amounts are in millions of dollars. ARAC = Atmospheric Release Advisory Capability, CAMS = Center for Accelerator Mass Spectrometry, CTBT = Comprehensive Test Ban Treaty Program, MI = Marshall Islands, PCMDI = Project for Climate Model Diagnosis and Intercomparison (excludes \$400,000 of work for others).

Figure 2. Breakdown of funding for E&ES in 1998 (in millions of dollars). Funding received directly from the Department of Energy totaled \$23.9 million. Funding received in work for others totaled \$8.2 million. Funding received to provide scientific expertise and program management for other LLNL programs totaled \$28.9 million.

In FY98, we managed an indirect budget of \$10.1 million to cover management and infrastructure costs of maintaining the directorate. This included program management, personnel management, facility maintenance, and computer operations. Program development activities within program management looked at future directions for our existing programs and potential new areas of relevant scientific interest. Development areas in progress at the end of FY98 included the Center for Fuels Assessment, the Hazards Mitigation Center, and various workshops to broaden exposure to E&ES capabilities. Plans in facility management included facility consolidation, review and upgrade of laboratory space, and integration of long-term needs. The directorate, along with LLNL, continued to take every opportunity to monitor and control infrastructure cost expenditures to stay efficient and cost-effective.

Facilities

We continue to make significant progress in our space-management process, begun when the directorate was formed in 1994. The challenge we continue to face is how to balance current and future operations of the directorate. Our emphasis, given the available funds for space, has been on the consolidation

of current facilities to improve the directorate's operations and its programmatic capabilities and to free funds to address future needs.

Aggressive facilities management has greatly increased efficiency by reducing our total number of facilities from 62 in 1994 to 31 in 1998 and total space from 300,000 to 195,000 square feet. 1998 facility infrastructure maintenance costs were \$3.7 million versus \$4.0 million in 1997. We also improved our use of the available space and thus the efficiency of our operations by combining and consolidating assets and by vacating obsolete buildings, which reduced the directorate's maintenance burden. Figure 4 shows our 1995–1998 accomplishments in reconfiguring and optimizing the directorate's facilities. In both office space and net space per person housed, we are well below LLNL averages. The directorate's six primary facilities are described in Table 2.

In the future, we plan to complete the consolidation process and release any remaining underused or low-quality space. An important focus is the renovation of a trailer complex that currently houses nearly 200 directorate and associated personnel. We also plan to improve the capabilities of key facilities to enhance programmatic success. We will be consolidating much of the Marshall Islands work into a soon-to-be-vacated area of Building 292 and refurbishing the 1400 complex trailers. We are committed to being one of Livermore's lead organizations in cost-effective research and programmatic operations.

Figure 4. Consolidation of facilities in E&ES between 1995 (green) and 1998 (orange).

Computational Capabilities

Our computational environment emphasizes cost-effective office computing and the integration of laboratory data acquisition and experiment control with very-high-performance scientific computing. The directorate performs much of its scientific work through the development and use of complex computational models of dynamic physical and chemical processes of the earth and atmosphere. The applications encompass a wide variety of computational effort. Scientific and engineering staff use high-performance UNIX workstations to develop the modeling codes, perform

Table 2. Major facilities in the Earth and Environmental Sciences Directorate.**National Atmospheric Release Advisory Center, Building 170**

44,000-square-foot facility
 Commissioned on February 26, 1996
 Award for architecture
 Fitted throughout with fiber-optic communication links
 120 offices, a library, and a conference and training center

Center for Accelerator Mass Spectrometry, Building 190

9,000-square-foot facility
 Multi-user Tandem Laboratory
 Houses two accelerators
 One 10-megavolt model FN Tandem Van de Graaff
 One newly installed 1.8-megavolt Tandem for particulate research
 Broad variety of applied research using ion-beam analysis and accelerator mass spectrometry

Health and Ecological Assessment Laboratories, Building 281

19,000-square-foot facility
 An older existing facility that was extensively renovated during 1996
 Used to consolidate closely related programs and experiments from six geographically separate facilities
 Includes both wet and dry chemistry, laser, and high-pressure laboratories and support space

Molten Salt Oxidation Demonstration Project, Building 292

3,500-square-foot facility
 Used to study performance of an integrated molten salt oxidation (MSO) system including primary unit, offgas, and salt recycle subsystems
 Construction completed and experimental work began in September 1997

Geoscience Technologies Laboratories, Building 243

18,000-square-foot facility
 Includes wet and dry chemistry, laser, and high-pressure laboratories, as well as a machine shop and support areas
 Used to conduct research in support of basic energy sciences, fossil energy projects, the Yucca Mountain project, the Accelerated Site Cleanup project, and other Laboratory-directed research and development

Environmental Microbial Biotechnology Facility, Building 446

1600-square-foot facility
 Includes a 1500-liter bioreactor and dedicated ancillary equipment
 Ability to grow, harvest, and radioactively label specific bacteria for bacterial cell or cellular DNA labeling and containment studies
 Used to conduct research in support of the Yucca Mountain Project, bioremediation, and microbial transport

calculations locally, and render graphic images from the data produced by the calculations. Complex large-scale simulations make use of the most powerful parallel computing platforms available.

Documents, budgets, presentations, and other office information are prepared, analyzed, and manipulated on low-cost Windows and Macintosh computers that take advantage of mass-market efficiencies and provide productive user interfaces. Similar systems are also used to control experiments and gather data in the laboratory or in the field.

The directorate has more than 1200 computers of various types, as shown in Figure 5. In addition to general office work computers, many researchers have systems that offer specific computational capability, support travelling or work from home, or control experiments. The Directorate also operates scores of computer systems for central services such as backup, file storage, database, and calendar/time.

The directorate's computer systems are interconnected with high-capacity switched networks. Nearly all offices have dedicated 10-megabits-per-second (Mb/s) bandwidth. In addition, the earth and atmospheric science facilities have 100-Mb/s bandwidth in the backbone. We are in the process of expanding the switched environment to all directorate computers, and will start deploying 100-Mb/s connections to selected offices as needed. In the near future we plan to bring 1-billion-bits-per-second (Gb/s) bandwidth to our backbone to accommodate the transfer of very large files of environmental data. We already provide essential central services over

the network that leverage economies of scale, including high-performance backup of several terabytes of data, multi-gigabytes of shared disk storage, high-quality color printers and plotters, and meeting scheduling. Our facilities are interconnected via LLNL's Open LabNet backbone through which we receive additional institutional services including electronic mail and an on-line directory. Open LabNet is also our path for access to supercomputers at LLNL and other institutions.

We are among the few institutions that can couple scientific expertise and laboratory and field measurements with sophisticated software engineering and high-performance computing techniques to enable first-ever and state-of-the-art scientific simulations. For example, our studies of the earth and atmosphere use platforms similar to LLNL's Accelerated Strategic Computing Initiative (ASCI) computer, the most powerful computer in the world, to carry out simulations of climate variability, weather, and sub-surface reactive flow, and to compare the results with data from international experiments. We developed a new model of fundamental turbulent mixing processes that served as a showcase for ASCI by sustaining a throughput of 1.2 trillion floating point operations per second and incorporating 10 billion zones, the highest sustained throughput ever obtained. This model will increase the understanding of the effects of turbulence; this can help in many simulations including the prediction of dispersion of airborne contaminants.

In addition to LLNL computing facilities, our researchers use supercomputers at Sandia National Laboratories, Lawrence Berkeley National Laboratory, Los Alamos National Laboratory, and NASA in their work. Their scientific expertise and understanding of high-performance computing enables ensembles of simulations across the various architectural platforms at these sites, leading to insights into the strengths and limitations of scientific models and to new scientific conclusions.

Many of the modeling codes we have developed and continue to maintain and enhance are in wide use in academia, at other national laboratories, and in industry. Table 3 lists some of the LLNL-developed codes that are most widely used.

Figure 5. The directorate has more than 1200 networked computers with applications ranging from office computing to control of laboratory experiments to high-performance computing.

Table 3. LLNL-developed modeling codes in wide use by academia, industry, and other national laboratories.

SAC 2000	<p><i>Description:</i> Processes and analyzes seismic signals and other time series</p> <p><i>Applications:</i> A number of geophysical problems including estimation and analysis of strong ground motions; earthquake, explosion, and volcanic source studies; seismic discrimination and identification studies; magnitude estimation, travel-time analysis, studies of wave-propagation phenomena such as path and site effects, and investigations of earth structure</p> <p><i>Usage:</i> Used by a large portion of the international seismological community, including over 400 academic, government, and business institutions; key component of Directorate work for the Comprehensive Test Ban Treaty</p>
EQ3/6	<p><i>Description:</i> Models the complex geochemical processes that occur when aqueous solutions react with rock, soil, or man-made materials including nuclear waste; includes a comprehensive set of thermodynamic databases, with data for thousands of inorganic and organic species</p> <p><i>Applications:</i> Geologic disposal of high-level nuclear waste; analyzing migration of radionuclides; modeling mineral dissolution, mineral precipitation, and waste form leaching; interpretation and design of laboratory measurements; study of natural geologic processes (e.g., ore deposit formation); chemical engineering and process design</p> <p><i>Usage:</i> Widely used in academia, national laboratories, and industry</p>
SUPCRT	<p><i>Description:</i> Calculates a set of internally consistent thermodynamic properties for organic and inorganic aqueous species, gases, and solids as a function of temperature and pressure</p> <p><i>Applications:</i> Generation of a set of internally consistent thermodynamic parameters used as input for EQ3/6 and many other geochemical models</p> <p><i>Usage:</i> Widely used in academia, national laboratories, and industry</p>
NUFT	<p><i>Description:</i> Simulates non-isothermal multi-phase flow and transport in porous media</p> <p><i>Applications:</i> Subsurface problems in high-level nuclear waste storage, environmental remediation, and petroleum recovery; containment of underground nuclear explosions</p> <p><i>Usage:</i> Used at universities and in the Yucca Mountain Project. Soon to be distributed as part of a textbook on hydrology (Bear and Nitao). Chosen by the Army to be included in the Department of Defense's system for modeling subsurface remediation. NUFT is the basis for a coupled chemical-reaction plus flow-and-transport code under construction at LLNL</p>
PARFLOW	<p><i>Description:</i> Simulates three-dimensional simulation of flow and transport in heterogeneous saturated or unsaturated hydrologic regimes using a parallelized architecture</p> <p><i>Applications:</i> Modeling migration of contaminants from nuclear tests, transport of environmental contaminants, and aquifer management</p> <p><i>Usage:</i> LLNL research; interest expressed by other national laboratories and academia</p>
IMPACT	<p><i>Description:</i> Models atmospheric chemical transport</p> <p><i>Applications:</i> Effects of aircraft emissions in the atmosphere; effects of energy-related nitrous oxide and sulfur emissions on ozone</p> <p><i>Usage:</i> The basis for the NASA Global Modeling Initiative (GMI) model that is used in the assessment of climatic impacts of aircraft; requested by academia, national laboratories, and industry</p>
Livermore Ocean Biogeochemistry Model	<p><i>Description:</i> Models oceanic distribution of carbon, carbon isotopes, nutrients, chlorofluorocarbons (CFCs), and other ocean tracers</p> <p><i>Applications:</i> Prediction of air/sea fluxes of carbon dioxide, CFCs, and other tracers, and to evaluate ocean general-circulation transport model</p> <p><i>Usage:</i> Used as DOE's participation in the Ocean Carbon-Cycle Model Intercomparison Project</p>
Artificial Neural Network Analysis (ANN)	<p><i>Description:</i> Interpolate the output of large subsurface transport codes in groundwater or oil reservoir prediction problems</p> <p><i>Applications:</i> Optimizing well locations for groundwater remediation and waterflood of an oil and gas reservoir</p> <p><i>Usage:</i> Published in <i>Solving Problems in Environmental Engineering and the Geosciences with Artificial Neural Networks</i>, Farid U. Dowla and Leah L. Rogers (MIT Press, Cambridge, MA, 239 pp.)</p>
ADPIC/LODI	<p><i>Description:</i> ADPIC solves the 3-D atmospheric advection-diffusion equation using a Lagrangian stochastic/Monte Carlo approach, and simulates the processes of mean wind advection, turbulent diffusion, radioactive decay, first-order chemical reaction, wet deposition, gravitational settling, and dry deposition. A new model, LODI, with these features plus improved numerical methods, grid systems, and physical parameterizations is under development</p> <p><i>Applications:</i> Modeling of local- and regional-scale atmospheric dispersion and surface deposition of toxic materials and air pollutants</p> <p><i>Usage:</i> LLNL research, LLNL emergency response system (ARAC), LLNL chemical and biological weapons nonproliferation studies, various international groups for nuclear accident preparedness and response</p>
FEM3C	<p><i>Description:</i> Three-dimensional CFD model for simulating local-scale atmospheric flow and dispersion of heavier-than-air gas releases</p> <p><i>Applications:</i> Simulations of the atmospheric dispersion of heavier-than-air gas releases. Could also be used as an incompressible flow code for engineering problems</p> <p><i>Usage:</i> Academia, national laboratories, and industry</p>

In addition to internally developed codes and models, we actively collaborate with other institutions for model development, model simulation, and data analysis. In atmospheric and climate modeling, we parallelized and performed science studies with the National Center for Atmospheric Research (NCAR) CCM3 climate model, the GFDL ocean dynamics model, and the LANL POP ocean dynamics and sea ice model. The Navy's COAMPS regional model and the LLNL LODI dispersion model are integrated into our Atmospheric Release and Advisory Capability (ARAC) program that provides information to emergency responders in the event of radioactive and other contaminant releases. These collaborative research and model development efforts are essential as we carry out programmatic goals and prepare for future scientific programs.

The results from climate models developed here and elsewhere are compared with each other and with real world data. We perform extensive analysis and data mining to ascertain areas in which models do not perform well and to detect signals in the data that may show a cause-and-effect relationship such as human effect on climate. Our expertise in geographic information systems and our library of extensive geospatial data are brought to bear on complex planning, resource management, and research problems involving environmental, physical, and temporal parameters tied to specific geographic locations.

As the work of the directorate increases in complexity and scope, our computational environment grows apace. We are planning increases in computing power, communications bandwidth, and storage capacity to meet the demands of our mission and our expertise.

Outreach and Collaboration

Research and development in E&ES is funded by a wide range of federal agencies. The directorate interacts with academic, industrial, and national laboratory organizations working on the development of the earth and environmental sciences and their application to challenges in environmental and national security. As in the past, no one agency or organization dominates this area, and multifaceted expertise is required in order to be a significant contributor. Over this past year, E&ES has continued its collaborations with other LLNL directorates and the external community to provide this expertise.

Our many interactions with the outside community allow us to assess our strengths, challenge us to improve, and provide a means to demonstrate our strengths. They provide us with insights into the strengths of other groups and the challenges that they face. In turn, the interactions provide the outside community with insight into and familiarity with elements of our expertise and infrastructure. This exposure complements that obtained from our more formal activities such as publications and workshop proceedings.

Major components of outreach in 1998 include the following:

- Ongoing and new collaborations with external research increased to 569 (from 500 in 1997).
- More than 70 faculty members and students and 49 other scientists visited for stays of more than one week.
- 8 on-site work-study programs involved 65 students.
- 23 conferences or workshops were organized or hosted.
- 153 tours of our facilities were given (the majority by the National Atmospheric Release Advisory Center).

- 126 directorate employees served as members of major national and international committees and review panels, as visiting lecturers, or as journal associate editors and reviewers.
- Our summer student program hired 34 students, including 19 women from a variety of academic institutions and programs. We hired students from many sources: International Atomic Energy Agency (IAEA); Summer Employment Program (SEP); Department of Energy Scholarship Program; Hawaii Scholarship Program; Associated Western Universities; Knowledge, Education, Reinforcement, Reach-out to Youth (KERRY) Program; Research Internship and Education Program (RIE), and Northern Arizona University Fellowship Program.
- 12 Basic Energy Sciences Geosciences PI-driven projects with a FY99 budget of \$1.5 million involving UC faculty and students were sponsored through the LLNL Institute of Geophysics and Planetary Physics.
- More than 60 employees participated in community activities such as special instruction, computer programs, classroom training, mentoring students, workshops and special conferences, community services campaigns, etc.

The E&ES Directorate is involved in other outreach efforts that could have significant impact on the Directorate in the near future:

- The E&ES Acting Associate Director is a major participant in efforts exploring partnering opportunities with UC-Merced, the new UC campus expected to be staffed by the year 2005. Collaboration between the

faculty and students and LLNL scientists in selected advanced degree programs is being planned as part of both the startup and ongoing operations. Environmental Sciences is to be one of the central campus programs.

- UC-Santa Cruz and LLNL are pursuing cooperative efforts in the general areas of (1) climate modeling, mechanisms, monitoring, and records (including carbon cycle and climate records); (2) environmental toxicology and risk assessment; and (3) water resources, environmental restoration, and seismic processes and hazards. Nine joint projects were proposed and five were selected in November 1998. These fund three graduate students and two postdoctoral fellows supervised jointly by scientists from both institutions.
- The Geographic Information Science (GIS) Center worked with officials at Los Positas College to establish a curriculum for GIS certification. Discussions are ongoing regarding placement of Las Positas students in the GIS Center while the students earn units of college credit and are paid under the Scholars Program.

Outreach and collaboration efforts are essential to the directorate's development and to its ability to help address both environmental challenges and threats to national security having geoscience components. Employee participation in these activities is a factor in our evaluation of the employees' professional development and their value to LLNL. These interactions can have significant impacts on our efforts to improve our strengths, correct our weaknesses, make our efforts relevant to society, and receive recognition for work well done.

Organization

Figure 6 shows the organization of E&ES. The major components are (1) the four divisions, which contain the scientific and support staff and have principal responsibility for the execution and maintenance of disciplinary science; (2) the program organizations, which execute focused missions for this directorate and others at LLNL; and (3) the infrastructure activities, which support our research and programmatic efforts. Each of these three components has a vital role to

play in creating and nurturing an organization that is scientifically excellent, capable of accomplishment that impacts national issues, and is safety-conscious, cost-effective, and agile in the current climate of national science and technology. A point particularly worth noting is the correlation between the Special Programs in Figure 6 and the breakdown of funding shown in Figure 3. The project organizations control a major fraction of the directorate's resources. The mission and capabilities of each division are described below.

Figure 6. Organization of the E&ES Directorate.

Atmospheric Science Division

The mission of the Atmospheric Science Division is to expand the scientific understanding of the response of the earth's atmosphere, oceans, and biosphere to anthropogenic and natural disturbances, to assess the impacts of hazardous materials released into the atmosphere, and to use the results to address significant national and international challenges. To meet these requirements, the division maintains expertise in

- Atmospheric climate dynamics, chemistry, and physics.
- Ocean dynamics, transport, and biogeochemistry.
- Mesoscale atmospheric prediction, transport, and dispersion.
- Terrestrial ecology and land surface hydrology.
- High-performance computing and computational physics.

This expertise is combined with the best available environmental simulation models, comprehensive real-time and archival observational datasets, and the most powerful computing resources to examine a range of problems. For example, we are studying the transport and dispersion of radioactive, chemical, and biological materials released into the atmosphere; global- and regional-scale impacts of changes in atmospheric chemical composition; variations in the earth's climate and carbon cycle; and the impact of aviation emissions on atmospheric processes. The division also provides the technical staff for several major programs, including the National Atmospheric Release Advisory Center, the Program for Climate Model Diagnosis and Intercomparison, and the Chem-Bio Nonproliferation Program.

For more information on the Atmospheric Science Division, contact the division leader, Bill Dannevik, at (925) 422-3132 (dannevik1@llnl.gov).

Geophysics and Global Security Division

The mission of the Geophysics and Global Security Division is to conduct basic and applied research that characterizes the physical and chemical properties and processes of the solid earth and to use the results of the research to address challenges in national security, environmental remediation, energy supply, civic infrastructure, and industry. The challenges include natural and anthropogenic hazards; test-ban-treaty violations; production of geothermal, oil, and gas energy; and containment of radioactive materials. The division's primary areas of research are

- Seismology, including empirical and computation studies of source and propagation effects on local, regional, and teleseismic ground motion, and signal processing, discrimination, and regional characterization in support of verification of a Comprehensive Test Ban.
- Computational physics, including shock physics, computer modeling, information sciences, weapons physics, sonoluminescence, and theoretical and applied physics.
- Experimental physics, including synthesis of materials; rock mechanics; flow in porous materials; physical and chemical properties of earth materials, cementitious materials, and metals at high pressures and temperatures; and experimental design.
- Geophysical site characterization, including theoretical and applied geophysics, geomechanics, engineering, containment science, field operations, on-site-inspection technologies, and instrumentation.

Division personnel provide the direction for a wide variety of LLNL programs including the Comprehensive Test Ban, Containment, Geothermal, Basic Energy Science, and Remote Sensor Test Range programs; the Hazard Mitigation Center; and a significant element of the Yucca Mountain Program.

For more information about the Geophysics and Global Security Division, contact the division leader, Norm Burkhard, at (925) 422-6483 (burkhard1@llnl.gov).

Geosciences and Environmental Technology Division

The mission of the Geosciences and Environmental Technology Division is to conduct basic and applied research to solve problems involving the geochemistry, geophysics, and hydrology of the earth's near-surface, and develop technologies to solve the nation's waste-disposal and waste-processing challenges. The division's research is focused on five basic areas:

- Subsurface characterization, especially the development of new geophysical and electromagnetic methods for characterizing the physical and chemical properties in the shallow subsurface and for identifying and mapping contaminant plumes.
- Subsurface remediation, with emphasis on developing new assessment techniques and innovative cleanup strategies for accelerated cleanup of subsurface contaminants.
- Nuclear waste disposal, including characterization and modeling of the thermally perturbed geochemistry, hydrology, and transport mechanisms expected in high-level nuclear waste repositories. We also design and test different disposal strategies and model the reactions of various nuclear waste forms after they are emplaced into a repository.
- Waste-processing technologies, including the development and testing of systems that provide alternatives to incineration for treating and stabilizing mixed hazardous and nuclear wastes.
- Basic geosciences research, such as studying the dissolution kinetics of minerals and glasses, determining thermodynamic and transport properties of geochemical systems, developing geologic information systems, producing computer models to simulate hydrologic and geochemical processes, and applying cosmogenic isotopes as tracers and age-dating tools.

For more information on the Geosciences and Environmental Technology Division, contact the division leader, Ken Jackson, at (925) 422-6053 (jackson8@llnl.gov).

Health and Ecological Assessment Division

The mission of the Health and Ecological Assessment Division is to conduct research to assess and manage the risks of chemicals released to the environment. The division's core expertise in the health, ecological, and measurement sciences provides a strong basis for multidisciplinary studies of toxic and

radioactive substances. An important asset of this division is a unique set of research facilities, which include:

- Laboratories for processing soil and vegetation samples for subsequent analysis.
- Alpha and gamma spectrometry for determining low levels of radionuclides in environmental media.
- Gas chromatography and high-performance liquid chromatography for measuring various organic compounds in different media.
- Atomic absorption spectrometry for analyzing metals.
- Accelerator mass spectrometry and proton-induced x-ray fluorescence for quantifying selected nuclides (such as ^{14}C , ^{129}I , ^{36}Cl , ^{59}Ni) and various elements.

Our measurement technologies support a broad range of field and laboratory studies within the division and the E&ES Directorate. We have developed both experimental methods and computer models to assess the nature and magnitude of

human exposures to chemical contaminants via inhalation, dermal contact, and ingestion. An important asset is our considerable experience in constructing dose-response functions for estimating the risk that such contaminants pose to humans. We also perform detailed studies involving the environmental chemistry and toxicology of various kinds of organic and inorganic substances, and we develop methods for managing the risks they pose to humans and ecosystems—an example is our work on identifying measures to allow resettlement of the Marshall Islands area used for a former U.S. nuclear test site. We are equipped to characterize pollutant-transport processes, such as the resuspension of contaminants deposited on soil. Finally, we conduct large-scale field programs, establish and maintain environmental databases, and create geographic information systems.

For more information on the Health and Ecological Assessment, contact the division leader, Dave Layton, at (925) 422-0918 (layton1@llnl.gov)a

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Awards

ERL/NOAA Outstanding Paper

A 1996 *Nature* paper by Benjamin D. Santer won the “Outstanding Scientific Paper” award from the Environmental Research Laboratories (ERL) of the National Oceanic and Atmospheric Administration (NOAA). The paper, written with contributing authors K. E. Taylor, T. M. L. Wigley, T. C. Johns, P. D. Jones, D. J. Karoly, J. F. B. Mitchell, A. H. Oort, J. E. Penner, V. Ramaswamy, M. D. Schwarzkopf, R. J. Stouffer, and S. F. B. Tett, is entitled “A Search for Human Influences on the Thermal Structure of the Atmosphere.”

Norbert Gerbier-MUMM International Award for 1998

Santer was informed by the Secretary-General of the World Meteorological Organization that the *Nature* paper had also won the “Norbert Gerbier-MUMM International Award for 1998.” The paper was the result of an international collaboration involving scientists at six research institutes on three continents.

MacArthur Fellow

Santer was named a MacArthur Fellow by the Chicago-based John D. and Catherine T. MacArthur Foundation. One of 29 new Fellows chosen from a wide variety of fields, he was selected for his “originality, creativity, self-direction, and capacity to contribute importantly to society, particularly in atmospheric science.”

In 1995, Santer led a key group of the Intergovernmental Panel on Climate Change (IPCC) through its review of the evidence regarding anthropogenic effects. The panel concluded that “the balance of evidence suggests that there is a discernible human influence on global climate.” The work of the panel provided important scientific foundations for recent international negotiations in Kyoto on greenhouse gas emissions.

American Institute of Chemical Engineers Research Project of the Year

LLNL was awarded the “Research Project of the Year Award” by the Northern California Section of the American Institute of Chemical Engineers for the Spent Salt Clean-Up/Recovery Process, which is a key module of the Lab’s Integrated Molten Salt Oxidation (MSO) Demonstration Project. MSO is a high-temperature chemical oxidation process designed to destroy organic wastes in an environmentally benign way. The recovery process, developed by Peter Hsu and Martyn G. Adamson, is the first of its kind; it is now being demonstrated at the pilot scale as part of the Integrated Technology Demonstration System.

Society of Exploration Geophysicists Special Commendation Award

Norman R. Burkhard received the Society of Exploration Geophysicists Special Commendation Award. This SEG award was established to give “recognition and special commendation to deserving persons for meritorious service to the public, the scientific community, or to our profession.” Burkhard led a group which, in concert with other SEG members, produced 3-D synthetic seismic data from two complex 3-D geologic models. The results were the culmination of the 3-D SEG/EAGE Modeling Project. The data sets, freely available worldwide to researchers, are aimed at (1) providing better understanding of problems in imaging data acquired over complex structures and intricate stratigraphy, (2) testing and validating processing algorithms, and (3) aiding in survey design. The data set will serve the industry as benchmark data for years to come.

The Mineralogical Society Award

James M. Brennan was recognized for outstanding published contributions to the science of mineralogy. This award recognized an outstanding series of eight papers dealing with partitioning of trace elements between minerals and aqueous fluids, published in *Geochimica Cosmica Acta*, *Earth and Planet Sciences Letters*, *Nature*, and *Reviews in Geophysics*.

National Academy of Sciences Case Histories Award

A team led by François Heuze, with members from LLNL, Los Alamos National Laboratory, Sandia National Laboratories, and the former Defense Nuclear Agency, received the Case Histories Award for outstanding achievements in rock mechanics from the National Research Council of the National Academy of Sciences. The award was given for the paper “Behavior of a Steel Liner-and-Bolt System Under Very High Thermal and Mechanical Loads” published in 1995 in the *International Journal of Rock Mechanics and Mining Science*. It described an experiment that demonstrated the feasibility of engineering underground cavities in rock to contain repeated low-yield nuclear explosions.

Administrative Achievement Workforce Excellence Award

Assistant to our E&ES Acting Associate Director Elizabeth Garrett won the LLNL Association of Black Laboratory Employees award for 1998 for Administrative Achievement Workforce Excellence, for “her dedication and commitment to excellence.”

Patents

Robert T. Taylor
Kenneth J. Jackson
Alfred G. Duba
Ching-I Chen

In Situ Thermally Enhanced Biodegradation of Petroleum Fuel Hydrocarbons and Halogenated Organic Solvents
U.S. Patent No. 5753122
(IL-9431)
May 19, 1998

Roger Aines
Robin Newmark

Active Cooling-Based Surface Confinement System for Thermal Soil Treatment
U.S. Patent No. 5,681,130
(IL-9479 [RL-12,666])
October 28, 1997

Joseph Lucas*
Tore Straume
Kenneth Bogen

Detection and Isolation of Nucleic Acid Sequences Using Competitive Hybridization Probes
U.S. Patent No. 5,616,465
April 1, 1997

Ananda Wijesinghe et al.

Nontoxic Chemical Process for In Situ Permeability Enhancement and Accelerated Decontamination of Fine-Grain Subsurface Sediments
U.S. Patent Number 5593248
January 14, 1997

*LLNL Biology and Biotechnology Research Program.

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