Lawrence Livermore
National Laboratory

Meeting National Needs

Earth & Environmental Sciences 1999 Annual Report

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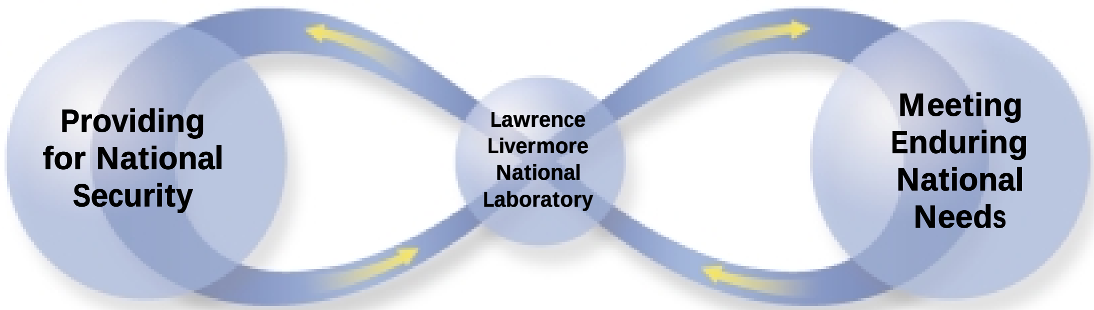
Contents

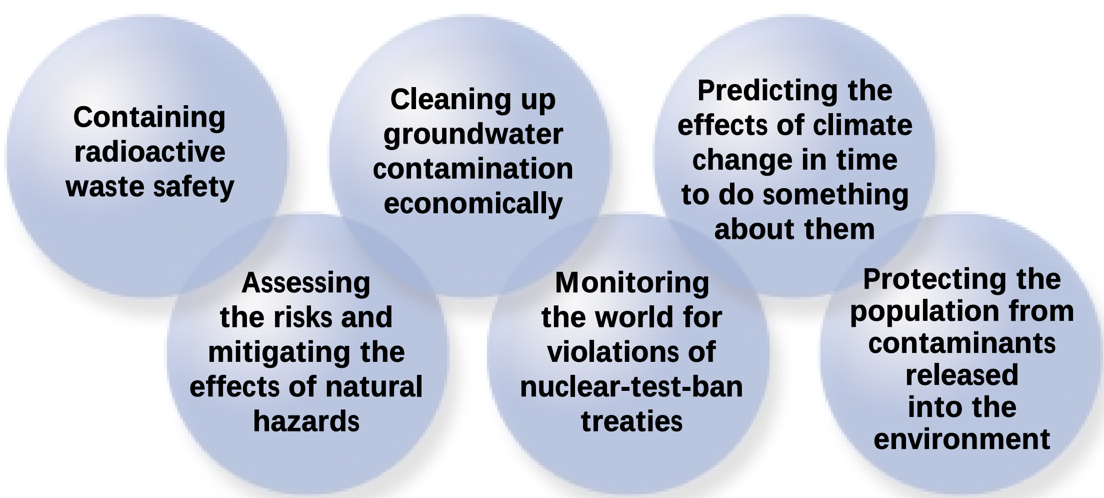
Earth and Environmental Sciences at Livermore— a unique resource for the nation

The Laboratory is in the unique position of being able to combine multidisciplinary science, world-class high-performance computing facilities, and decades of experience in designing and deploying experimental and field-scale systems.

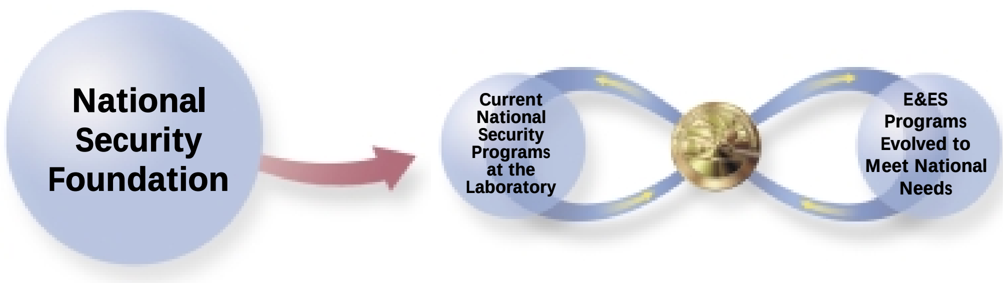
As part of Lawrence Livermore National Laboratory, a U.S. Department of Energy laboratory with an essential national security mission, the Earth and Environmental Sciences (E&ES) directorate has its roots in programs that began during the years of nuclear weapons testing. The major investments made for national security research at the Laboratory, which now supports the U.S. mission in the current non-testing era, provide it and E&ES with special capabilities to respond to critical national needs in energy and environment.

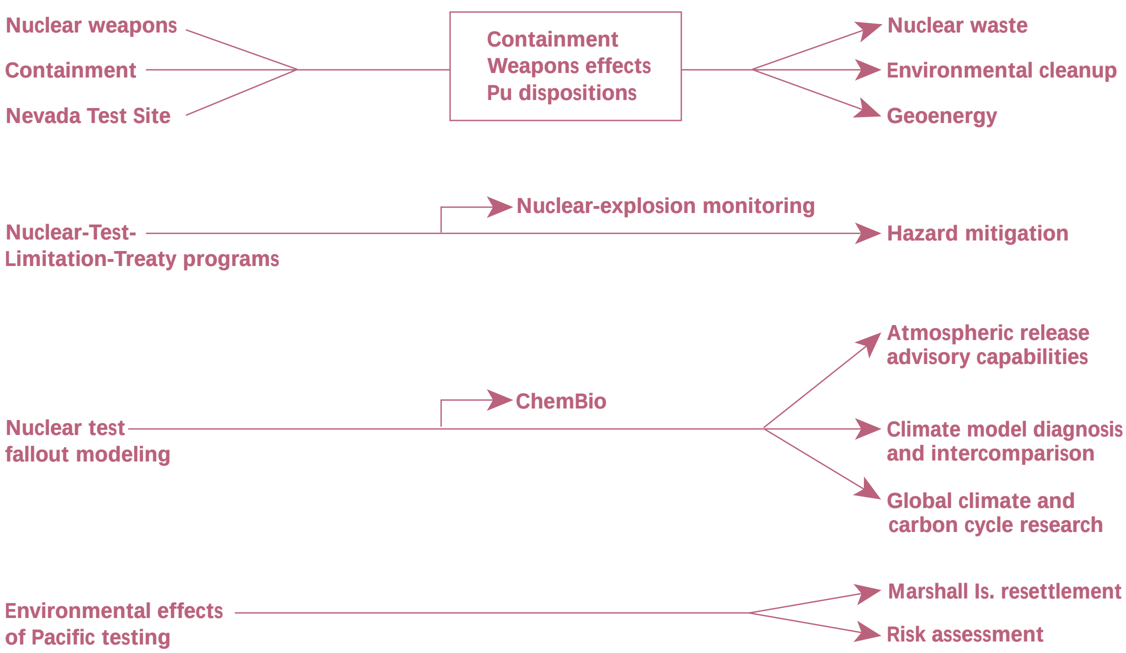


E&ES programs search for solutions to problems that are vital to our national interest:



E&ES has its roots in National Security





What makes E&ES work?

Cutting-edge capabilities in multiple areas of science and technology:

Experimental and analytical laboratories

Theory, modeling, simulation

A committed, vital, and talented staff

Collaborations that promote creativity

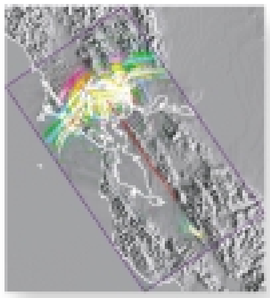
Enabled by:

Management, business practices, and operations that support mission goals

Science and technology in an environment that creates spin-off applications:

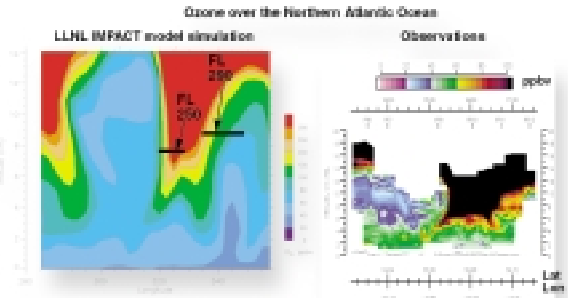
E&ES cutting-edge capabilities

Modeling

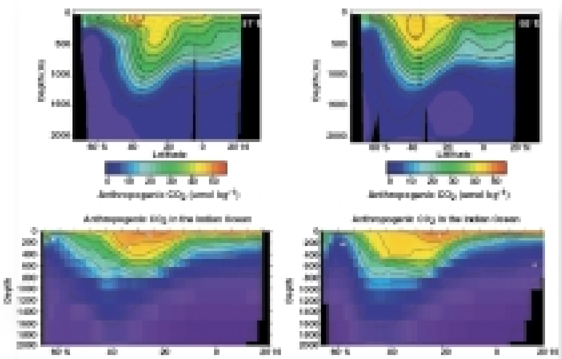


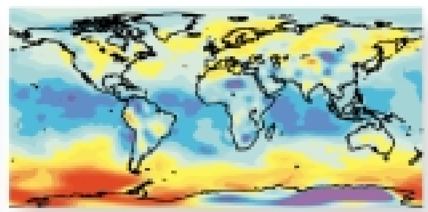
Ground-motion models show land areas of greatest concern for earthquake preparedness (here, 45 seconds after an earthquake on the Hayward, CA, fault).

Models of chemical and dynamical processes reveal their influence on ozone in the lower and upper atmosphere.



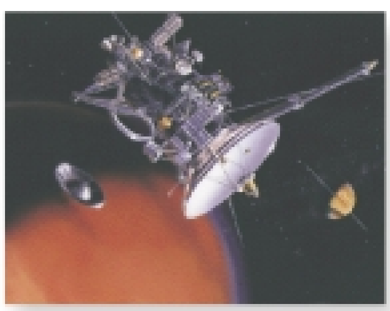
Ocean circulation and ocean carbon cycle models are used to predict rates of uptake of fossil-fuel carbon by the ocean.





The Program for Climate Model Diagnosis and Intercomparison works to improve climate models by identifying errors through intercomparison among models and comparison with observational data.

Operations



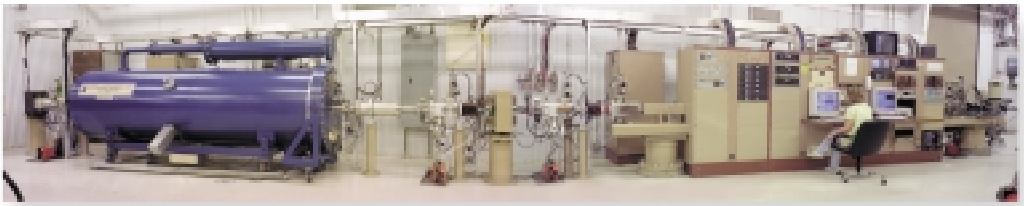
The National Atmospheric Release Advisory Center provided hazardous release modeling for the Cassini launch.

The National Atmospheric Release Advisory Center tracks hazardous airborne emissions anywhere in the world.

Remote Sensor Test Range wind tunnel produces a uniform chemical plume for remote sensor development.

Laboratories

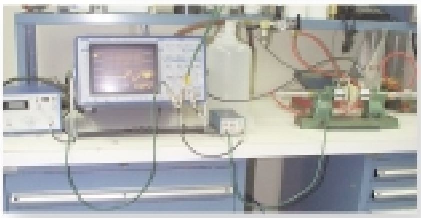
The Center for Accelerator Mass Spectrometry nuclear microprobe facility performs quantitative elemental and density microanalysis of biological, materials science, and particulate specimens.



The multidisciplinary Environmental Chemistry Lab performs basic and applied research in environmental chemistry.

Research on the risks of chemicals and radionuclides includes experiments studying the effects of alpha radiation on liver cells in minnows.

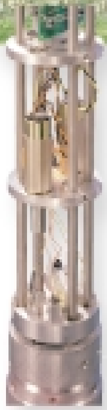
Geophysics apparatus measures shear-wave velocity in unconsolidated media.



Field experiments

Experimental work on Bikini Island tests the effectiveness of various methods of reducing cesium-137 uptake into food crops.

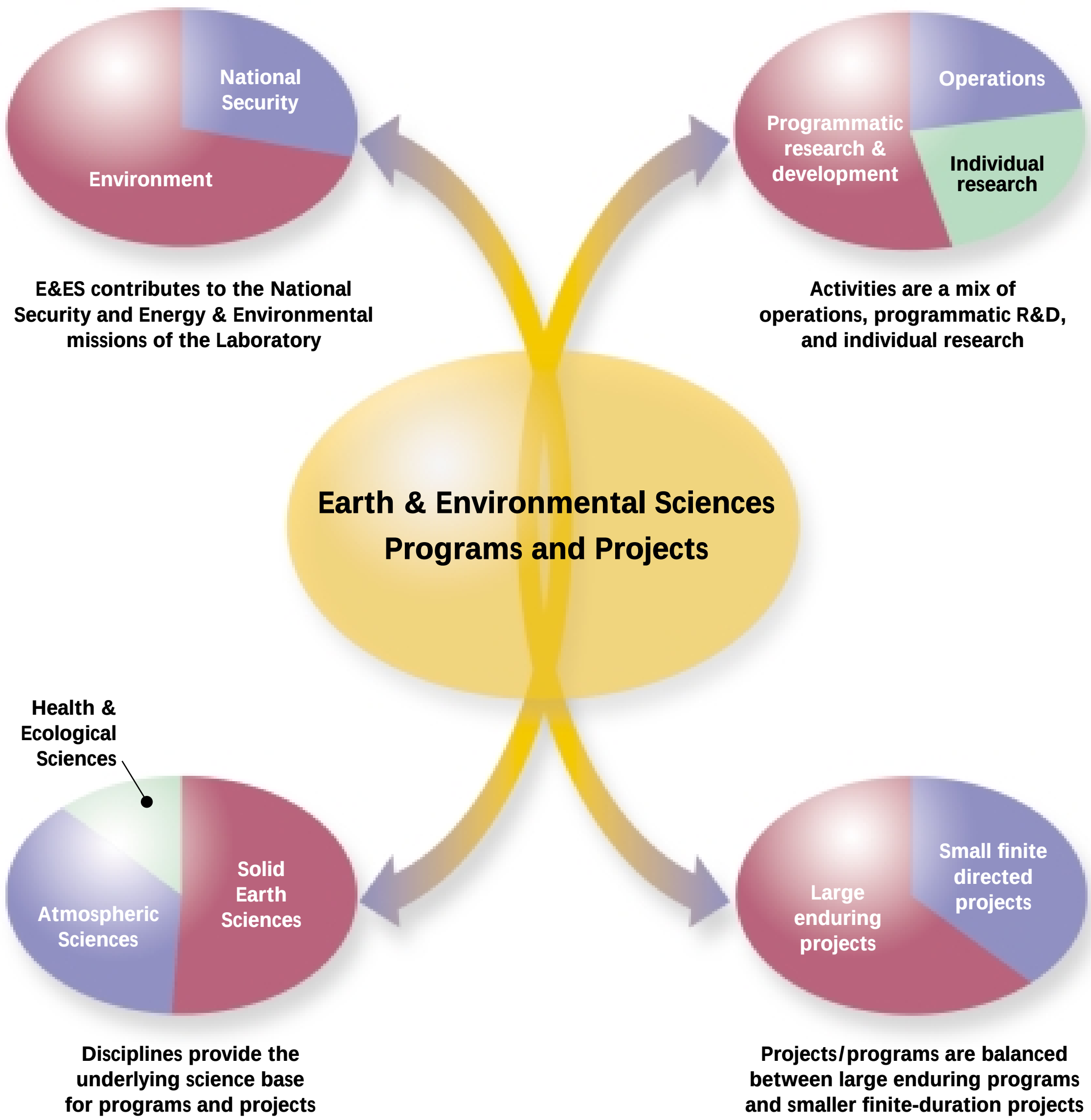
Large block of tuff from the proposed Yucca Mountain nuclear waste repository allows testing of conceptual models and understanding of processes.



Tiltmeter can measure hydrofracture orientation at depths exceeding 10,000 feet.

Dynamic Underground Stripping combined with Hydrous Pyrolysis/ Oxidation, and controlled using electrical resistance tomography, is successfully cleaning one of the first Superfund sites in Visalia, CA.

These capabilities combine in an environment that allows flexibility and the ability to draw on large projects or small—enabling powerful synergy



E&ES research areas align with national needs

National Security

Treaty Verification

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

Stockpile Stewardship

Geophysical and computational support to the Stockpile Stewardship mission

Atmospheric Release Hazards

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

Providing for National Security

Lawrence Livermore National Laboratory

Earth and Environmental Sciences

Basic Science Research

Science and technology projects complementary to programmatic funding

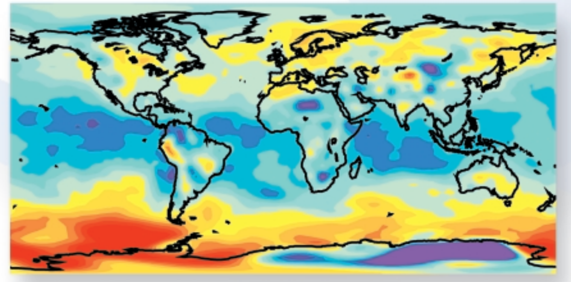
Energy and Environment

Nuclear Materials

Options for storage, immobilization, and sequestration of radioactive materials

Meeting Enduring National Needs

Climate, Carbon, and Energy



Models and impact assessments of current and future climatic conditions

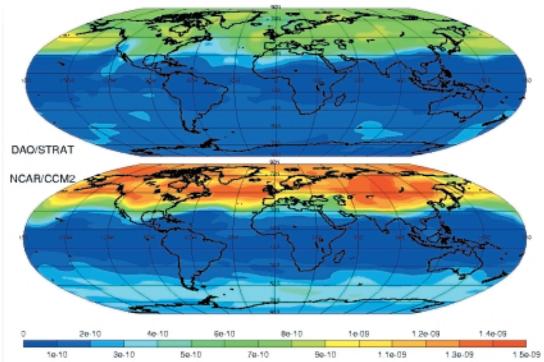
Environmental Risk Reduction

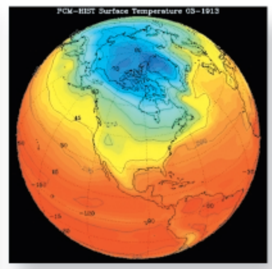
Systems to characterize and remediate environmental hazards

E&ES synergy enables our research to align with national needs in many areas

Collaborations with the greater scientific community range over many levels

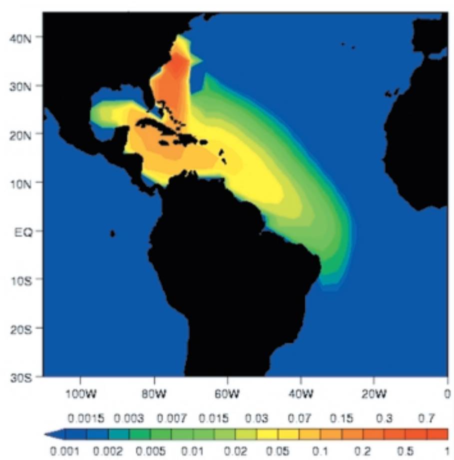
Global Modeling Initiative: E&ES leads a consortium of 19 members from academia, industry, and government research labs to conduct assessments of the impact of aviation on the atmosphere.

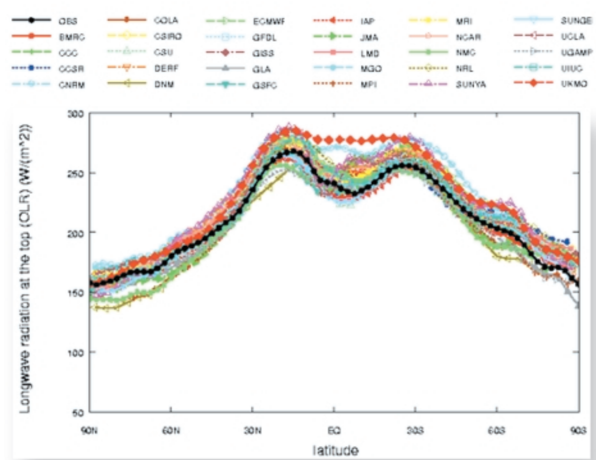




Distributed Climate Model Development Team: E&ES partners with three other DOE labs, the National Center for Atmospheric Research, and the National Aeronautics and Space Administration to develop the next-generation community climate model.

Center for Research on Ocean Carbon Sequestration: E&ES and Lawrence Berkeley National Laboratory, along with academic collaborators, conduct research on marine carbon management strategies.





Program for Climate Model Diagnosis and Intercomparison: PCMDI provides scientific diagnostics and the infrastructure for systematic intercomparison and improvement of climate model performance.

E&ES accomplishments

National Security

Treaty Verification

Developed and applied innovative statistical techniques to characterize seismic location and identification capabilities in large parts of the Mid-East and North Africa.

Led international efforts on development of the On-Site Inspection Regime for the Comprehensive Nuclear-Test-Ban Treaty Preparatory Commission.

Providing for National Security

Stockpile Stewardship

Developed and fielded successful containment designs for the Clarinet and Oboe series of subcritical experiments at the Nevada Test Site.

Atmospheric Release Hazards

Implemented the new modeling and operating system in the National Atmospheric Release Advisory Center as the primary NARAC emergency response system.

NARAC produced consequence assessments on three scales—local, regional, and hemispheric, using a source term of noble gas and iodine nuclides that evolved over several days to assess the consequences of the Tokaimura Nuclear Fuel Conversion Facility criticality accident.

Basic Science Research

During 1999 more than 60 E&ES basic science projects totaled $13.3M (about 22% of the Directorate's programmatic budget).

Energy and Environment

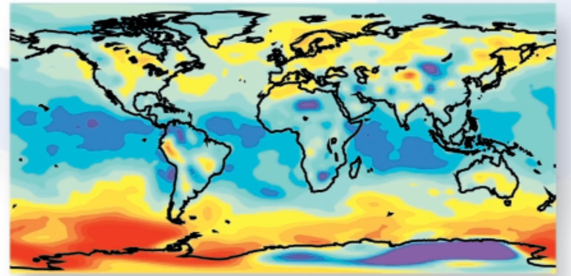
Nuclear Materials

Assessed radiological conditions and developed mitigation measures for resettlement of the Marshall Islands and completed a final detailed dose assessment for Utirik Atoll.

Conducted thermal–hydrologic calculations for repository designs and the total system performance assessment for Site Recommendation for the Yucca Mountain Project.

Meeting Enduring National

Climate, Carbon, and Energy



Won DOE competition to establish the National Center for Research on Ocean Carbon Sequestration (operated jointly with Lawrence Berkeley National Laboratory).

Initiated co-development of the next-generation Community Climate Model as a member of the DOE Distributed Model Development Team (Livermore, three other DOE Laboratories, the National Center for Atmospheric Research, and the National Aeronautics and Space Administration).

Environmental Risk Reduction

Using hydrous pyrolysis/oxidation technology, characterized, cleaned up and removed more than 150,000 gallons of pole-treating compounds (approximately 600,000 cubic yards of material in about 2 1/2 years) from a contaminated Superfund site.

Led the development of a novel tritium accelerator mass spectrometry technology that will have broad applications in environmental and biomedical research.

Our capabilities, environment, and collaborations produced many accomplishments in 1999

Leading Into the Future: Environmental Simulation

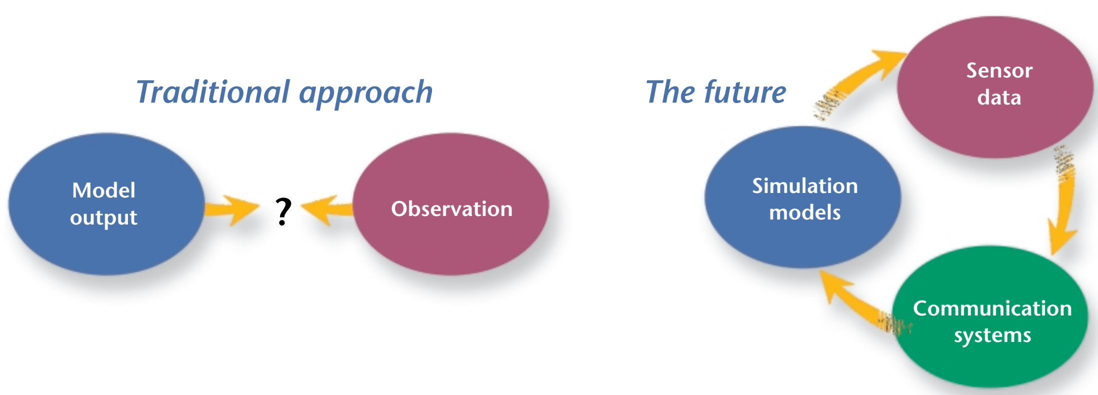
Recent technology advances have enabled us to simulate the environment as never before, and the trends continue. The traditional approach to validating environmental simulation models has been to compare model data with observations, and then to adjust the model to improve the level of agreement. This open-loop "confrontation" between models and observation has served well for several decades. However, radical changes are in sight—changes that will combine to allow an unprecedented ability to measure the environment and to link the measurements in real time to simulation models that are used to monitor, characterize, and predict complex environmental processes.

First, computing power will continue to grow at the Moore's Law rate, roughly doubling every 18 months (and thus the cost of computing will go down). Second, wireless communication systems will become smaller, cheaper, more adaptive, and more seamlessly connected with communication channels such as the internet. Similarly, environmental sensors will be smaller, smarter, cheaper, less invasive, and more mobile.

These trends mean that timely collection and use of sensor data in "live" simulation models will enable the models to "learn" about the details of environmental media, to adapt and reconfigure for rapidly changing conditions, and to "train" dynamic mobile sensor configurations to optimize the quality and usefulness of information. In essence, the traditional open-loop confrontation of model and observations will be transformed into a closed-loop symbiotic relation through which model and sensor data are mutually optimized.

Several E&ES applications in environmental simulation will benefit: for example,

Closing the Loop Between Models and Observation



Model-to-data intercomparison

Full integration of models and sensor data

- Understanding of complex subsurface material properties and distributions will improve when sparse *in situ* observations (borehole measurements, for example) and more abundant but "fuzzy" path-wise data (such as tomographic images or streamflow measurements) can be fused with predictive models.
- Contaminant source location, strength, and time signature can be estimated (and downwind dose prediction enhanced) when atmospheric-concentration measurements can be inserted into plume-dispersion models in real time.
- Probable damage from seismic or blast events can be better assessed when data from sensors embedded in engineered structures and from ground-motion detectors can be fused in real time.

The notion of "real time" varies from fractions of a second to weeks or even longer, depending on the time scale of the controlling physical processes. For some time-urgent applications (such as the second and third examples above), emerging mobile wireless communication and sensor systems will play a crucial role. Timely integration of models and data for these applications will require mathematical methods to be developed for estimating with random variables in the context of parameter uncertainty and dynamical chaos.

Exploiting new technologies in a coherent framework for integrating models, sensors, communication systems, and advanced mathematical algorithms will be a major challenge—and will deliver important new capabilities. With our partners in the Computations and Engineering directorates, for example, we are pursuing new initiatives in sensor-driven prediction and inversion of atmospheric plumes and in subsurface characterization and process optimization.

These and other projects will provide components of a comprehensive system for environmental simulation and observation that could establish the foundation of an expanding research partnership with the University of California, including the new campus at Merced.

Modeling Thermohydrologic Processes at the Proposed Yucca Mountain Nuclear-Waste Repository

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James Gansemer
Kenrick H. Lee

Collaborator:
Yunwei Sun
Weiss Associates

***National need: Contain radioactive waste safely*—we need to understand the effects of heat and water on the radioactive waste packages inside the repository to ensure its long-term integrity.**

Yucca Mountain (Figure 1), located 145 kilometers northwest of Las Vegas on federally owned land on the edge of the U.S. Department of Energy's Nevada Test Site, has been studied intensively for more than 15 years. It may become the nation's first permanent geologic repository for high-level nuclear waste. If the site is licensed, cylindrical waste packages will eventually be placed in about 50 horizontal tunnels, approximately 5.5 meters in diameter and 1 kilometer in length, several hundred meters below the ground surface in partially saturated volcanic tuff.

The repository would accommodate the emplacement of both spent nuclear fuel from nuclear power plants and high-level waste from nuclear weapons production. Radioactive decay of this material will produce an initial heat flux on the order of many times larger than the heat flux in the natural geothermal systems. This heat flux will change the thermal and hydrologic environment, affecting both the host rock and the conditions within the tunnels (called drifts) in ways significant to repository performance. Understanding the thermohydrologic behavior in this coupled natural and engineered system is critical to the assessment of the viability of Yucca Mountain as a nuclear-waste repository site and for repository design decision-making. Since the Yucca Mountain Project's inception, Laboratory scientists and engineers have played an important part, particularly in the area of understanding thermohydrologic behavior.

Figure 1. Yucca Mountain, located northwest of Las Vegas on DOE's Nevada Test Site, is being studied as a potential site for the nation's first permanent geologic repository for high-level nuclear waste.

Thermohydrologic Processes at Yucca Mountain

Under ambient conditions, liquid-phase flow in the repository host rock arises as a result of the infiltration of rainfall and snowmelt. Although most of the total fluid-storage capacity is contained in the matrix pores of this rock, the permeability in the matrix is very low and fractures dominate liquid-phase flow. After the emplacement of nuclear waste, the thermally driven transport of water vapor away from the heat source causes a redistribution of the pore fluids within a potentially large volume of rock; depending on the thermal design of the repository, this volume can extend from the ground surface to some distance below the water table and over an area larger than the repository footprint. Water in the matrix pores evaporates, creating dryout zones around the emplacement drifts and condensation zones outside of the dryout zones. As the heat pulse decays, the system slowly rewets.

In the host rock, local thermohydrologic behavior is dominated by whether that location is inside or outside of the zone of boiling temperatures (Figure 2). Although thermohydrologic processes such as evaporation occur at below-boiling temperatures, the most important processes (refluxing and dryout) require boiling temperatures. Two important factors influence the thermohydrologic conditions within the emplacement drift. The first is whether or not temperatures at the drift wall are above the boiling point, which strongly affects the likelihood of water seeping into the drift. The second is the temperature

For further reading on this topic, see page 79.

gradient between the waste package and drift wall, which strongly affects how much lower the relative humidity on the waste package is than at the drift wall.

Multiscale Modeling Approach

In response to the specific modeling challenges posed by the Yucca Mountain Project, we have developed a suite of sophisticated numerical tools referred to collectively as the Multiscale Thermohydrologic Model. The need for a multiscale modeling approach stems from the fact that the performance measures depend on thermohydrologic behavior within a few meters of the emplacement drifts and also on thermal and thermohydrologic behavior on a much larger repository (or mountain) scale. A single numerical model would require an unfeasible number of grid blocks. The goal of the Multiscale Thermohydrologic Model is to provide results that would be obtained if such a single model were possible, and at a computational cost that makes it possible to be an effective performance assessment and engineering design tool.

The Multiscale Thermohydrologic Model (Figure 3) consists of four major submodels and includes various scales, dimensionality, and assumptions regarding the heat-transfer processes considered and coupling of heat transfer to fluid flow. These four submodels all use NUFT (Nonisothermal Unsaturated–Saturated Flow and Transport), a flexible multipurpose computer code developed by E&ES for modeling fluid flow and transport in porous media. These submodels are:

- **SMT** (Smeared heat source, Mountain scale, Thermal conduction)
- **LDTH** (Line averaged heat source, Drift scale, Thermohydrologic)
- **SDT** (Smeared heat source, Drift scale, Thermal conduction)
- **DDT** (Discrete heat source, Drift scale, Thermal conduction)

The DDT submodel also accounts for thermal radiation in open drift spaces. The integration of these four submodels is accomplished with the Multiscale Thermohydrologic Abstraction Code.

The LDTH thermohydrologic submodels are two-dimensional (2-D) drift cross-sections run for multiple locations spaced evenly throughout the repository area (31 locations in the latest model implementation), with stratigraphy appropriate for each location. These submodels assume a heat-generation history that is effectively that of an "average" waste package. The LDTH submodels are also run for several lower heat-loading values. The coupling of 3-D mountain-scale heat flow to 2-D drift-scale thermohydrologic behavior is accomplished by integrating the LDTH submodels with the SMT and the SDT submodels. The 3-D SMT submodel accounts for the actual repository footprint in Yucca Mountain, allowing consideration of important thermal processes such as edge-cooling effects. The LDTH submodels at lower than the nominal heat-loading levels are used in calculations at the repository edges and corners. The SDT submodel is a 1-D vertical submodel, run at the same locations and for the same heat loadings as the LDTH submodels.

Output from the LDTH and SDT models is used to modify the output from the SMT submodel, creating a 3-D LMTH (Line-averaged-heat-source, Mountain-scale, Thermohydrologic) model. The DDT submodel is then used to further modify the LMTH model to account for waste-package-specific deviations from average waste-package behavior. The DDT submodel is a

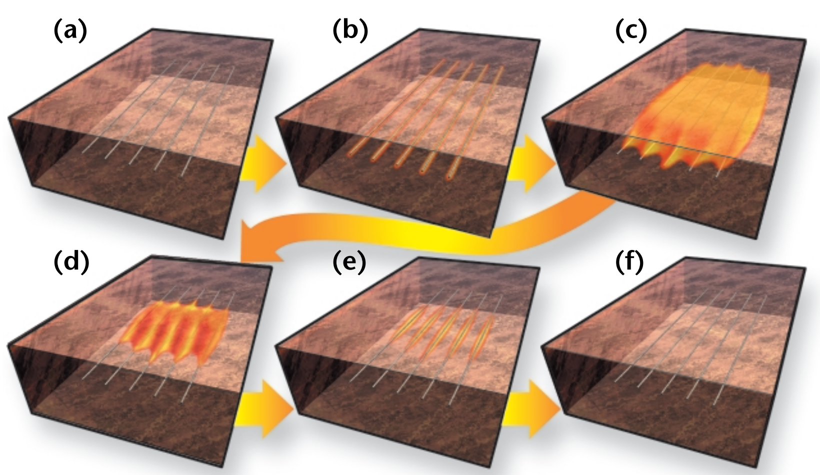
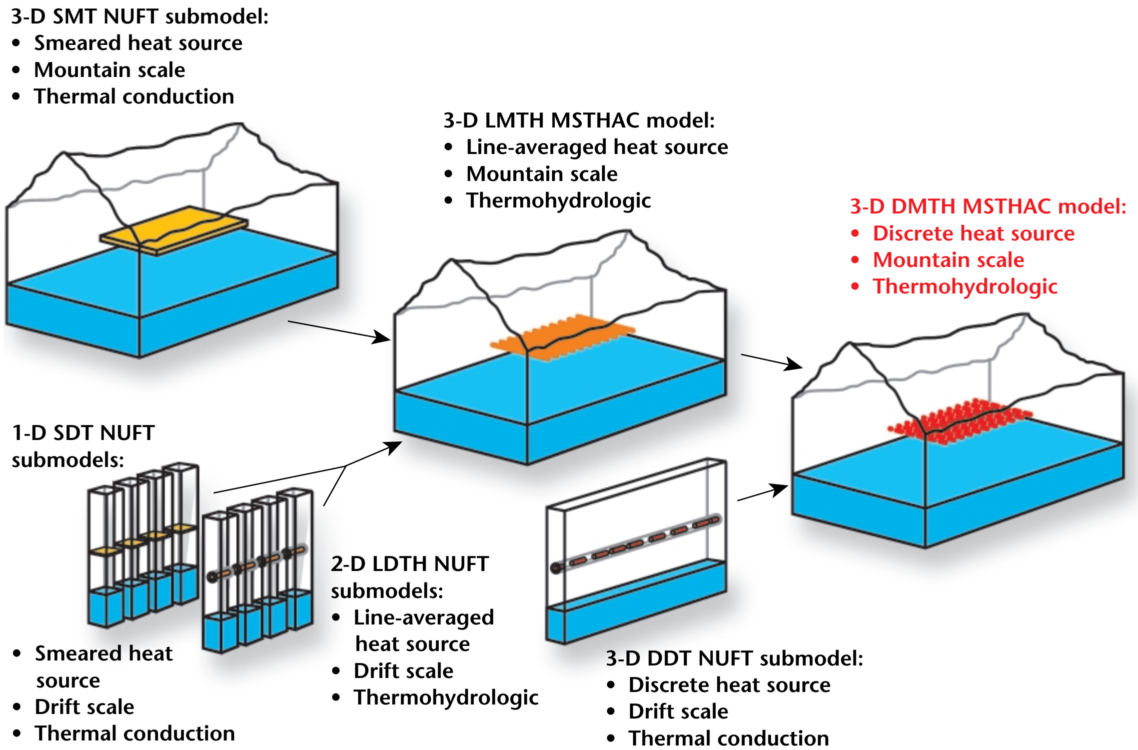


Figure 2. The "boiling envelope" at a Yucca Mountain nuclear waste repository will evolve through time, depending on the details of repository design and the response of the natural system to thermal loading. For some designs, coalesced boiling zones never form and the system evolves directly from (b) to (d).

Figure 3. The Multiscale Thermohydrologic Model consists of a family of four NUFT-based submodels of various scales, dimensionality, and processes, which are integrated with the Multiscale Thermohydrologic Abstraction Code (MSTHAC). The Multiscale Thermohydrologic Model was specifically developed to meet the challenges posed by the Yucca Mountain Project.



3-D drift-scale submodel that includes individual waste packages with distinctive heat-generation histories. The end result is a 3-D DMTH (Discrete-heat-source, Mountain-scale, Thermohydrologic) model.

Assessing Repository Performance

In December 1998, the Department of Energy issued a Viability Assessment on Yucca Mountain based on the reference repository design at that time. The Laboratory provided key model results for this effort. Specifically, the model viability assessment used model results from our Multiscale Thermohydrologic Model to assess several dozen thermohydrologic variables at several locations within repository drifts (for example, waste-package surface temperature and relative humidity, water vapor and air fluxes, and evaporation rates at the drift wall) for hundreds of repository map locations for three different climate scenarios.

One of the major strengths of our modeling contribution is the ability to provide predictions for the range of expected performance across the entire repository footprint rather than simply considering average repository behavior. This is important because the thermohydrologic environment that will arise as a result of the emplacement of heat-producing radioactive waste is influenced by factors that vary across the repository, including infiltration flux, hydrologic and thermal properties in the repository horizon host-rock unit, proximity to the repository edges, and depth from the surface to the repository horizon. Our Multiscale Thermohydrologic Model has the capability to assess thermal management strategies that take into consideration this variation across the repository, for example, placing hotter waste packages close to repository edges where cooling is more rapid.

Thermal Hydrology and Repository Design

One of the Laboratory's most significant accomplishments in 1999 was to help the Yucca Mountain Project evolve a thermal management strategy by assessing thermohydrologic behavior and repository performance for a number of alternative repository designs. The Yucca Mountain Project's License Application Design Selection (LADS) effort was conducted to develop and evaluate a range of conceptual repository designs and recommend a design concept for further consideration by the project.

The repository design selection process involves trade-offs between competing goals, including performance, economic costs, uncertainty, and constructability. Thermal design goals include:

- Keeping temperatures below critical temperatures for engineered materials.
- Keeping waste packages dry (that is, low relative humidity) until cool.
- Limiting water seeping onto waste packages.
- Limiting the spatial extent of boiling conditions in host rock.

These four thermal-design goals are interdependent. For example, backfill may be used to keep relative humidity low, but may make peak waste packages too hot. Similarly, the reduction in uncertainty that comes from limiting boiling conditions comes at the cost of a loss in relative humidity reduction in the drifts due to decreased rock dryout.

There are many design variables in the engineered system that affect thermohydrologic behavior in the repository:

- Overall heat-generation density of waste inventory.
- Average heat-generation density along the drifts.
- Age of the nuclear waste.
- Waste-package spacing and sequencing.
- Duration and heat-removal efficiency of drift ventilation.
- In-drift design and materials (backfill, dripshields, for example).

There are a large number of combinations of the various thermal-design variables described above. Fortunately, the most significant aspects of the thermohydrologic response of Yucca Mountain to thermal loading can be described, to first order, by considering only a few major attributes, including whether boiling or sub-boiling conditions occur in the host rock, whether or not the boiling zones around individual drifts coalesce, the degree of heterogeneity of heating along drifts, and the relative humidity gradient between the drift wall and surfaces of engineered components within the drifts.

The LADS study recommended a repository design referred to as Enhanced Design Alternative II (EDA-II). In EDA-II, with a heat loading equivalent to 60 metric tons of uranium per acre, only a small volume of host rock would reach boiling. The design includes waste-package blending to reduce the heat-source heterogeneity along the drift, end-to-end spacing of the 3–6-meter-long waste packages so that the line of waste packages will act as a homogeneous line-source of heat, a distance between emplacement drifts of about 80 meters which would allow for condensate drainage between drifts, and pre-closure ventilation to reduce peak temperatures. The recommended design also includes a titanium dripshield covered by backfill.

Site Recommendation

Our current thermohydrologic modeling efforts focus on assessing performance of the current repository design, EDA-II (with and without backfill, since in January 2000 the Yucca Mountain Project modified the design selection to remove the backfill). This work is part of a series of Analysis and Models Reports and Process Model Reports being prepared to support the formal project Site Recommendation, due to be released by the Department of Energy in 2001.

Thermal Field Tests

In addition to our work in performance assessment and repository design, we have also played a major role in thermohydrologic modeling of the Yucca Mountain Project's major thermal field tests to date, which include the completed Single-Heater and Large-Block Tests and the ongoing Drift-Scale Test. The primary purpose of these tests is to improve our understanding of thermohydrologic processes at Yucca Mountain and our ability to predict these processes. Results from our NUFT-based thermohydrologic models have shown good agreement with experimental data.

Dose Assessments and Resettlement Support on Rongelap Atoll in the Marshall Islands

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William Robison

National need: Protect the population from contaminants released into the environment— **information derived from the radiation-cleanup success at an early nuclear test site is important knowledge for other cleanup efforts.**

During the 1950s the United States conducted 66 atmospheric nuclear weapons tests on Bikini and Enewetak Atolls in the northern Marshall Islands. The most significant contaminating event in the entire Pacific test program was the Castle–Bravo denotation of March 1, 1954. Prior to Bravo, little consideration was given to the potential health and ecological impacts of fallout contamination beyond the immediate vicinity of the test sites. The explosive yield of Bravo (15 megatons) exceeded expectations and resulted in the deposition of radioactive fallout over the inhabited islands/atolls of Rongelap and Utirik to the east of Bikini (Figure 1). A total of 290 people were unexpectedly exposed to Bravo fallout, including 239 Marshallese, 23 American servicemen, and 23 Japanese fishermen. Sixty-four people were evacuated from Rongelap Island about 50 hours after the Bravo blast—most were taken to Kwajalein Atoll for decontamination and health care, and moved onto Ejit Island (Majuro Atoll). Rongelap Atoll was originally resettled in 1957; the scientific and medical investigations that followed only raised concerns and the level of fear within the community about exposure to residual fallout contamination on the atoll. Consequently, in 1985 the Rongelap people voluntarily left the island and took up residence on Mejatto Island (Kwajalein Atoll) and only recently have initiated a resettlement plan.

Beginning with the first relocation of the Bikini people to Rongerik Atoll in 1946, and following the tragic events of the Bravo test, problems in establishing long-term resettlement of Rongelap (1957–85) and Bikini Island (1972–78), and numerous and sometimes conflicting scientific investigations, the Marshallese people have struggled to come to terms with the technical and health-related

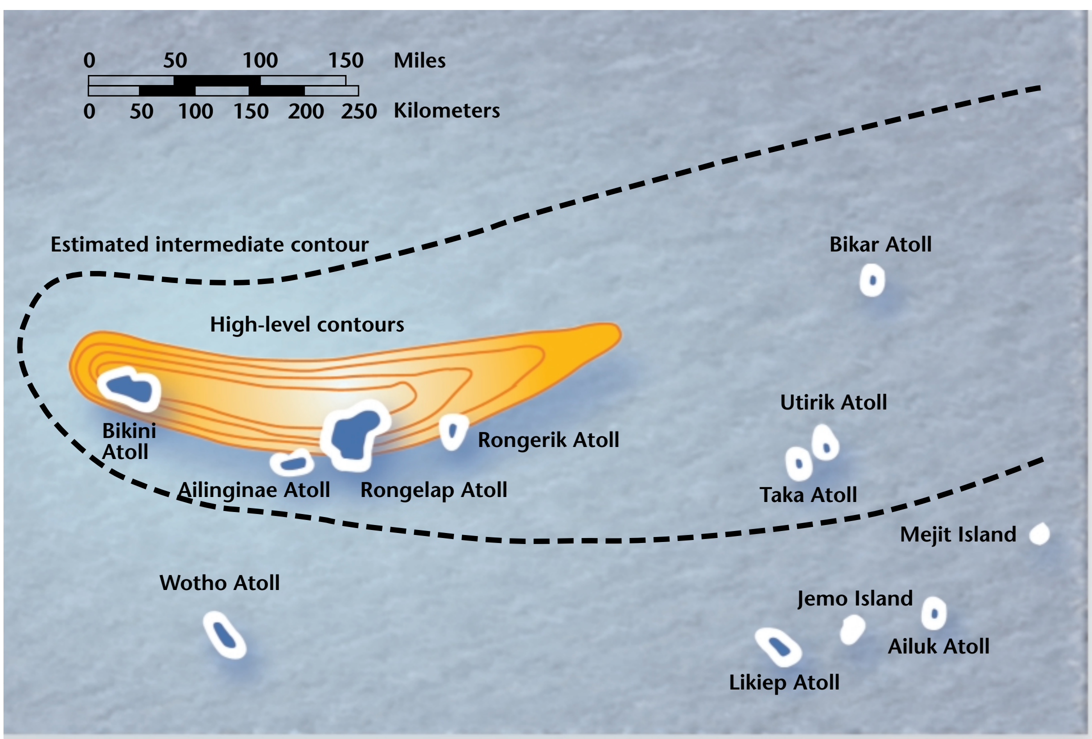

Figure 1. The Republic of Marshall Islands; dashed line shows the fallout pattern of the Bravo test conducted in 1954.

For further reading on this topic, see page 79.

information presented to them and have developed a societal fear of radiation. The social, political, and economic impacts of nuclear testing in the Marshall Islands have created a life of debate, conflict, and distrust of U.S. authorities. The opportunity to learn from previous mistakes is invaluable. It is within the context of these historical events that the Department of Energy, in cooperation with scientists from the Laboratory, is seeking to develop a new partnership with the atoll communities in order to formulate shared responsibilities for ensuring the radiation protection and general well-being of the Marshallese people into the new millennium. Our scientific studies form the basis for recommendations concerning resettlement, help guide the continuing environmental monitoring program, and provide the U.S. and the local atoll governments with current knowledge of radiological conditions on the islands.

Resettlement of Rongelap Island

In September 1996, the Clinton Administration announced a $45 million grant to the Rongelap community to enable resettlement of their atoll. The settlement provides for environmental remediation and cleanup, development of community intrastructure, and building of homes and schools. The Rongelap Atoll Local Government, the Republic of Marshall Islands, and the Department of Energy in consultation with the Laboratory have a signed a Memorandum of Understanding that formally outlines shared responsibilities in support of Rongelap resettlement. An important milestone underlying this memorandum was the acceptance by the Rongelap community and its leaders of the use of a preferred remedial strategy developed by scientists from the Laboratory to help reduce the dose to the resettling population.

Dose Assessments

Scientific investigations carried out at the Laboratory over the past 25 years have provided enormous quantities of data on the levels and distributions of fallout radionuclides at the atolls from which detailed and updated dose assessment have been made. We have developed a good understanding of all the important exposure pathways and identified the key radionuclides. Rongelap Atoll was one of eleven atolls surveyed as part of the Northern Marshall Islands Radiological Survey in 1978. The survey included an aerial radiological survey to map external gamma-ray exposure rates over islands of each atoll, and an environmental sampling program to assess the radiological dose for people living on islands and consuming local foods. More extensive environmental studies were conducted during the 1990s, including assessments of potential dose contributions from radionuclide resuspension and inhalation. We estimate that the ingestion pathway will contribute about 60% of the dose to residents, mostly through uptake of cesium-137 (^{137}Cs) from the soil into terrestrial foods such as coconut, *Pandanus* fruit, breadfruit, and papaya. External gamma exposure from ^{137}Cs accounts for most of the rest of the dose; other radionuclides and pathways contribute about 2%. The estimated annual effective dose on Rongelap Island, assuming a resettlement date of January 1, 2000, is 0.24 millisieverts per year (mSv/y, a measure of dose equivalent) without remediation. This is the dose that people would receive if they were to resettle the islands and eat a balanced diet containing locally grown and imported foods. Food gatherers using the island only periodically would receive a lower dose from the islands.

Coral atoll soils make ^{137}Cs more available to plants than do soils from continental regions. This is attributed to the high cation-exchange capacity of the soil, the absence of clay mineral binding sites, and the very low concentrations of potassium in the soil. Any procedure leading to a reduction in the uptake of ^{137}Cs into food crops and/or the elimination of ^{137}Cs in the soil column would substantially reduce the dose. Extensive field trials on Bikini Island have demonstrated that the application of potassium to agricultural areas (containing coconut, *Pandanus*, breadfruit, or any other food crop products) reduces ^{137}Cs uptake into plants to 5–10% of pretreatment levels. Furthermore, the supporting strategy of limited soil removal in and around the housing and village area helps eliminate most of the external and internal doses from soil ingestion and/or inhalation. Use of this "combined" option on Rongelap Island would reduce the estimated dose from about 0.24 mSv/y to about 0.04 mSv/y.

The natural background radiation dose in the Marshall Islands is about 1.4 mSv/y of which a very significant fraction comes from polonium-210 ingested via consumption of fresh fish. The estimated combined annual effective dose from natural background and weapons-related exposures on Rongelap Atoll is around 1.7 mSv/y without remediation and about 1.5 mSv/y with remediation (Figure 2). For comparison, the average background dose in the United States is 3.0 mSv/y and in Europe is 2.4 mSv/y (Figure 2). Consequently, the total radiation dose on Rongelap Atoll is expected to be no different than that of people living in most other parts of the world.

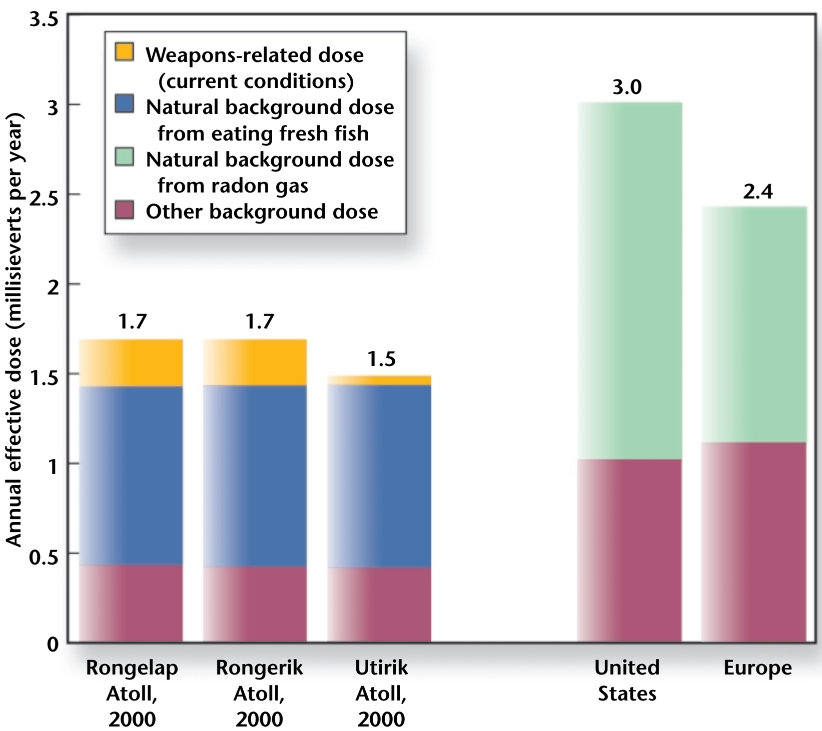

Figure 2. Comparison of the total annual effective dose on different islands in the northern Marshall Islands (current conditions) with doses in the United States and Europe.

Whole-Body Measurements of ^{137}Cs

An important strategic initiative of the Rongelap Atoll resettlement support plan is to install a whole-body counting system on the island, and have local Marshallese technicians operate and maintain the system so that workers (and future residents) can satisfy themselves that their ^{137}Cs body burdens do not increase significantly. The Rongelap Whole-Body Counter (WBC) is designed with a large-volume sodium iodide (NaI) detector and will detect small quantities of high-energy gamma-emitting radionuclides such as potassium-40, cobalt-60, and ^{137}Cs. The NaI detector is a solid crystal 28 centimeters in diameter and 10 centimeters thick, housed inside a shield that can be rotated to allow for maximum observation of the entire body. A Canberra Inspector and associated whole-body counting software are specifically designed for use with the detector interfaced to a laptop computer. The patient sits inside a shadow-shielded enclosure. This design of the whole-body counter is typically referred to as the "Masse Chair" design (Figure 3). The Masse Chair design is sufficient to monitor for radionuclides in most of the body and all of the internal organs. Calibration of the system is performed using a phantom filled with a known amount of a mixed gamma-emitting radionuclide standard (shown in Figure 3).

We have been performing WBC measurements on workers living on Rongelap Atoll since October of 1999. These data are summarized in Figure 4, showing the WBC measurements taken by the Brookhaven National Laboratory leading up the period when the Rongelap people decided to leave the island (1977–84) and then again after they had resettled on Mejatto Island (1989–94). ^{137}Cs body burdens have been interpreted on the basis that cesium is maintained in the body under steady-state conditions as a result

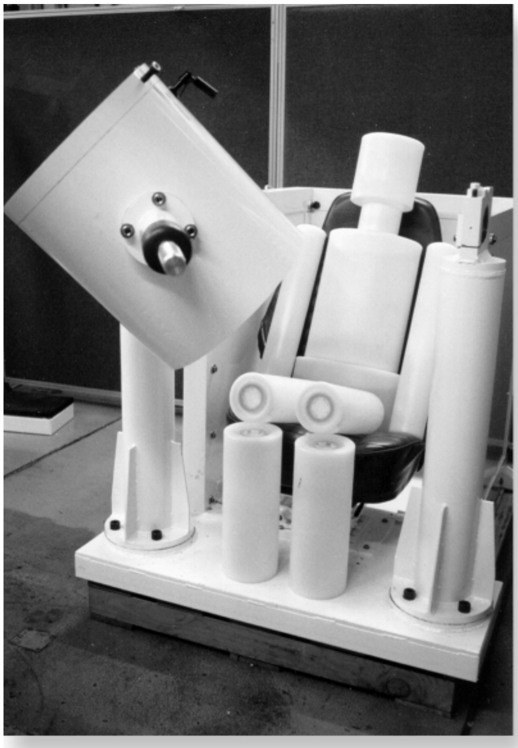

Figure 3. Rongelap Atoll Whole-Body Counter, with the phantom calibration source "seated" in the Masse Chair.

of a series of chronic intakes. The biokinetic model for ^{137}Cs uptake, transport, and distribution in the human body is well documented. The half-time for cesium retention in the human body is relatively short, around 110 days. The radiological conditions on Mejatto Island are close to worldwide fallout concentrations, so estimates of ^{137}Cs in the Rongelap population taken between 1989 and 1994 provide a baseline (mean value ~3 microsieverts per year) for the current workforce on Rongelap Atoll. We have made the important finding that there is only a slight increase in the mean ^{137}Cs body burdens in the workforce (mean value ~8 microsieverts per year) compared with Mejatto measurements; this slight increase is of no radiological significance. These data also represent largely adult males, who would normally tend to have a high ^{137}Cs body burden when compared with the total adult population. Workers living on Rongelap Atoll are known to be consuming some of the local foods containing elevated levels of ^{137}Cs—hence the whole-body measurement data should help provide a level of assurance for the workers and Rongelap community.

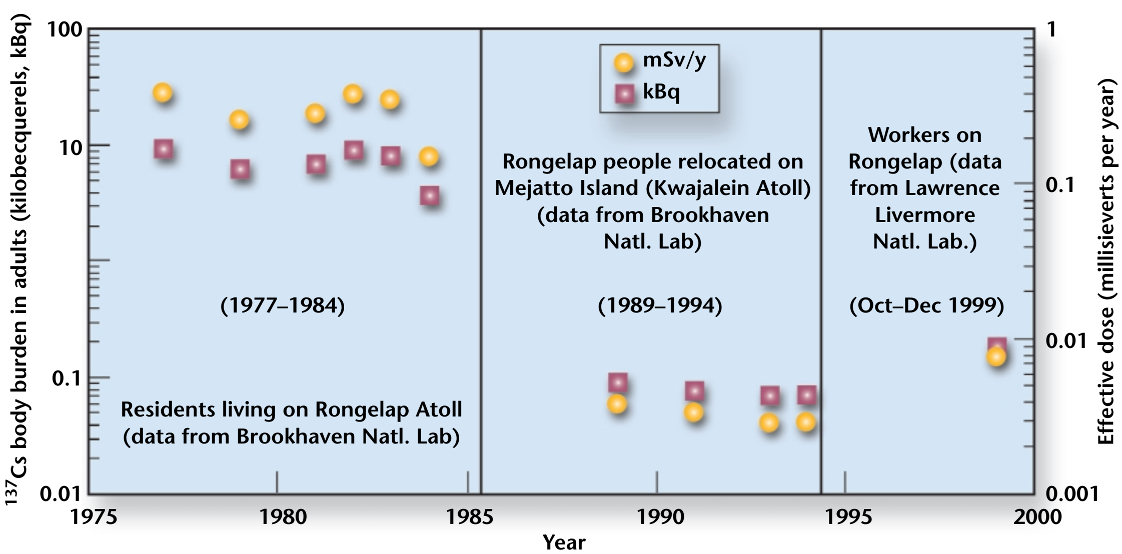

Figure 4. ^{137}Cs body-burden measurements and the effective doses in the Rongelap population show that workers currently on Rongelap have no significantly different exposure than the Rongelap people relocated in 1985 to another atoll.

Incorporating Surprise into Models of Global Climate Change: A Simple Climate Demonstrator Model

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National need: Predict the effects of climate change— **climate-simulation computer models will enable policy makers to see the possible future effects of energy policy choices.**

Climate analysts need to do a better job of characterizing climate "surprises"—the low-probability yet high-consequence scenarios that are driving much of the international concern about climate change. Currently, most analyses rely on models or projections that assume that climate responds slowly and predictably, gradually warming as atmospheric carbon dioxide (CO_2) concentrations increase from fossil fuel burning. In fact, the global climate is a complex system that could behave quite erratically. The circumstances that could drive such behavior depend on the physical characteristics of the climate system itself, as well as the magnitude and rate of the CO_2 buildup.

During 1999, we developed a climate-simulation model that is both simple enough to use in economic studies, and complex enough to explore the causes and consequences of one major type of "climate surprise"—the collapse of the overturning circulation of the North Atlantic Ocean. This model will enable researchers and policy makers to see more clearly the range of possible climate futures that could result from current policy choices.

A New Way to Simulate the Unexpected

The new model, the Simple Climate Demonstrator (SCD), is designed to mimic the response of complex climate models used for global warming research. Unlike earlier simple models, SCD allows for "surprise" effects on ocean circulation, including effects produced by the rate of increase of CO_2 concentrations.

Large, three-dimensional computer models of Earth's climate system, such as the ones run on the Laboratory's supercomputers, exhibit what was once thought of primarily as a mathematical curiosity: the ability to produce two very different global climate conditions given identical climate-controlling factors. The two climate conditions can be likened to the positions of a light switch (on/off), where each position is stable indefinitely unless "switched" by an external force—a finger in the case of a light, or man-made greenhouse gases in the case of climate.

For climate, the two stable conditions relate to the strength of the overturning circulation in the Atlantic Ocean. The Gulf Stream that warms Europe is part of this circulation. The overturning circulation is driven by the sinking of cold, dense water at high latitudes. The circulation is called "thermohaline" because the differences in density that drive it are determined by temperature and salinity. The thermohaline overturning circulation can be idealized as the localized sinking of dense plumes of water at high northern latitudes followed by transport southward in the deep ocean. Upwelling at lower latitudes and return flow northward in the upper ocean completes the circuit. The two idealized stable states for this flow are (1) similar to present day and (2) little or no flow at all. The case of no flow is referred to as "overturning collapse" or the "thermohaline catastrophe."

Ocean Circulation in the Future

The possibility of a thermohaline catastrophe has profound implications for the climate of the Northern Hemisphere, especially Europe. Western Europe is up to 15°C warmer in winter than it would be if the heat transported northward by the thermohaline overturning circulation were to cease.

For further reading on this topic, see page 79.

It is significant that the potential for thermohaline circulation collapse is now known to be more than a mathematical oddity. The geologic record of past climate change clearly shows a dozen or more incidences of reduced or collapsed thermohaline circulation. Although the circulation collapsed during cold climates in the past, this history is still highly relevant to a much warmer future. Any process that acts to lessen the density of the northern Atlantic Ocean can reduce or possibly collapse the overturning circulation. Increasing temperature and precipitation from global warming may be just such a trigger.

The Simple Climate Demonstrator

Climate modelers now understand the importance of correctly simulating the response of ocean circulation in their models. However, current comprehensive supercomputer models differ not only in their overall climate sensitivity, but also in how well they simulate the present-day thermohaline circulation and its response to global warming scenarios. Our goal was to develop a simple climate model that would demonstrate behaviors similar to those found in the current supercomputer models. The model had to be simple enough to understand thoroughly, and computationally efficient enough to be useful for coupling to similarly simplified economic models. Thus, the SCD model represents only five geographic regions in the Northern Hemisphere.

Circulation or No Circulation

As found in other models, SCD exhibits two stable climate states. One state has a substantial overturning circulation of about 20 sverdrups (1 sverdrup = 1 million cubic meters of seawater per second). The second state has no overturning. Lowering the density of the water in the northern upper ocean box can trigger a jump from the overturning to the no-overturning state. This can be accomplished by increasing either the temperature or the rainfall, both of which are likely to occur with increasing CO_2.

To move from the no-overturning, "collapsed" state back to a "normal" circulation requires a large decrease in global temperature. In fact, the temperature decrease must be larger than the increase that triggers the collapse. The inability to reverse a thermohaline collapse causes concerns about such an event in the real world.

Climate Change for 1800–2500 AD

The SCD model was used to simulate global climate change for the years 1800–2500 AD for four atmospheric CO_2 scenarios (Figure 1). In each case, the scenarios start from pre-industrial CO_2 concentrations of about 280 parts per million by volume (ppmv) and follow the actual historical curve until 2000 AD. After 2000 AD the concentrations follow a "business as usual" (BAU) curve, which effectively has a 0.61% per year exponential growth rate. The curves in Figure 1 depart from the BAU

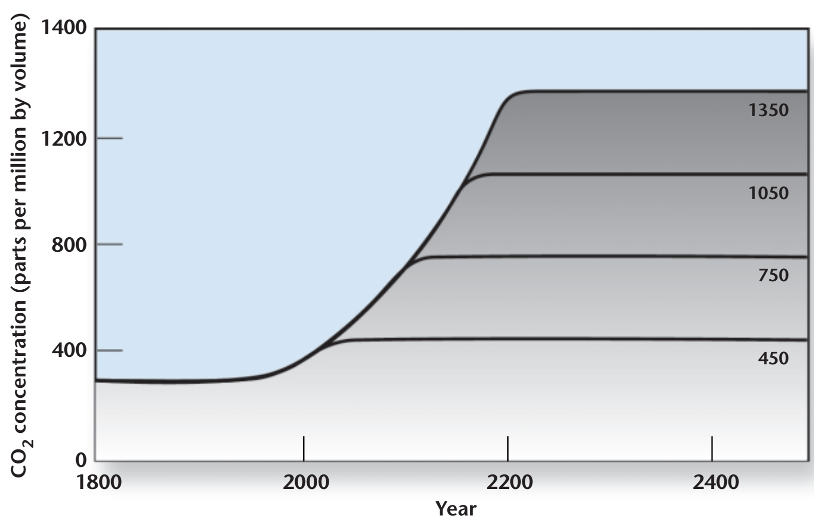

Figure 1. Four time-dependent atmospheric CO_2 concentration scenarios used in the SCD model. Each starts with the historical CO_2 increase to the present day, then moves into the future following a "business-as-usual" scenario. The effective exponential CO_2 increase rate after 2000 AD is 0.61% per year. Each scenario falls away from the exponential increase and stabilizes at the value shown.

exponential growth and stabilize at the arbitrary values of 450, 750, 1050, and 1350 ppmv. For comparison, current concentrations are about 370 ppmv.

The values of 450 and 750 ppmv have often been used to bracket a plausible range of stabilization values. However, when atmospheric concentrations are calculated for 2150 AD and beyond, large CO_2 increases are expected unless there is a significant shift away from fossil-fuel-based energy systems, a major improvement in energy efficiency, or massive carbon sequestration programs implemented over the next 50–100 years. Thus, the higher values of 1050 and 1350 are plausible scenarios as well, although it is often assumed that humans would act to curb CO_2 emissions before such high levels were reached.

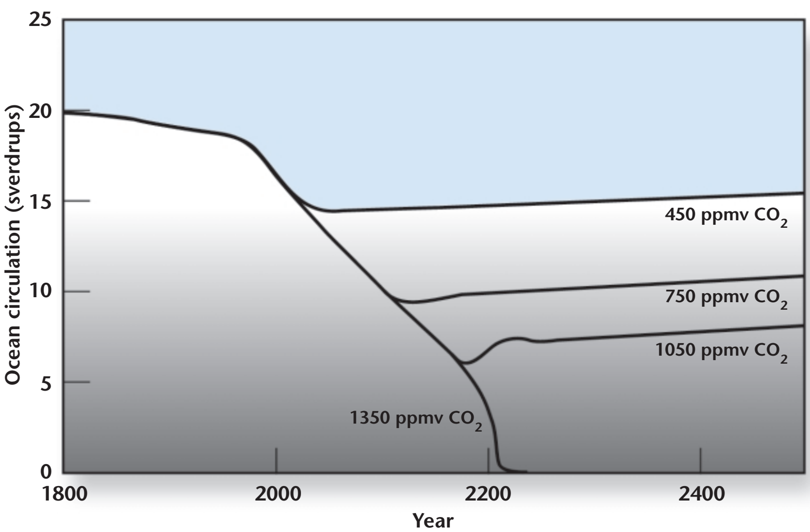

Figure 2. Response of the North Atlantic overturning circulation strength for the four CO_2 scenarios shown in Figure 1. The present circulation strength is thought to be roughly 20 sverdrups (1 sverdrup = 1 million cubic meters per second). The strength of the overturning circulation decreases with increasing CO_2 until a point is reached where the overturning ceases entirely (the so-called "thermohaline catastrophe").

The SCD model was run with a global climate sensitivity of 3.0°C (that is, a 3.0°C global surface-air temperature warming for an equilibrium CO_2 doubling), which is in the middle of the current uncertainty range of 1.5–4.5°C.

Figure 2 shows the behavior of the overturning circulation for each of the four CO_2 scenarios shown in Figure 1. In the case of the highest CO_2 concentration increase, the overturning circulation collapses permanently, as opposed to merely slowing.

CO_2 Effects on the Ocean

Tests were done to see if reducing the CO_2 back toward pre-industrial levels could force the case having a collapsed circulation back to normal. The model showed that the CO_2 would have to be reduced to around 100 ppmv to accomplish this. This value is probably lower than has ever occurred on Earth, and not likely to be photosynthetically acceptable for natural ecosystems and agriculture, even if it were physically possible to attain. An emergency reduction of atmospheric CO_2 concentration is an unlikely remedy for reversing a thermohaline catastrophe once it occurs.

After a thermohaline collapse, the north ocean box stabilizes at a temperature that is colder than the present day by about 8°C, even though the globe as a whole warms by 3.6°C. This would lead to the ironic condition where the world warms well beyond the range experienced over the past 10,000 years—during which human civilization evolved—while northern Europe and the North Atlantic cool to temperatures reminiscent of those during the transition from the last ice age.

Some comprehensive models have recently indicated that the rate of increase of CO_2, not just the absolute amount, can influence thermohaline collapse. Figure 3 illustrates the behavior of the SCD model's thermohaline circulation as a function of both stabilized CO_2 amount and the annual rate of increase of CO_2 used to reach stabilization. In this example, we are only interested in whether the circulation collapses permanently or recovers after it is allowed to reach its equilibrium many centuries in the future. As can be seen, the stability of the circulation does depend on the rate of CO_2 increase as well as the stabilization value of CO_2 amount. For a CO_2 increase rate of 0.9% per year, the circulation collapses at 1125 ppmv. However, a higher stabilized concentration of 1450 ppmv can be reached without collapsing the circulation, if the CO_2 increase rate is restrained to only 0.2% per year.

The dependence of thermohaline circulation collapse on the rate at which CO_2 is allowed to increase is contrary to the standard assumption that only stabilization levels matter, not rates at which stabilization is achieved. This could have a marked impact on some policy options in which it is argued that early abatement is costly and thus delayed abatement is preferable on cost-effectiveness grounds. If rates of CO_2 increase are important in determining surprise in the climate system, then such conventional assumptions about the costs of delayed abatement could be incorrect.

The SCD model should prove to be a useful tool for understanding and simulating the behavior of much more expensive models. However, substantial uncertainties remain in the comprehensive models themselves. In Figure 3, the true location of the dividing line between the "collapse" and "recovery" zones is controlled by uncertain socioeconomic and geophysical factors.

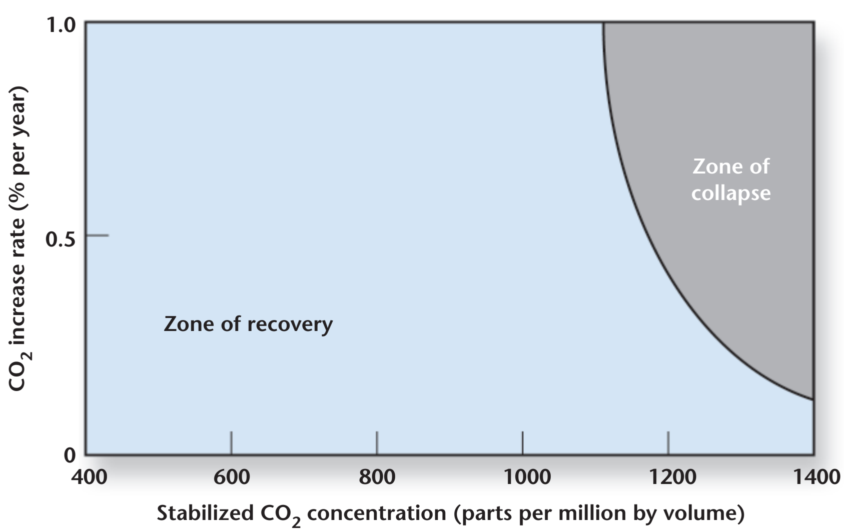

Figure 3. The strength of the thermohaline overturning circulation is shown as a function of the stabilized CO_2 concentration and CO_2 annual increase rate. All the model simulations used to create this figure start from an equilibrated pre-industrial state, follow the historical CO_2 increase, and then follow the path defined by the given increase rate and stabilization value. The model climate sensitivity is set at 3°C. Note the permanent thermohaline circulation collapse ("zone of collapse") for a combination of sufficiently high stabilized CO_2 concentrations and CO_2 increase rates.

The NASA Global Modeling Initiative: Analyzing the Atmospheric Impacts of Supersonic Aircraft

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John Tannahill
Peter Connell
Dan Bergmann

***National need: Predict the effects of climate change*—the effects of emissions from a proposed fleet of supersonic aircraft must be analyzed by simulation before production decisions can be made.**

The National Aeronautics and Space Administration (NASA) is investigating and assessing the possible environmental impacts from a proposed fleet of high-speed civil transport (HSCT) aircraft. These aircraft, proposed to be built in the United States within the next 20–30 years, would fly in the lower stratosphere at a speed of near Mach 2, thereby reducing the flight times for long cross-ocean trips by at least a factor of two. The primary environmental effect of interest has been the effect of the combustor's emission of oxides of nitrogen (so-called NOx emissions) on stratospheric ozone. It is feared that these nitrogen species would alter the catalytic cycles of nitrogen and hydrogen to deplete stratospheric ozone. Over time this NOx has remained a constant issue, but especially over the last 5 years, the combustor's emission of water has also peaked people's interest. First, because the water emission can alter the hydrogen catalytic cycle and the occurrence of polar stratospheric clouds; also, research (especially in Europe) has shown that water emissions from aircraft can increase contrails and cirrus cloud formation, and thus influence climate.

NASA is sponsoring a Global Modeling Initiative to better simulate the effects of these aircraft. The goal is to produce an assessment model that is well understood and validated against observations and to carry out multi-year simulations to provide a meaningful assessment. Because of the Laboratory's history in the science of aircraft assessment, its capabilities in high-performance/parallel computations, and its willingness to actually carry out assessment simulations, it was selected as the NASA "core modeling site."

Background

During the 1970s NASA's research moved forward; however, the economic difficulties associated with these aircraft slowed interest. By the late 1980s Boeing began to voice interest in building the aircraft. Their vision was a fleet of 500–1000 HSCTs used on flights across the oceans (sonic-boom issues still preclude flights of these aircraft over land). At that time, the Office of Aeronautics at NASA took up the challenge and created a program to assess the atmospheric impact of these aircraft.

For most of the 1980s and early 1990s, the research and assessments were done by various teams across the United States (and Europe) using zonally averaged (two-dimensional in latitude and altitude) chemical-transport models. Three-dimensional chemical-transport models were still being developed and, furthermore, their computational requirements were far beyond current computing capabilities. NASA funded multiple institutions to perform the assessments to provide a "collective" analysis of the multiple assessment runs. Over time, each institution had developed its own model using different algorithms, different assumptions, and different model structures. To provide better understanding of the models' scientific performance, NASA conducted model-to-model and model-to-data intercomparisons in which all models performed a series of identical calculations with given boundary conditions. These intercomparisons and comparisons with data provided the basis for trying to understand model differences in the aircraft-assessment simulations. However, simulation results differed to a large degree and the models were complicated; producing a meaningful and well-understood aircraft impact assessment was difficult.

By the mid 1990s, the scientific community began to question the continued use of two-dimensional models as the primary scientific assessment tool. The proposed aircraft are intended to fly in the lower stratosphere—exactly the region of the atmosphere where the zonally averaged assumption inherent in two-dimensional models breaks down. NASA agreed that future aircraft-assessment

For further reading on this topic, see page 79.

models would necessarily require three dimensions, but it did not have the funds to support multiple three-dimensional modeling efforts; moreover, the number of institutions that could actually develop and run a three-dimensional chemistry model was very limited.

It was at this point, in 1995, that NASA made a decision to carry out aircraft-assessment simulations using a collaboratively developed three-dimensional chemical-transport model. This new program was called the Global Modeling Initiative (GMI). The computational issues were a major concern since few (if any) institutions in the United States had run multi-year chemistry simulations, especially with the detail required for the aircraft assessment; the Laboratory's experience and its high-performance computing facilities earned it selection as the core modeling site.

The Global Modeling Initiative

The GMI followed a new methodology in which science team members provided modules and data into a single model structure. Modules were interchangeable and allowed numerical experimentation that greatly enhanced our ability to understand model sensitivities and model results. Each institution on the team provided either model software, data for validation, or analysis of results. All 3-D assessment model creation, development, integration, and simulations were done at the Laboratory in close collaboration with team members. The Laboratory's parallelized IMPACT chemistry model formed the basic structure for the NASA GMI model. Members of the science team for the past three years are listed below.

National Center for Atmospheric Research (NCAR)
Guy Brasseur, Peter Hess, Jean-Francois Lamarque, Phil Rasch

NASA GSFC
Ricky Rood, Anne Douglass, David Considine

NASA GISS
David Rind, Jim Hansen

Univ. of California, Irvine
Michael Prather

AER Corp.
Malcom Ko, Jose Rodriguez, Debra Weisenstein

Univ. of Maryland
Ken Pickering

Harvard Univ.
Daniel Jacob, Jennifer Logan

Univ. of Michigan
Joyce Penner

State Univ. of New York, Stoneybrook
Marv Geller

Boeing Corp.
Steve Baughcum

ONERA–France
Richard Ramaroson

Lawrence Livermore National Laboratory
Doug Rotman, Doug Kinnison, Peter Connell, John Tannahill, Deanne Proctor

Our job at the Laboratory was to take in all the model software, design, develop, and integrate all of these into a working 3-D chemistry-assessment model for use on parallel computers, and finally to carry out the required assessment simulations. At times this was simply integrating the provided subroutines, but other times this required extensive rewrites of routines to parallelize or to make them usable and understandable.

The 3-D Model

Through close collaboration with NASA and the GMI science team, the GMI 3-D assessment model was created here. It includes three different algorithms to solve the coupled set of stiff ordinary differential equations representing the chemistry, two different photolysis (short-wave radiation) algorithms, three different transport/advection algorithms, and a polar stratospheric cloud algorithm. As input meteorological data, the model provides three different choices—data from the NCAR MACCM2, the GISS Model II', and the NASA Data Assimilation Office. The model was implemented, validated, and run on Cray C90s and J90s, the IBM SP2, SGI Origin 2000, and the SGI/Cray T3E.

Validation of the GMI model occurred in two phases. First, to ensure proper implementation, the model must duplicate a test case provided by the originator of each module. Second, the GMI model was compared with a myriad of observed data, including satellite, balloon, aircraft, and laboratory data. Figure 1 shows seasonal vertical ozone profiles for 40–50° north latitude (near the latitude location of maximum aircraft traffic). The figure includes climatological data along with GMI simulation results using all three meteorological input datasets. In addition to showing the GMI model's capabilities to scientifically represent the distribution of ozone, this figure also presents an example of a unique capability of this model. The GMI model was designed and configured to provide flexibility in which scientific modules are used to carry out simulations. Hence, one can select particular advection and chemistry algorithms to carry out simulations, then swap one particular module and re-run the simulation. This provides an ability to observe the sensitivity of a model's output to algorithms, model assumptions, or any other model-dependent aspect. This important capability enables us to carry out tightly controlled numerical experiments and allows us to more fully understand model simulations, leading to much improved assessments. In Figure 1, the GMI model is identical in all ways except for the input dataset. All three datasets underestimate ozone quantities at 45–60 kilometers. Further analysis showed this to be directly attributable to our choice to not include a particular chemical reaction whose reaction rate and yields are not finalized. (Addition of our best guess to that reaction cured this ozone problem.) Between 10 and 20 kilometers in altitude, the simulation using the NASA Data Assimilation Office (DAO) fields produced an overabundance of ozone. Further analysis showed this to be caused by a short stratospheric residence time and an overly aggressive exchange of material between the troposphere and the stratosphere. Comparing simulations from 3-D and 2-D models, these validation simulations indicated an improved ability to model lower-stratospheric ozone, stratospheric circulation, and exchange of material across the tropopause. For example, Figure 2 shows distributions of a

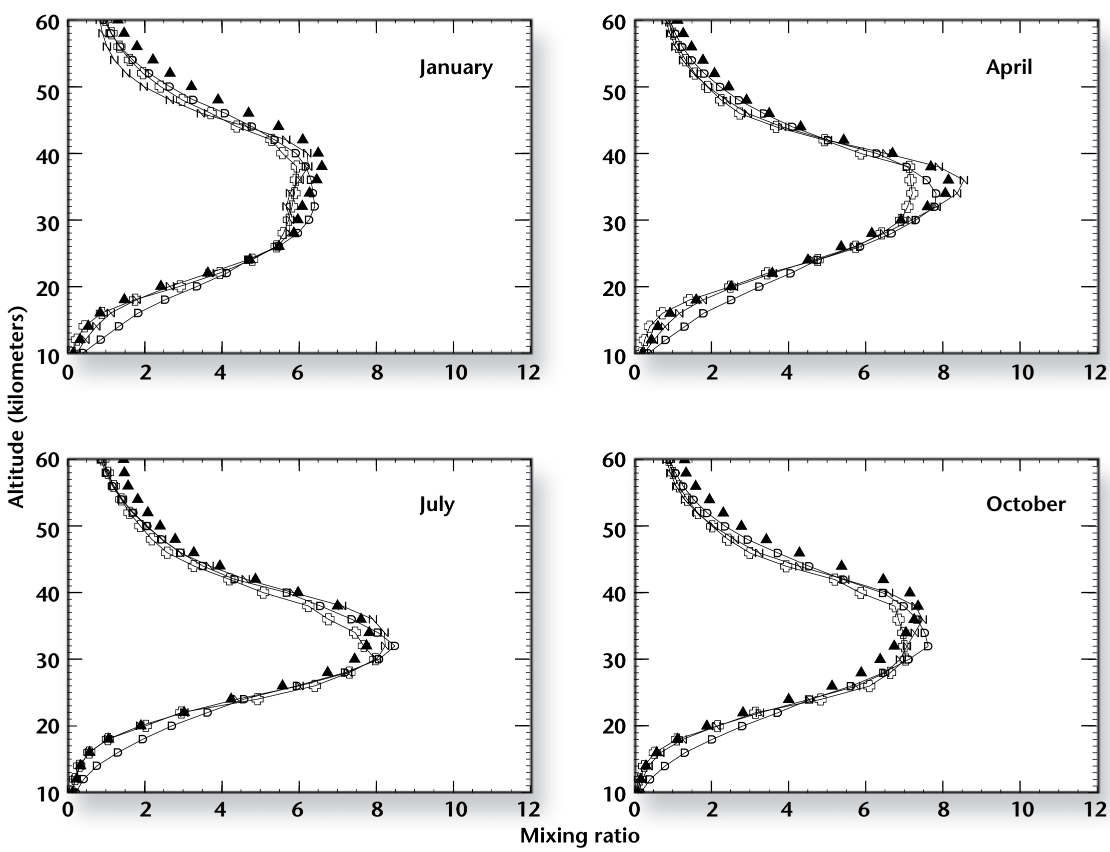

Figure 1. Vertical profiles of ozone at 40–50° north latitude from measurements and from the GMI model run with three different meterological input datasets illustrate that the model provides improved ability to simulate lower-stratospheric ozone circulation. (N = NCAR MACCM2, D = NASA DAO, G = NASA GISS II'.)

proxy HSCT tracer in the lower stratosphere. This tracer is emitted using Boeing projected flight patterns and is conservatively advected throughout the stratosphere and upper troposphere. The figure shows tracer simulations using an identical model except for the meteorological input. Higher concentrations of tracer in the MACCM2 simulations suggest a longer stratospheric residence time and slower transport of stratospheric material into the troposphere. This parameter is crucial to HSCT aircraft assessment since there is a strong correlation between how long the aircraft emissions of NOx remain in the lower stratosphere and their impact on ozone.

Using this capability to interleave different numerical algorithms and model input data and using observed data as ground truth, we carried out a very large set of numerical experiments to ascertain the optimal combination of model components that produces a simulation that best represents real-world atmospheric-species distributions. To do this, we developed a grading and scoring system. Measured quantities used as testing criteria included

- Temperatures—absolute values with added emphasis on ability to reproduce cold polar regions.
- Vertical and horizontal gradients of nitrous oxide and methane to analyze stratospheric circulation.
- Carbon dioxide and “total water” (equal to water plus methane) to establish the models’ ability to propagate seasonal cycles.

Using these criteria, we established the optimal combination of model components producing the highest-quality comparisons with the observed data. Each combination had its problem areas and issues, but our goal was to find that which produced the integrated best scores. This combination was the formulated GMI assessment model that was used for the final assessment simulations. It was made up of the following:

- Input meteorological data: NCAR MACCM2

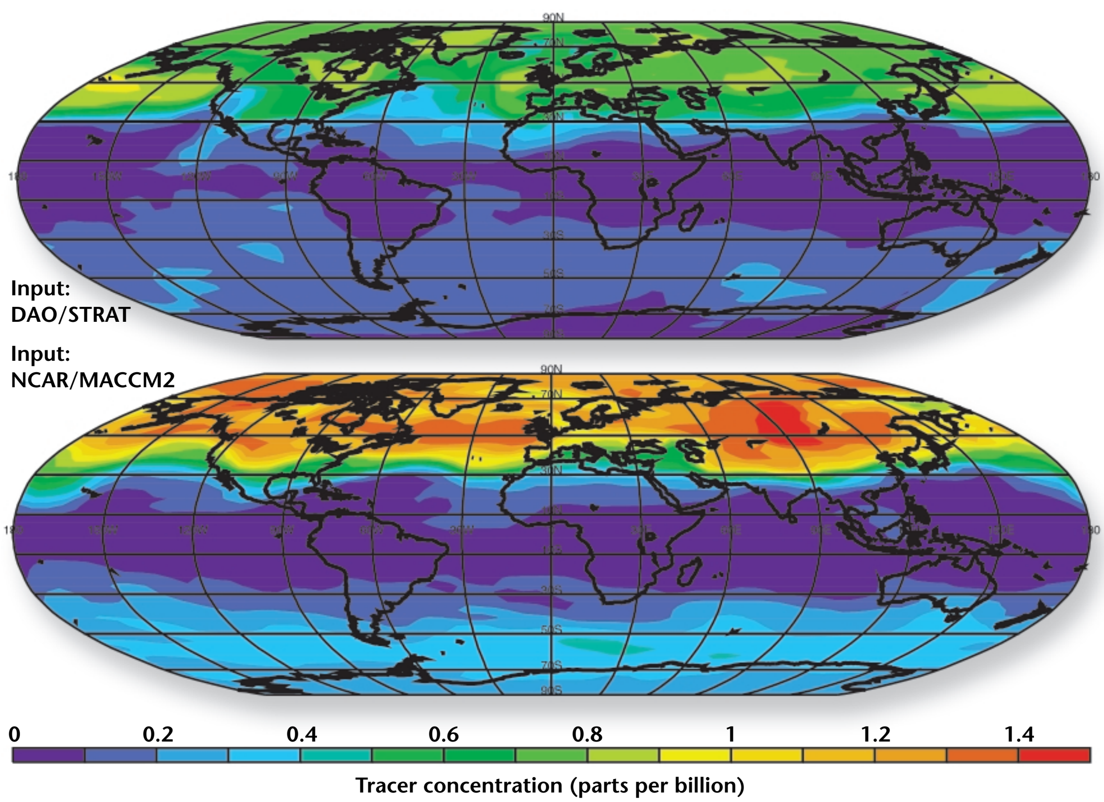

Figure 2. A core model framework allows intercomparison of model components. Here the influence of the input meteorological data on the simulation of transport of HSCT aircraft emissions (100 hectopascals pressure) is shown.

- Advection algorithm: NASA DAO Lin/Rood Flux Form semi-Lagrangian
- Chemistry algorithm: MEDIANTE algorithm from ONERA (France)
- Photolysis: Look-up table from NASA Goddard
- Cold sulfate algorithm: NASA Goddard/Univ. of Maryland

All assessment simulations have been completed and the NASA report is published. All final simulations were done on parallel computers, primarily the 1024 node T3E at NASA Goddard and clusters of SGI Origin 2000 machines at NASA Ames.

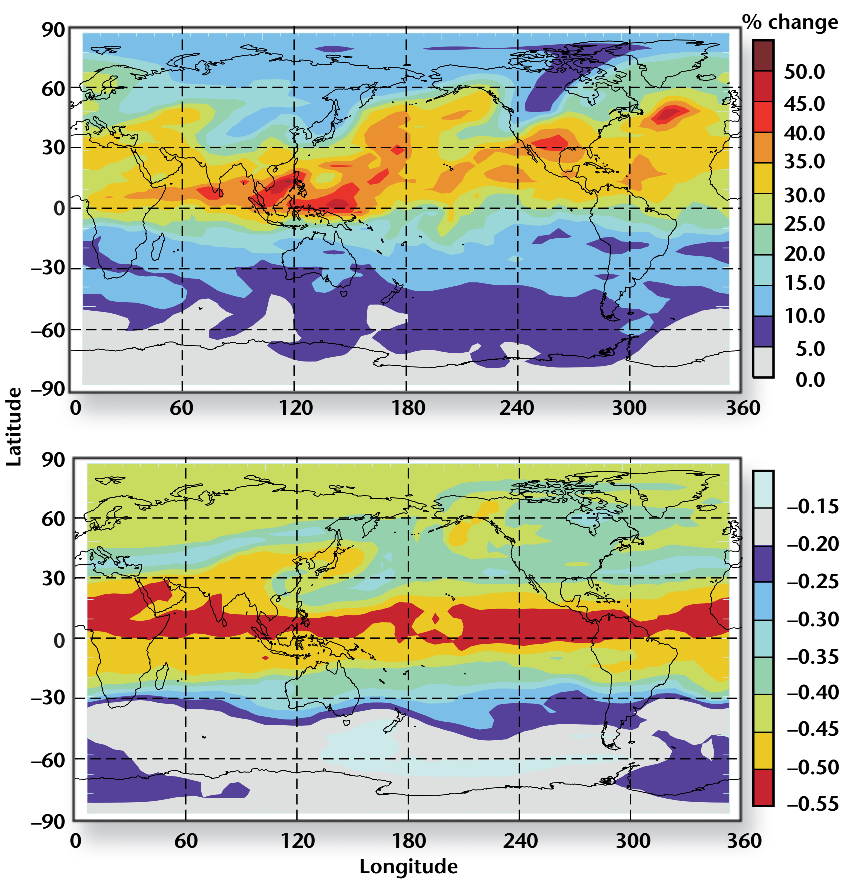

Figure 3. (*top*) Predicted changes in nitrogen oxide levels in the stratosphere due to aircraft emissions and (*bottom*) the associated changes in ozone.

Aircraft Impacts

The final assessment by the GMI model showed a near-zero global ozone impact from a fleet of 500 HSCTs. This small global impact is made up of an increase in the very lower stratosphere and a decrease in the upper stratosphere. Figure 3 shows the HSCT-induced buildup in reactive nitrogen species (known as NO_y) and the resultant change (decrease) in ozone in the middle stratosphere. Lower-stratospheric increases are caused by aircraft emissions into a region where the model simulates too-low background levels of total reactive nitrogen compared with observations. These low nitrogen levels combined with a complicated interaction of chlorine, hydrogen, and nitrogen catalytic cycles allow ozone to be produced in this region. In addition, overly warm temperatures in the polar lower stratosphere never allowed the important ozone depletion from heterogeneous chemistry on polar stratospheric clouds.

As part of our validation and assessment, we integrated a total of nearly 50 simulated years. Calculations of that magnitude could not have been carried out without using massively parallel computers.

Over the next three years, NASA is continuing this collaborative development in carrying out an assessment of the existing and proposed fleet of commercial subsonic (tropospheric) aircraft. The Laboratory will continue to be the integrating core model site. In addition, NASA is moving forward with plans to expand the application of the GMI process, science team, and model to a more comprehensive set of anthropogenic and natural influences on atmospheric chemical species. These may include, for example, chlorofluorocarbons, volcanic eruptions, short-lived compounds such as methyl bromides, sulfate aerosols, and many others.

Atmospheric Release Assessment Programs

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***National need: Protect the population from contaminants released into the environment*—we operate the U.S. resource for assessing contamination and human exposure from natural or man-made hazardous releases.**

For further reading on this topic, see page 80.

The Atmospheric Release Assessment Programs (ARAP) conduct research, development, and operational assessments to track the dispersal of hazardous material released into the atmosphere. Central to the ARAP is the National Atmospheric Release Advisory Center (NARAC), managed and staffed by ARAP personnel and located at the Laboratory. NARAC is an emergency response and assessment service; it predicts the probable spread of contamination and resulting population exposure from an atmospheric release of hazardous material. NARAC's primary function is to support the Department of Energy and the Department of Defense (DoD) for radiological releases at their facilities and to assist them and other agencies (from local to international) in responding to natural and anthropogenic hazardous releases, at the direction of the DOE.

Since 1979, NARAC personnel have responded to more than 100 incidents involving radiological and chemical releases, smoke from fires, and plumes from volcanic eruptions. Notable examples include the Three Mile Island and Chernobyl nuclear reactor accidents, various smoke and chemical releases during and following the Persian Gulf War, and, more recently, the criticality accident in Tokaimura, Japan. Our work is supported by the DOE Atmospheric Release Advisory Capability (ARAC) program, the DOE Chemical and Biological Nonproliferation Program, and by several agencies within the DoD.

Over the past few years, much of our research and development has focused on the potential threat of chemical–biological terrorism. The hazard from a chem–bio agent release within an urban area can be confined to a localized area within or around a single building or extend out to a larger portion of the city or even out into the surrounding suburbs, depending on the type of agent, release characteristics, and ambient meteorological conditions. We are addressing this threat by developing a coupled suite of multi-scale (regional- and building-scale) dispersion models, expanding our supporting databases and operational infrastructure, and developing an internet remote access capability to effectively respond to a chem–bio release. We are also pursuing new initiatives that require the use of high-performance computing, including wildfire prediction, plume uncertainty estimation, and sensor-driven plume modeling.

A continuing challenge for the ARAP staff is to expand our capabilities in keeping with advances in science and technology and in response to changing national security concerns—while maintaining NARAC operational emergency preparedness and response readiness. Our accomplishments in 1999, discussed below, illustrate this challenge.

NARAC Responds to Real Emergencies

On September 30, 1999 at 8:10 a.m. PDT, NARAC was notified by the DOE of an ongoing nuclear accident that had begun about 13 hours earlier at a nuclear fuel conversion facility in Tokaimura, Japan. Television showed a facility with a hole in its roof, suggesting a severe explosive accident with potential for large releases of nuclear material into the atmosphere.

NARAC and the Japanese Atomic Energy Research Institute (JAERI) had previously established a data link and agreed to exchange information during non-military nuclear emergencies involving the dispersion of nuclear material releases into the atmosphere. Calls placed that morning by NARAC staff to JAERI verified that a criticality event was ongoing, but no explosive release to the atmosphere was evident.

NARAC immediately calculated a regional-scale spread of dispersed material using a unit release rate for noble gases and iodine aerosols—the commonly released suite of radionuclides produced during a criticality accident. This initial calculation was provided to JAERI and sent to the DOE Operations Center, the DOE Oakland Regional Office, and the DoD Joint Nuclear Accident Coordinating Center. The White House, the DOE Office of the Secretary of Energy, and the Environmental Protection Agency were requesting guidance on if and when the cloud of nuclear material might impact the continental United States. NARAC used 6-day global forecasts provided by the U.S. Navy to predict that the Aleutian Islands could be potentially impacted within 6 days and the Pacific Northwest within 7 days. The consequences were unknown because the magnitude of the release was uncertain at that time.

Other U.S. government agencies requested NARAC results. With DOE's approval, NARAC electronically sent its consequence predictions to emergency operations centers at the Environmental Protection Agency, the Nuclear Regulatory Commission, the National Oceanic and Atmospheric Administration, and the U.S. Marine Corps in the Pacific. JAERI and NARAC used these data to estimate the amount of radioactive material released and transported downwind. Over the 20-hour accident period, the wind direction varied considerably, thus dispersing the radioactive material in a fan pattern and reducing potential dose in any one direction. Predicted doses from material released into the air were below guidelines for sheltering people at Tokaimura and negligible across the Pacific Ocean and the United States (Figure 1).

Implementation of the New NARAC Modeling and Operating System

We replaced NARAC's primary operational capability with a completely new atmospheric modeling and operating system using redesigned and upgraded models, software, and hardware. The modeling system consists of a new modeling suite, the coupled COAMPS/ADAPT/LODI models, which are state-of-the-science tools for predicting the consequences of atmospheric releases of hazardous materials over multiple spatial and temporal scales (Figure 2).

Our in-house version of the Naval Research Laboratory's COAMPS model provides NARAC with an operational regional weather forecasting capability. The new atmospheric data assimilation model ADAPT constructs meteorological fields including nondivergent mean winds, pressure, precipitation, temperature, and turbulence from real-time observational and forecast model data. The two meteorological models are used to drive NARAC's new atmospheric dispersion model, LODI, which simulates a broad range of hazardous-material transport and removal processes. The models are coupled to NARAC's extensive databases which provide elevation, geographical data, chemical–biological–nuclear material properties and health effects, real-time meteorological observational data, and global and mesoscale forecast model analyses and predictions.

The highly flexible design of the operating system provides an improved ability to quickly respond to evolving customer

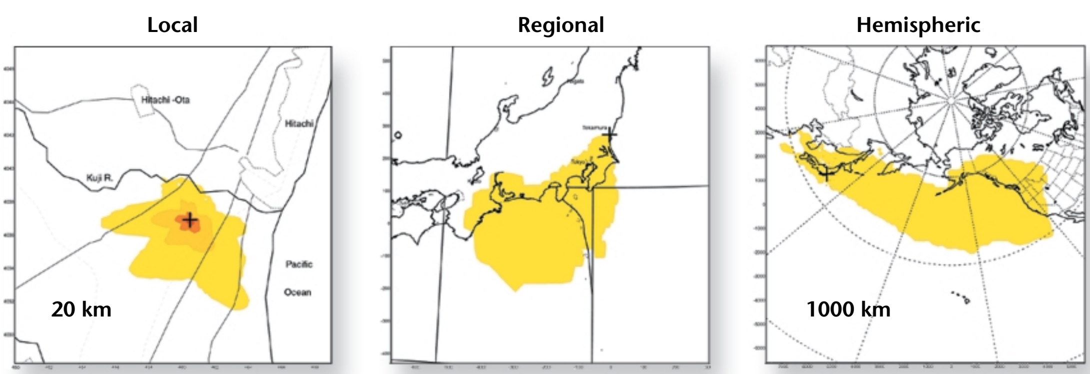


Figure 1. Multi-scale NARAC simulations of the criticality accident in Tokaimura, Japan. Colors show potential combined dose from noble gases and iodine aerosol released into the atmosphere, but represent different dose threshold levels at each scale. All doses are well below guidelines for sheltering population.

requirements. A major structural enhancement is the use of a distributed architecture, allowing software components to run on multiple computer systems. Platform-independent access to NARAC products is provided as well as standardized graphical user interfaces and sophisticated model preprocessors to support the input requirements of the new models. Customer products are produced by post-processing model output to incorporate health effects and to determine populations at risk.

Urban Dispersion Modeling

Emergency Response

We are expanding NARAC capabilities to treat events involving chemical and biological agents, with a focus on predicting the consequences of releases occurring in urban areas. This requires modification of both our regional dispersion models and our supporting model infrastructure. Additional databases of chemical and biological agent properties, health effects, and source models are being integrated into the NARAC system and coupled to physical processes in the models such as biological agent degradation.

The presence of a city alters the mean winds, temperature, and turbulence, significantly affecting the dispersion of hazardous materials. We have therefore incorporated urban physics into NARAC's regional COAMPS/ADAPT/LODI model suite. Since regional models have a spatial resolution on the order of a kilometer and cannot explicitly resolve individual buildings, we have parameterized the area-averaged effects of urban structures. One of the primary physical processes represented is the transfer of energy between the mean flow and the turbulence caused by the presence of buildings. Temperatures are affected by the addition of anthropogenic heat, the incorporation of rooftop thermal energy balances, and the modification of the radiative transfer due to multiple reflections and attenuation. We are also integrating the new urban models with land-use and building data that provide inputs to drive the urban parameterizations.

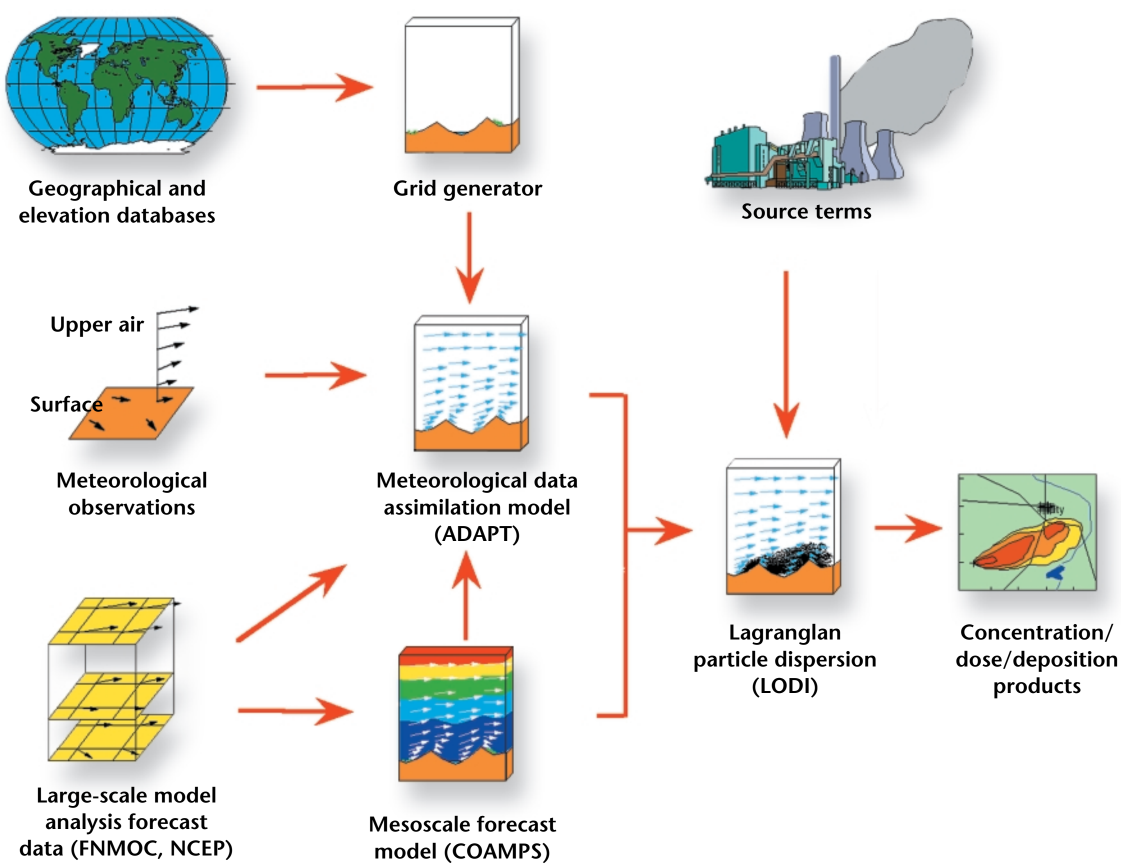


Figure 2. The new NARAC suite of models and some of the major connections to NARAC databases. Topographical, geographical, meteorological, and source properties are input to the ADAPT/COAMPS/LODI models. The final model outputs show concentration and health-effects predictions.

Urban areas cool less rapidly than the surrounding rural region due to heat retention in the buildings and the anthropogenic production of heat. Urban areas can also increase turbulence production by drawing energy from the mean flow, decreasing low-level wind speeds and changing the wind direction. Our model simulations show that this can produce significant modifications in both the windfield and dispersion patterns.

Planning and Consequence Assessment

We have developed a new high-fidelity numerical model to assess the transport and fate of hazardous releases within urban areas with the capability of resolving individual buildings at high resolution. This state-of-the-art computational fluid dynamics model (FEM3MP) has been designed to run on massively parallel platforms and contains many physics submodels that are relevant to the simulation of chemical and biological agent releases. The results of this model have been used to support counterterrorism emergency planning for specific government sites during special events and has aided in the preparation and design of field experiments. Other applications of this model include enhancing NARAC's emergency response capability with building-scale dispersion information, calculating very-high-resolution wind flow and dispersion patterns around building complexes, and providing data linkage to indoor and regional models.

Over the past year, validation studies for our model have included comparisons with both wind tunnel and field data. We recently performed a coupled field test and model validation study of the atmospheric flow around the NARAC building. The purpose of the field experiment was to collect wind field data around a single but relatively complexly shaped building to validate FEM3MP.

In the first phase of the field experiment, model calculations provided guidance for placing the wind sensors. Additional calculations were made after the field tests were performed to compare the model results against the field data. Figure 3 depicts a comparison of the 10-meter-height wind vectors from the model versus measurements for the 225° mean wind direction. The blue areas in the figure reflect the reduction in momentum of the flow due to the building itself and the row of trees east of the building. Momentum drag from the trees is included in the model via a canopy parameterization. The model was successful in capturing the flow channeling induced by the gap between the buildings and the trees as well as the mean recirculation zones downwind of the building. The average difference between the model calculations and observation was approximately 10° for wind direction and 15% for wind speed.

We have also applied the model to an urban downtown four-city-block section containing more than 80 buildings to study the flow and dispersion pattern in street canyons around building complexes. The flow pattern becomes extremely complex because of flow separation and interacting wakes from neighboring buildings. Figure 4 depicts a concentration cloud from an instantaneous release at the source location shown. The resulting concentration pattern shows the strong influence of the flow recirculations around the high-rise building, causing the elevated pollutants to be carried down toward ground level. This and similar simulations

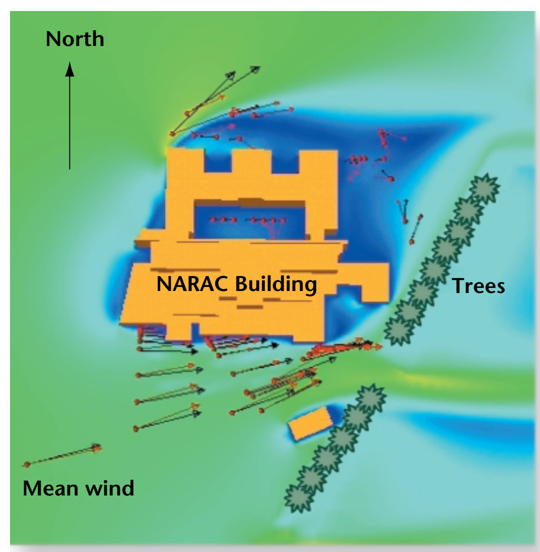


Figure 3. Comparison of the observed and model (FEM3MP) velocities of the wind field around the NARAC building. Red vectors = observations, black vectors = model results. The mean wind direction is at 225°. Note the flow acceleration within the gap southeast of the building and the recirculation zones north and east of the building.

are being performed to support field experiments that will be conducted in 2001.

Expanding NARAC to Wildfire Prediction

In response to congressional inquiry, we have developed a plan for a National Wildfire Prediction Program (NWPP). The goal of the NWPP is to provide guidance to wildfire management planners throughout the country, assisting them in the management of limited fire-fighting resources. The proposed program will be a collaborative effort by NARAC and the Wildfire Modeling Team at Los Alamos National Laboratory. The NWPP will build upon existing physics-based atmospheric and wildfire modeling, a proven emergency response infrastructure, state-of-the-art computer science, and the world's most advanced computers to create a comprehensive wildfire prediction system.

With key members of the wildfire management community, we have defined four primary missions for the NWPP: real-time firefighting support (on-demand, internet-accessible predictions of fire behavior and of the relative effectiveness of various firefighting procedures), tactical planning (such as predictions of the fire and smoke behavior from prescribed burns, and analyses of current fire threats), strategic planning (for long-term forest management and community development), and firefighter training (using computer simulations to help firefighters better understand the effects on fire behavior of weather, terrain, fuel conditions, and various firefighting techniques).

A unique aspect of the NWPP's planned capability is that it will take into account many complex fire–atmosphere interactions. Historically, wildfire behavior models have been based on a limited number of idealized experiments, and have used greatly simplified relationships between weather, fuel conditions, and idealized terrain to predict fire behavior. Real wildfires, however, are strongly affected by changing local atmospheric conditions that, in turn, are affected by the intense heat of the fire itself, as well as by changing regional weather patterns. In addition, the terrain in fire-prone regions is often very complex. The NWPP will provide much more accurate predictions by using advanced, generalized, physics-based models to simulate these fire–atmosphere interactions over realistic terrain at extremely fine spatial resolution.

Recently we have been working closely with officials from Los Angeles County to explore the concept of a Southern California Regional Response Center for Wildfires and Atmospheric Releases. We have also been working with the management of the East (San Francisco) Bay Regional Park District to develop a collaborative study of wildfire behavior in the East Bay Hills, where 25 people died and 3,000 homes were destroyed by a catastrophic wildfire in 1991. These collaborations are helping to demonstrate the

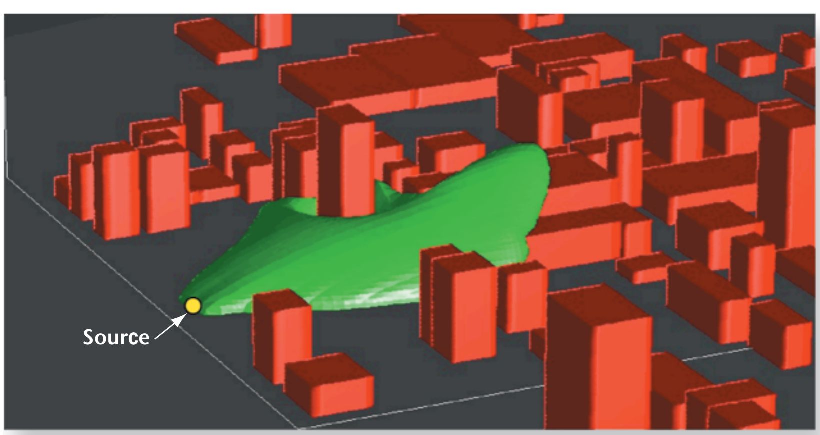


Figure 4. Concentration cloud from an instantaneous release in a downtown urban area, simulated by FEM3MP.

need for and benefits of science-based wildfire prediction (Figure 5).

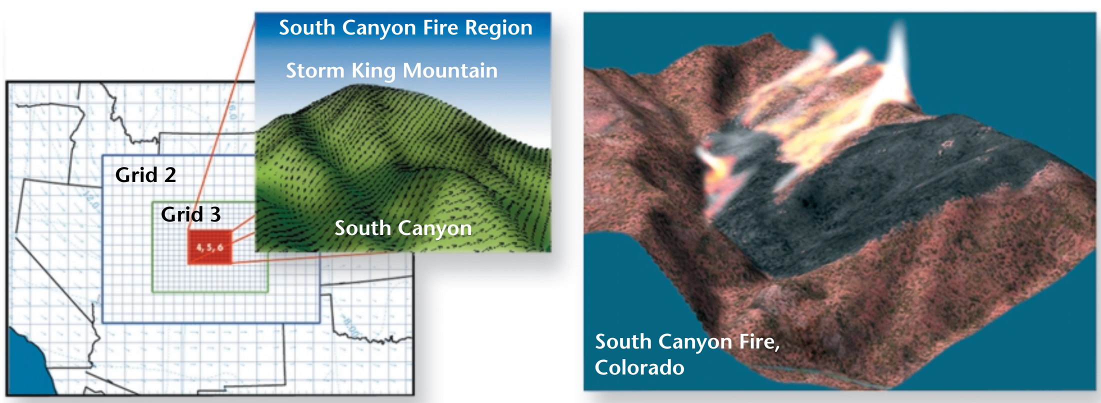
Internet Access to NARAC

Currently, NARAC provides services and products through dedicated workstations installed at over 40 federal emergency operations centers around the country which communicate to the NARAC central system via a dedicated DOE intranet or a dial-up modem. In order to expand access to NARAC services and products to many other organizations and customers, we are developing an internet remote access (IRA) system that will not require any dedicated or specialized hardware or communications links.

NARAC IRA software will be usable on computers already available to most authorized users. This could be a desktop personal computer with Internet access, or a laptop equipped with a cellular modem at the scene of the incident. With this technology, potential users of the IRA system could include local emergency managers and first responders such as fire departments, police departments and hazmat teams.

We have successfully developed and demonstrated a prototype version of the NARAC IRA software. This version provides the ability to enter basic information about an atmospheric release of selected hazardous material, communicate with the NARAC central system, and view maps of NARAC-predicted health hazard zones. Interactive graphical displays allow the user to select a release location by pointing on a map, as well as view model predictions and maps. A communication monitor provides status information on the progress of the NARAC central system model calculation and product transmission. A user can download and install the NARAC IRA software by accessing a NARAC Web site using a Web browser.

In the near future, we will be expanding the capabilities, security, and performance of the prototype IRA system. For example, we will (1) develop a centralized global database of maps for users to download and display, (2) expand support for simultaneous access by many users (including sharing of information between users), and (3) integrate a rapid-local-dispersion modeling tool.



Images courtesy of Los Alamos National Laboratory

Figure 5. The proposed National Wildfire Prediction Program will use advanced models to predict interactions between fire and atmosphere for firefighting support and planning. For example, in 1994, a rapid, unexpected change in the behavior of a South Canyon, Colorado, wildfire claimed the lives of 14 firefighters. This high-resolution, interactive fire–atmosphere simulation successfully captured the behavior of the tragic fire: (*center*) wind simulation and (*right*) the simulated fire.

Advances in Technology at the Center for Accelerator Mass Spectrometry

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National need: Protect the population from contaminants released into the environment**—our world-class facility provides the sensitivity necessary to assess the progress of radioactive and other dangerous compounds through the human body.**

The Center for Accelerator Mass Spectrometry (CAMS) is the most versatile and productive AMS facility in the world. AMS is an exceptionally sensitive technique for measuring concentrations of specific isotopes in relatively small samples (less than 1 milligram). CAMS routinely measures low-abundance isotopes for multidisciplinary applications.

The development and dissemination of AMS technology, coupled with the needs of scientific users, is of special value to the scientific community. The expertise of the CAMS staff and the high throughput of the CAMS facility have resulted in more than 60 collaborative and fee-for-service relationships with universities, research institutes, and government agencies. These relationships have resulted in unique applications and breakthroughs in earth, environmental, and biological sciences. A continuing thrust is the development and application of new AMS technologies as well as the improvement of existing ones; we recently added capabilities for analysis of tritium and actinides, and improved our exceptionally powerful ion source (the Laboratory's ion source produces the highest ion currents of any AMS source presently operating in the world). These capabilities and advances will allow us to continue to lead the field of AMS.

A Compact Tritium AMS System

Tritium (^3H) is a radioisotope that is extensively used in biological and environmental research. For biological research, ^3H is generally quantified by liquid scintillation counting, requiring gram-size samples and counting times of several hours. For environmental research, ^3H is usually quantified by helium-3 (^3He) ingrowth, which requires gram-size samples and ingrowth times of several months. In contrast, the Laboratory demonstrated that AMS can be used to quantify ^3H in milligram-size samples with a comparable sample preparation methodology and a 100-fold improvement in detection limit when compared with scintillation counting. This technique will advance biological and environmental research by providing the sensitivity necessary to trace environmentally relevant concentrations of compounds.

To make the technique of ^3H AMS more broadly accessible, we collaborated in the design and construction of a compact and relatively low-cost prototype system (Figure 1). The new system is smaller, simpler, and less expensive than existing technology. It is the result of a collaboration with AccSys Technology, Inc. of Pleasanton, California,

Figure 1. The new tritium AMS system. The ion source/sample changer is on the right; the linear accelerator in the center simultaneously accelerates tritium ions to 1.5 MeV and ^1H ions to 0.5 MeV. Final mass analysis is performed using a small magnetic spectrometer. Compared with standard scintillation counting, AMS can quantify tritium in milligram-size samples with 100-fold improvement in detection limit. It advances biological and environmental research by providing the sensitivity necessary to trace environmentally relevant concentrations of compounds.

For further reading on this topic, see page 80.

and was funded by a National Institutes of Health/National Cancer Institute Small Business Innovation Research grant.

System Description

The ^{3}H AMS system is based on a Laboratory ion source/sample changer and an AccSys Technology, Inc. radio frequency quadrupole (RFQ) linac. The ion source/sample changer design was chosen because of its high output currents (more than 30 milliamps of H^{-} is typical) and its large-capacity sample changer. An RFQ was chosen because of its inherent compact size (in this case, less than 1.5 meters long) and its ability to simultaneously accelerate all three hydrogen isotopic species to energies sufficient for each to be measured using a simple magnetic spectrometer. Particles with masses greater than that of ^{3}H are not accelerated by the RFQ, a feature that greatly reduced the complexity of the input-beam transport line because no mass analysis is required. With this system, we have measured $^{3}H/^{1}H$ ratios ranging from 1×10^{-10} to 1×10^{-13} from milligram-size samples.

Applications

Our ^{3}H AMS capability will advance biological and environmental research for several reasons. First, ^{3}H is the most widely used radioisotope in biological tracer studies (the number of commercially available ^{3}H-labeled compounds far exceeds the number of commercially available carbon-14 [^{14}C]-labeled compounds). Accordingly, a ^{3}H AMS measurement capability will facilitate experiments using compounds that are either unavailable in ^{14}C-labeled form or are prohibitively expensive. Second, a ^{3}H AMS capability, when used in conjunction with ^{14}C AMS, permits unique low-level double-labeling experiments in which two compounds can be traced simultaneously. Finally, ^{3}H AMS will enable experiments in which the relatively large sample size and the long counting times of the ^{3}He ingrowth technique are not practical.

We recently performed a dual-isotope labeling study to determine the fate and distribution of two dietary carcinogens, PhIP and MeIQx, in a laboratory animal model. These compounds were chosen because they are both found in the diet at very low levels and they cause cancer in rats when administered at much higher doses. In this experiment, low doses of ^{3}H-labeled PhIP and ^{14}C-labeled MeIQx were administered to rats. The tissues were subsequently analyzed by ^{3}H- and ^{14}C AMS to determine the PhIP and MeIQx contents, respectively. The results of the analyses of liver tissues demonstrate that PhIP and MeIQx can both be measured following low exposures (the lowest doses were equivalent to the amount of PhIP one would find in a single well-cooked hamburger). Importantly, the results of this work indicate that co-exposure does not appear to increase the hazard posed by these compounds, compared with exposure to only one compound at a time.

Heavy-Element Spectrometer

Low-level measurements of long-lived actinides and fission products such as plutonium and iodine-129 (^{129}I) have important applications throughout the Department of Energy complex. These radionuclides are distributed throughout the environment because of nuclear weapons testing, fuel reprocessing, reactor operations and, to a lesser extent, accidental releases. In the case of actinides, many present-day applications require a combination of high analytical sensitivity and sample throughput beyond that of currently available techniques. Development of a robust analytical tool with the sensitivity to detect these prominent products of the nuclear fuel cycle at environmental levels will have a broad impact in many of these core mission areas.

Spectrometer Description

An ongoing project at CAMS has been the design and construction of a spectrometer intended for analysis of heavier ions (100–250 atomic mass units, AMU). In work funded by DOE's Office of Nonproliferation and National Security, we are developing a new low-level measurement capability for plutonium and other actinides, and improving our existing ^{129}I AMS capability. For actinide AMS, the most important design consideration is rejection of nearby, abundant isotopes (±1 AMU). For example, a dominating interference for plutonium-239 (^{239}Pu) measurements is the naturally occurring isotope uranium-238 (^{238}U). The heavy-element spectrometer will improve the ^{129}I capability by allowing transport of ^{129}I ions at higher energies, which translates into a higher detection efficiency. It also is expected to improve the ^{129}I abundance sensitivity through improved rejection of the stable isotope ^{127}I.

The new heavy-element spectrometer (Figure 2) relies on a combination of magnetic and energy analysis, followed by particle identification. Magnetic analysis is provided by a 30° bending magnet. Scattering and energy spread in the ion beams exiting the accelerator allow some ions of incorrect mass (for example, ^{127}I or ^{238}U) to pass through the magnetic-analysis stage, so additional suppression of these backgrounds is provided by an energy-analysis stage consisting of a 45° electrostatic analyzer. The filtered ions are counted and identified in nuclear-physics-type ion detectors for identification by energy, mass, and atomic number, allowing additional rejection of backgrounds.

Applications

The heavy-element spectrometer has enabled an Laboratory-Directed Research and Development project to develop the necessary sample preparation and measurement protocols to bring the plutonium capability to routine application. The initial focus of this work is the quantitation of plutonium concentrations and isotope ratios in urine bioassays, for use in support of the Marshall Islands Program in Earth and Environmental Sciences. The technical goals of this project are a sensitivity less than 1×10^6 atoms per sample, an initial throughput of several hundred samples per year, and a cost per sample similar to that of standard alpha-spectrometry measurements.

We recently demonstrated the basic components of our capability and successfully applied this technology to a set of soil samples that included International Atomic Energy Agency (IAEA) reference materials. Measured $^{239+240}Pu$ concentrations showed good agreement with the IAEA reference value and $^{240}Pu/^{239}Pu$ isotope ratios, and matched recently published inductively coupled plasma–mass spectrometry (ICP–MS) results. Measurements of ^{241}Pu, a difficult-to-detect beta emitter that could provide an important additional isotopic signature, were also made. Though not a primary focus of this project, measurement of ^{241}Pu comes with no added cost. Similarly, we expect capabilities for other isotopes, such as neptunium-237 (^{237}Np), as direct byproducts of the present project.

Once complete, our new AMS capability will provide ultratrace sensitivity for plutonium isotopes with high rejection of interferences and low susceptibility to matrix components. These advantages will lead to reduced demands on the sample preparation chemistry, high throughput, and rapid turnaround of results.

Evolution of a Cesium Ion Source

A corollary to the extreme sensitivity of AMS is the need for high-intensity ion sources to provide good counting statistics in reasonable counting times (preferably seconds or minutes rather than hours). AMS ion sources must have steady output to allow precise measurements, must have multi-sample capability to achieve high throughput, and must be easily maintainable. As well as

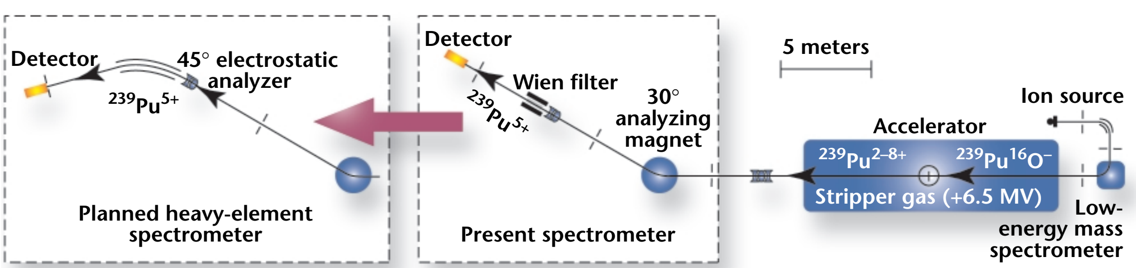

Figure 2. The heavy-element spectrometer uses a combination of magnetic and energy analysis, followed by particle identification. Shown are the present configuration and the upgrade in progress. In the final spectrometer, an electrostatic analyzer, designed to fully resolve neighboring isotopes at 250 atomic mass units, will provide the final separation of interferences.

producing the highest ion currents of any AMS source now operating in the world, the Laboratory's ion source allows more samples to be run in a given period, or the same number can be run to far better precision.

Most AMS ion sources are based on a high-intensity design developed at the University of Pennsylvania in the 1970s. Our source thermally ionizes cesium (Cs) vapor from an oven. The shape of the ionizer and the surrounding beam-forming electrode focus the Cs^+ beam on to the source cathode, which is maintained at a potential of –3 to –11 kilovolts relative to the ionizer. A socket in the cathode structure contains a sample of the element of interest, mounted in a small hole on the front of a sample holder. Sixty-four holders are stored in a magazine or wheel (Figure 3) and can be inserted into the source and withdrawn under computer control. Negative ions sputtered from the sample by the Cs beam are focused by an immersion lens at the end of the cathode and accelerate back toward the ionizer, passing through the central hole and accelerating to the full source energy of 33–41 kiloelectronvolts as they leave the source and enter the spectrometer-beam transport system.

Our Modifications

In 1989, we purchased a prototype AMS ion source from General Ionex Corporation. It represented a major improvement in terms of output over most AMS sources available at the time, but had significant design problems. We have since made several modifications to the source with the aim to: (1) improve reliability and ease of maintenance, (2) increase output, and (3) reduce sample-to-sample memory.

To reduce the ion source's vulnerability to sparks, we completely redesigned and rebuilt the sample changer using pneumatic logic and an optical shaft encoder to sense the wheel position. For easier access and easier cleaning the ion-source body and sample wheel chamber were redesigned from stainless steel. The Cs feed tube was redesigned as a double-walled tube with vacuum insulation to prevent clogging, and a new reservoir for a larger (5-gram) Cs charge was installed to reduce the frequency of Cs changes. Additionally, the original single-jet Cs feed, which pointed directly at the central hole of the ionizer, was replaced with a version having six jets aimed at the actual ionizing surface.

Increased ion-source output was obtained by improving source vacuum and by operation of the ion source at higher sputtering voltages. Improvements in ion-source and injection-line vacuum have consistently resulted in higher output. Better vacuum was obtained by increasing the ionizer assembly–cathode clearance, and reducing the supports for the ionizer and extraction electrode assemblies to thin ribs to improve pumping around the ionizer/extraction region. Additionally, changing the source vacuum pump from a 500-liter-per-second turbo-pump to a 2000-liter-per-second cryopump reduced source pressure by two-thirds, increased ion currents by 25%, and reduced pumpdown times after wheel changes and source maintenance by 30%. Increased ion-source output was also obtained by achieving higher sputtering voltages. To achieve higher sputter voltages we increased the immersion lens-to-ionizer assembly clearance and provided proper shielding of the cathode insulator. An reduction in sample-to-sample memory was achieved primarily by better pumping and improved thermal isolation of critical components around the sample. The geometry changes also improved the thermal isolation of the immersion lens, the ionizer baseplate, and the extraction ground electrode, and increased their operating temperatures. Electrostatics calculations suggest that space-charge buildup presently limits the efficiency with which $Cs+$ can be pulled off the ionizer surface, and/or the extraction of negative ions from the sample holder. We have tested experimental modifications that increase the electric field at the ionizer surface and at the sample, and these suggest that further increases in output will be possible.

Figure 3. The redesigned and rebuilt cesium ion source can store 64 samples in a wheel, insert them into the source, and withdraw them under computer control: (*right*) the changer and its pneumatic controls, (*left*) the cathode insulator and ion-source body.

Experimental Geophysics: Investigating Material Properties at Extreme Conditions

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National need: *All of the needs shown on page 2—* **experimental observations using innovative techniques support environmental, energy, and defense programs.**

For further reading on this topic, see page 80.

The Experimental Geophysics Group develops new techniques and apparatus to investigate material properties at extreme conditions for diverse problems. Problems of interest range from studying the composition of polar ice caps on Mars, to determining electrical conductivity at pressures representative of the earth's mantle and core, to measuring soil properties at low pressures for environmental cleanup applications. These experiments support a wide range of programs including environmental, defense, geothermal, and basic research. We provide experimental observations that can be used to constrain computer modeling of explosions, test theories about composition of the earth and other planets, improve underground imaging at contaminated sites, guide decisions about nuclear waste repository designs, and enhance production of geothermal reservoirs. The projects described below highlight some of our capabilities. We integrate theory and modeling with experiments, and collaborate on different projects to increase our understanding of imposed pressure and temperature on the behavior of elements, minerals, rock, and man-made materials. Formal and informal collaborations with university researchers, postdocs, and scientists in other disciplines enrich our basic research and further increase our ability to make our results relevant to national needs.

Reactive Flow in Single Fractures

To understand some of the key processes involved in dissolution and precipitation when fluids pass through fractured rock formations, we are undertaking an experimental study of the changes that occur to the surfaces of individual rough fractures in rock in a very carefully controlled laboratory environment. Many phenomena important to the Laboratory's interest in energy and nuclear waste isolation depend on the movement of groundwater through fractures, for example, mineralization of fractures, exploitation of geothermal heat, and transport of toxic and radioactive waste. Our current interest is finding the relationship between rate of fluid flow and rate of mineral dissolution in a fracture. We introduce single large fractures in a sample of marble (which is very simple mineralogically, and reacts readily with slightly acidic water), and then map the full shape of the two facing surfaces of the fracture using a specialized three-dimensional surface profiler built in our laboratory. Precise knowledge of the shape of the fracture allows us to numerically simulate fluid flow when the fracture is put back together (see Figure 1a). When we do reassemble the fracture and pass reactive fluid—our slightly acidic water—through the fracture for a few hours, material dissolves from the fracture surfaces. We map the fracture surfaces again, and again simulate the flow pattern (Figure 1b). In our first

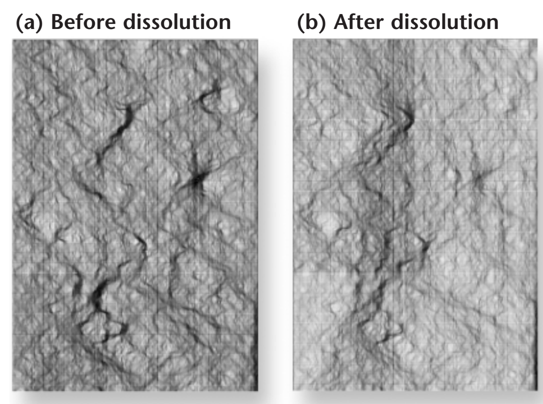

Figure 1. Simulated fluid flow patterns in a fracture in marble. The view is normal to the fracture, and fluid flows from top to bottom. The images are actually composed of thousands of tiny arrows pointing in the local flow direction, with their length proportional to local flow volume (flux). The dark regions thus mean higher fluid flux. The flow pattern before the fluid started to dissolve the material (a) is distributed but rather heterogeneous. After dissolution (b), the pattern is smooth at fine scale, but shows a broad dissolved channel near the center of the fracture.

experiment of this sort, we see in the marble sample that the flow has become more uniform across the face of the fracture, which means that the dissolution has smoothed the fine-scale roughness. However, at the same time, the fluid has dissolved a single broad channel along the fracture (in the direction of flow), meaning that at coarse scale the fracture has actually gotten rougher. This is the first time that reactive flow in fractures has been studied at this level of detail, and the observation of stable-vs-unstable dissolution at fine-vs-rough scale was quite unexpected. It turns out that the effects can be explained in terms of reactive flow models that consider fluid velocities and the rates of reaction. Our quantitative observations have provided sound parameters for those models.

Electrical Properties of Geothermal Reservoir Rocks During Boiling

We have undertaken laboratory core studies at elevated temperatures and pressures to determine how geothermal fluids are stored, released, and transported at reservoir conditions. Electrical measurements are used as a tool to study physical properties of fluid-saturated rocks because these properties are sensitive to many factors, including porosity and microstructural properties, the nature and amount of pore saturant, temperature, and pressure. In geothermal reservoirs, the water's state as liquid or steam is an important factor that has a major effect on electrical resistivity. Saturation with insulating liquid (or steam) decreases resistivity by eight orders of magnitude or more. As water in pores flashes to more resistive steam because of lower pressure, possibly caused by geothermal power production, electrical pathways are cut off and the resistivity of the sample increases. If boiling-induced changes are sufficiently large, such regions could be sensed remotely using surface- and borehole-based electrical surveys. Employing electrical sensing techniques could provide the means to evaluate changing geothermal reservoirs, track re-injected fluids, or follow steam fronts.

Laboratory measurements were performed on hydrothermal breccia, metashale, welded tuff, sandstones, and fused-glass-bead samples from 23 to 250°C and pressures between 100 kPa and 10 MPa. Tracking the resistivity of the rocks as boiling conditions were achieved revealed a number of interesting phenomena. First, as pore pressure is lowered, boiling occurs gradually rather than all at once (Figure 2) and is controlled by the microstructure and pore size distribution. Individual pores do not boil until the capillary pressure (or suction) is offset by a corresponding lowering of the overall pore pressure. Each pore that boils effectively cuts off a conductive pathway with the result that as pressure is continually lowered a higher percentage of the pores are boiling. Some samples also demonstrated porosity enhancement and permeability modification caused by salt deposition and crystal shattering during the boiling process.

Although the current experiments are aimed at understanding how fluid is stored and transported in geothermal reservoirs, the results apply to all situations where two-phase aqueous fluids are important at high temperature. Boiling "below the phase boundary" has been observed in a wide variety of rocks as well as sintered glass beads and is probably the norm *in situ*.

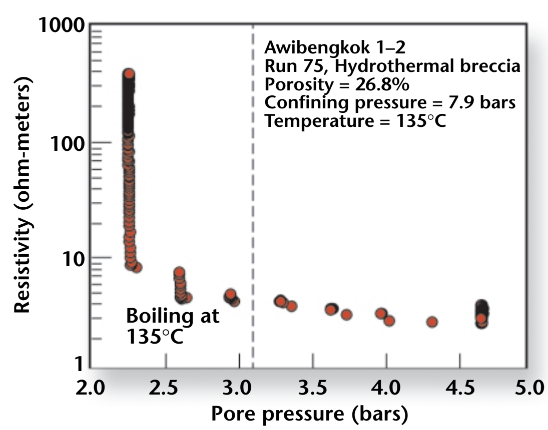

Figure 2. Laboratory measurements of the high-temperature resistivity of rocks revealed that boiling occurs gradually, not all at once, and is controlled by microstructure and pore size distribution. Aimed at understanding fluid transport in geothermal reservoirs, these studies also apply to nuclear-waste storage, enhanced oil recovery, and environmental remediation.

Additional examples include nuclear-waste repositories, enhanced oil-recovery operations, and environmental remediation sites that use steam flooding.

Rock Mechanics Modeling

Many applications in civil, environmental, and mining engineering require accurate predictions of the strength and mechanical behavior of large rock masses. While a great deal of experimental and theoretical work has been done to improve understanding of rock behavior at the grain scale, empirical relationships are generally used to predict large-scale behavior. The objective of our rock mechanics research program is to study the scaling behavior of rock by taking advantage of recent advances in numerical methods and computational power. At all scales, cracks and fractures play a major role in the mechanical behavior of rock. Our approach is to use the displacement discontinuity (DD) method to model cracks and fractures. This method has the advantage that it accurately captures the behavior of fractures within a rock mass by explicitly accounting for discontinuities. Unfortunately, traditional approaches to the DD method are computationally expensive for large problem sizes such as those that include crack formation and crack propagation.

We have developed a new approach to the DD method that performs the necessary calculations in optimal time using less memory. Our solution employs an approximate summation technique, the fast multipole method (FMM), to calculate the interactions between N crack elements in time proportional to N. The relative error between the original DD method and our approximation is very small. Our approach greatly reduces the time taken per crack element. The performance of the FMM can be further optimized for specific problems by adjusting the trade-off between efficiency and accuracy as appropriate. The FMM approach permits much larger problems to be solved using desktop computers, opening up a range of applications. Currently we are investigating the relationship between the strengths of small samples and larger field-size rock bodies. Our initial results are for simulations of Brazilian tests in which a disk of rock is loaded in diametral compression. Samples loaded in this geometry fail by formation of a tensile crack along the diameter. The results of one of our simulations are shown in Figure 3. Other results predict the decrease of rock strength with increase in size and degree of heterogeneity. The results of this study, once completed, can help provide bounds for rock strength in many applications, leading to increased safety and reductions in construction cost.

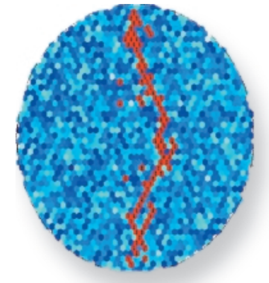

Figure 3. Simulation of a test in which a disk of rock is loaded in compression. Samples loaded in this geometry fail by formation of a tensile crack along the diameter. Such simulations can help predict the effect of heterogeneity on rock strength.

Designer Diamond Anvils for Measuring High-Pressure Electrical Transport

Measurements of the electrical conductivity of materials under ultra-high pressure are fundamental to understanding how matter behaves under extreme conditions. Such behavior is not only of fundamental scientific interest, but is critical for modeling and simulating explosions and their effects. There also are direct applications to mantle geophysics, particularly in inferring temperatures at depth from magnetotelluric data. In an effort to extend these laboratory measurements to higher pressures, we have modified the diamond anvils used to apply ultra-pressure in Mbar experiments (1 Mbar = one million earth atmospheres = 100 gigapascals = pressure at the core–mantle boundary). To construct these “designer anvils,” metallic probes with micron dimensions are precisely deposited at the tip of the diamond anvil using advanced microlithography techniques. This allows electrical currents to enter the sample volume. These conducting probes are then encapsulated with epitaxial, chemically vapor-deposited diamond to protect them from extreme pressures and to prevent shorting to the metal gasket that contains the microscopic test sample.

With this method, the electrical resistances of potassium iodide (KI) and wustite (FeO) have been determined for pressure up to 1.8 and 1.7 Mbar, respectively. The resistance of FeO decreases gradually up to the maximum pressure, agreeing with literature values obtained at 0.8 Mbar and theoretical predictions of metallization above 2 Mbar. In contrast, the resistance of KI decreases exponentially with increasing pressure, reaching low values at 1.31 Mbar, as shown in Figure 4. This observation agrees well with band-structure calculations, which predict metallization by band overlap at 1.25 Mbar.

Improving Underground Imaging in the Shallow Subsurface

Porosity, permeability, and saturation are the hydrogeological properties that control the distribution and movement of fluids in soils and rock. These properties cannot be measured directly in all parts of a contaminated site because of cost constraints and concerns about spreading contaminants when drilling boreholes. Geophysical measurements such as seismic surveys or electrical resistance tomography can provide information about the geophysical properties in the shallow subsurface in regions where drilling must be minimized. But such subsurface imaging describes geophysical properties rather than the hydrogeological properties of soil and rock.

The DOE Environmental Management Science Program provided funding for a group of scientists, mainly from Experimental Geophysics, to investigate ways to improve geophysical underground imaging by studying the relationships between measured geophysical properties and needed hydrogeological properties in soils. This interdisciplinary group included researchers with expertise in soil science, rock physics theory and modeling, inverse theory, and laboratory measurements of geophysical and hydrogeological properties of soils.

We designed new laboratory apparatus capable of measuring electrical properties of soils at frequencies ranging from low frequencies typical of field resistivity measurements, up to high frequencies approaching ground-penetrating radar. We also designed a first-of-its-kind apparatus for simultaneously measuring the ultrasonic compressional and shear-wave velocities in soils at low pressures representative of the top few meters of the subsurface, for comparison with seismic field data. Initial results from rock physics modeling and joint inversion using our lab data suggest that field experiments should be designed to collect more than one kind of geophysical data, and that such data can be inverted to provide information about the distribution of soil types and hydrogeological properties in the shallow subsurface. We are currently investigating how fluid distribution affects measured geophysical properties in soils in the lab (see Figure 5).

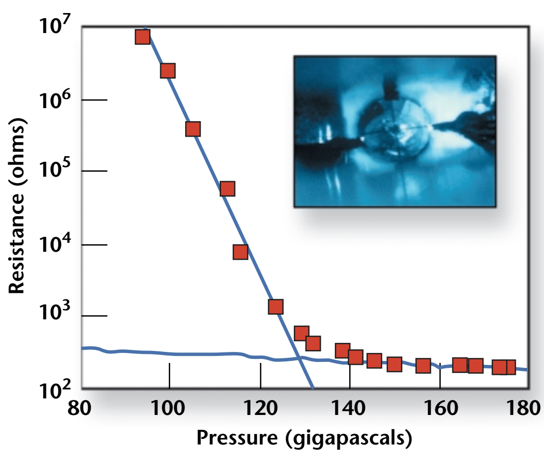

Figure 4. Our newly designed diamond anvil (*inset*) extends the range of pressure possible in studies of the electrical conductivity of materials under high pressure. Experiments show that the resistance of KI, for example, decreases exponentially with pressure; this result agrees well with band-structure calculations.

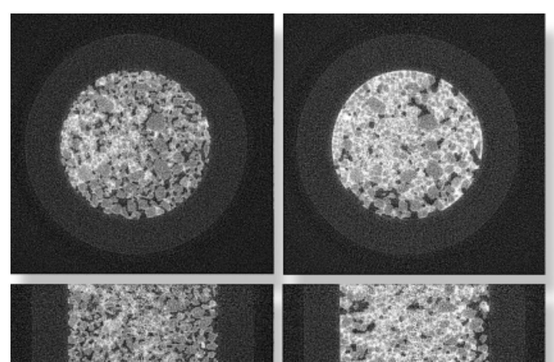

Figure 5. Tomographic slices through a packed-sand core in identical positions. Grey is sand grains, white is water, and black is air. (*left*) After the core has been drained slowly to a final capillary pressure of 490 cm using a multi-step approach. (*right*) After the core has been drained very quickly using one large pressure step of 490 cm. Note the difference in overall water content and distribution.

The Role of the Earth and Environmental Sciences Directorate in the Greater Scientific Community

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The E&ES Directorate plays a strong role in the greater scientific community. We interact with academic, industrial, national laboratory, and international collaborators on many levels, working on the development of the earth and environmental sciences and their application to challenges in environmental and national security.

These interactions range in character from collaborations between individual researchers to large-scale joint research efforts between organizations (Figure 1). This strong and diverse range of collaborations is a hallmark of the directorate's research portfolio. They 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 research groups and the challenges that they face. In turn, these 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.

Outreach in 1999

Over this past year, E&ES has continued its collaborations with other Laboratory directorates and the external community. As in the past, no one agency or organization dominates this area; multifaceted expertise is required in order to be a significant contributor.

Major components of outreach in 1999 include the following:

- 392 ongoing and new collaborations with external research members of industry, government, academic and international areas.
- Visits by more than 45 faculty members and other scientists and 88 students for stays of more than one week.
- 9 on-site work-study programs.
- Hosting or organization of 22 conferences or workshops.
- 178 tours of our facilities, most of the ARAC facility.
- Participation by 125 Directorate employees on major national and international committees and review panels, as visiting lecturers, or as journal associate editors and reviewers.
- Summer student hiring program for 34 students, including 19 women, from a variety of academic institutions and programs: International Atomic Energy Agency, Summer Employment Program; Department of Energy Scholarship Program; Hawaii Scholarship Program; Associated Western Universities; Knowledge, Education, Reinforcement, Reach-out to Youth Program; Research Internship and Education Program; and Northern Arizona University, Fellowship Program.

Individual Collaborations: The Foundation for the Directorate's Role

Individual-to-individual collaborations are the most common in the Directorate research world. By exploring the nature of these collaborations and how they initiate, we can begin to address the question of how the Directorate impacts the larger scientific

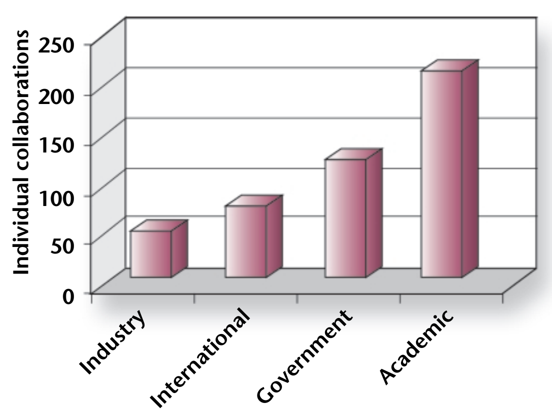


Figure 1. Breakdown of E&ES 1999 collaborations by organization character. Each collaboration constitutes an individual interaction or project.

community and how the Laboratory has benefited from them as well. Most initial contacts occur because of the direct participation of E&ES researchers in the scientific community. Key activities include publication of research in peer-reviewed journals, acting as editors and reviewers for scientific journals, participating in research panels, committees and working groups, giving invited lectures at scientific meetings and universities. Participation in the peer-reviewed journal process is important; directorate technical staff include 13 journal editors and provided 94 reviews of scientific papers. E&ES technical staff fulfilled 62 major committee, working group, panel or academic thesis advisor responsibilities. Our technical staff presented nearly 50 invited lectures and seminars over the past year, 24 of which were given by one individual.

Meaningful interactions often require close proximity; in the past year, nearly 90 academic faculty and students have visited E&ES researchers for periods of a week or more. Through these interactions, we provide academic researchers and students with a unique opportunity to interact with a larger group interested in their research area, in many cases broadening their applicability. Some of these interactions have come full circle; once-student visitors now send their students to learn techniques developed at the Laboratory. Other Laboratory programs benefit from such exchanges as well; by collaborating with outside researchers, E&ES investigators gain access to cutting-edge technology, enhancing our ability in new areas.

Individual collaborations often begin as informal interactions, and grow. A developing interaction may begin with an informal request (1), and result in a service whereby one participant is providing an analysis, data or interpretive input to another (2), to collaborations recognizable by co-authorship in a peer-reviewed journal article (3), to joint research between co-investigators (4) (Figure 2). At any moment, potential projects are being developed through this pipeline. A healthy research organization has some level of activity throughout the cycle.

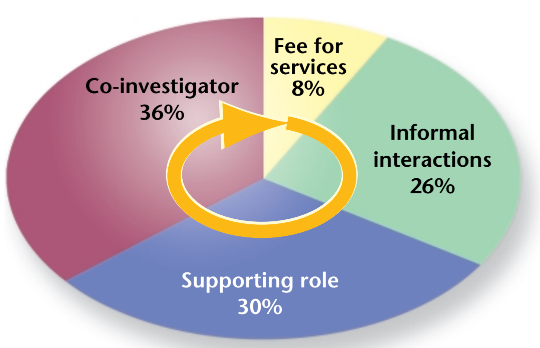


Figure 2. Nature of collaborations (110) between external investigators and E&ES researchers in the Health and Ecological Assessment and the Geosciences and Environmental Technology divisions. One type of collaboration can evolve into another.

Programmatic Impacts: Supporting Participation in the Greater Community

Programmatic interactions are similarly of mutual benefit to the Laboratory and the greater scientific community. A close inspection of the number and character of the external interactions that occur within a single program illustrates their synergistic nature. One example is the Ground-Based Nuclear Explosion Monitoring (GNEM) R&D Program (formerly CTBT Program), which supports collaboration on all levels, ranging from scientist-to-scientist joint research to very structured organizational collaborations. The very nature of the program involves both technical and policy aspects; because of the Laboratory's demonstrated technical leadership, we are asked to represent the U.S. government in international negotiations involving technology and policy development pertinent to the treaty. The program supports the participation of its researchers in a variety of aspects involving the greater scientific community through both formal and informal collaborations. These include supporting post-doctoral research and the participation of Program personnel in major committee and panel commitments (Figure 3).

The Directorate partners with other institutions to develop programs to address national needs. Some examples from the Atmospheric Sciences arena include the following:

- In the Global Modeling Initiative (GMI), part of an effort by NASA to assess the impact of aviation on atmospheric chemistry, E&ES plays the role of a modeling integrator. The Laboratory maintains the global modeling effort, whereas the consortium members (about 20) contribute process models. Consortium members include individual academic researchers, companies, government organizations and other national laboratories. The Laboratory's GMI budget is approximately $750K for 3 years.
- In the Program for Climate Model Diagnosis and Intercomparison (PCMDI), the Laboratory acts as an impartial clearinghouse to compare different global climate models; these models are contributed by about 30 collaborating institutions worldwide. In collaboration with this international community, the PCMDI program designs experiments for model testing, providing comparisons and analysis. This is a large effort, with a budget of about $5000K/year. As part of this work, the program provides and maintains software and a database that is available for global use, on the web. This introduces yet another form of exchange: the anonymous interaction, where interactions occur largely through data exchange. This is perhaps the most difficult to quantify, unless the external investigator contacts Directorate researchers directly.
- In response to a DOE request, a Distributed Model Development Team has been formed, whose members include the Laboratory, the National Center for Atmospheric Research, Los Alamos National Laboratory, and the National Aeronautics and Space Adminstration. Their goal is to develop a (common) community model.
- E&ES has partnered with Lawrence Berkeley National Laboratory as co-directors of DOE's Center for Research on Ocean Carbon Sequestration (DOCS), with a budget of $1000K/year. DOCS participating institutions include academic and research institutions from across the country.

Facilities: Unique Capabilities as National Resources

E&ES's unique facilities attract researchers external to both the directorate and the Laboratory. Our Center for Accelerator Mass

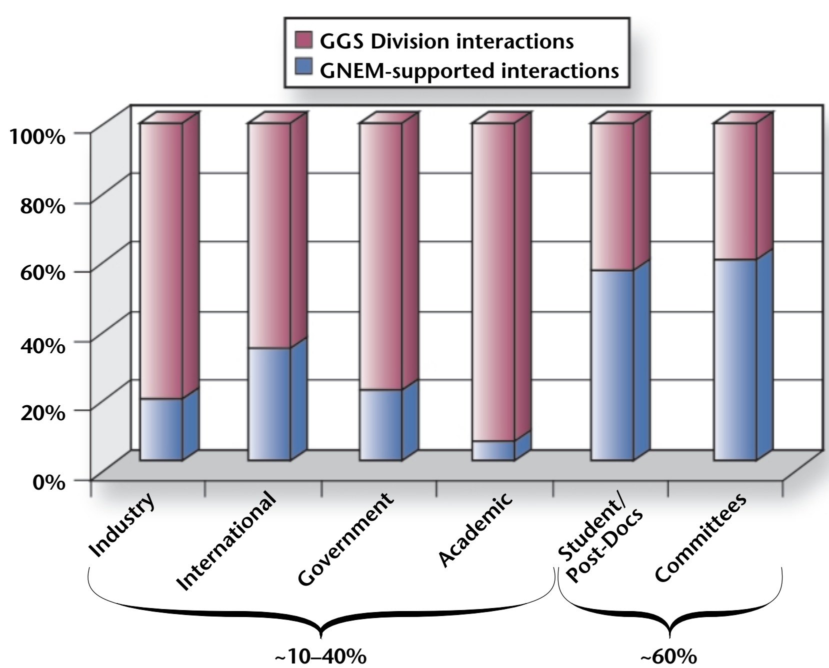


Figure 3. Impact of programmatic support for various interactions. The Ground-Based Nuclear Explosion Monitoring (GNEM) Research & Development (formerly CTBT) Program supports about 10–40% of collaborations between researchers in the Geophysics and Global Security (GGS) Divison and external investigators. The Program supports about 60% of the long-term student visitors and post-doctoral fellows hosted by the Division. Program personnel play a lead role in 60% of the significant committee commitments and panels in which Division personnel take part.

Spectrometry (CAMS) is one such unique capability because it functions as both a facility and a research institute. Without the research staff, the impact CAMS makes on the Laboratory programs and national research would not be possible. Consider the various ways that the CAMS capability interacts with research interests outside the Laboratory, listed in increasing size and impact:

Fee-for-Service mode: Provide sample analyses as a service; by design, limited to industrial suppliers, who service a wide range of academic and government customers for which CAMS receives no direct credit. (Fees range from $60/sample for bioAMS, or $275/sample for radio carbon dating). There are currently five industrial suppliers.

Collaboration on a project: Although external researchers may lead the effort, CAMS personnel contribute significantly to the analysis and interpretation, generally appearing as co-authors on peer-reviewed papers. (CAMS funding range: $10K–$100K.) There are currently 66 such collaborations.

Co-Investigators: Joint research, in which CAMS researchers appear on the grant itself and in joint publications. (CAMS funding range: $50K–$150K.) There are currently six such projects.

Principal Investigator: CAMS researchers lead the effort, with little or no external collaboration. (CAMS funding range: $150K–$400K.) There are currently 10 PI-driven projects.

Research Resource: CAMS is recognized as a national resource for the technology, and funded by the National Institutes of Health (NIH) to provide service to NIH-funded projects, collaborate with other NIH-funded investigators, and advance the technology. (For this 5-year effort, CAMS funding is about $7000K.)

A major role of CAMS is to nurture the use of its technology in the scientific community in general and the University of California (UC) system in particular. As a UC Institute, about 10% of its operating budget is accompanied with a mandate to interact with the UC campuses, and to make its technology available to faculty and students. CAMS manages a mini-grant program of about $250K/year, most of which is spent at UC campuses. This program is broadcast nationally; the intent is to educate academic researchers in CAMS technology and provide them access to it. Many of these approximately $25K projects develop into more substantial collaborations, funded through the Campus–Laboratory Collaboration or other external sponsors.

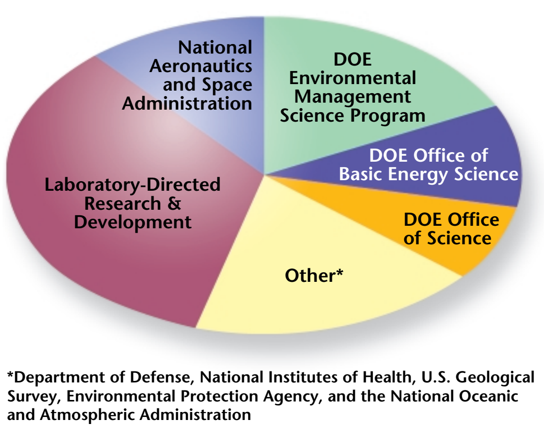


Figure 4. Competitive research budget by sponsor for 1999. Budget total is $1300K.

Competitive Research: Participation in Peer-Reviewed Processes

The Directorate encourages and supports individual efforts for individual and group efforts in areas of science related to Directorate disciplines and programs. Participation in these PI-driven, peer-reviewed processes provides the staff with opportunities to pursue research in areas outside of, but often complementary to, current programmatic funding and generate new internal and external interactions. During 1999, more than 60 E&ES projects were of this type. They make up $13.3M (about 21%) of the Directorate's Programmatic budget. About 35% of these projects are funded by Laboratory-Directed Research and Development and about 40% are funded by a combination of DOE's Office of Basic Energy Science, Office of Science, and Environmental Management Science Program. The National Aeronautics and Space Administration also funds some projects (Figure 4). Other sponsors include the Department of Defense, the National Institute of Health, the United States Geological Survey, the Environmental Protection Agency, and the National Oceanic and Atmospheric Administration.

Resources: An Overview of the Earth and Environmental Sciences Directorate

The E&ES Directorate operates programs and pursues basic and applied research to support Laboratory 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.

Organization

Figure 1 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 the Laboratory; and (3) the infrastructure activities, which support our

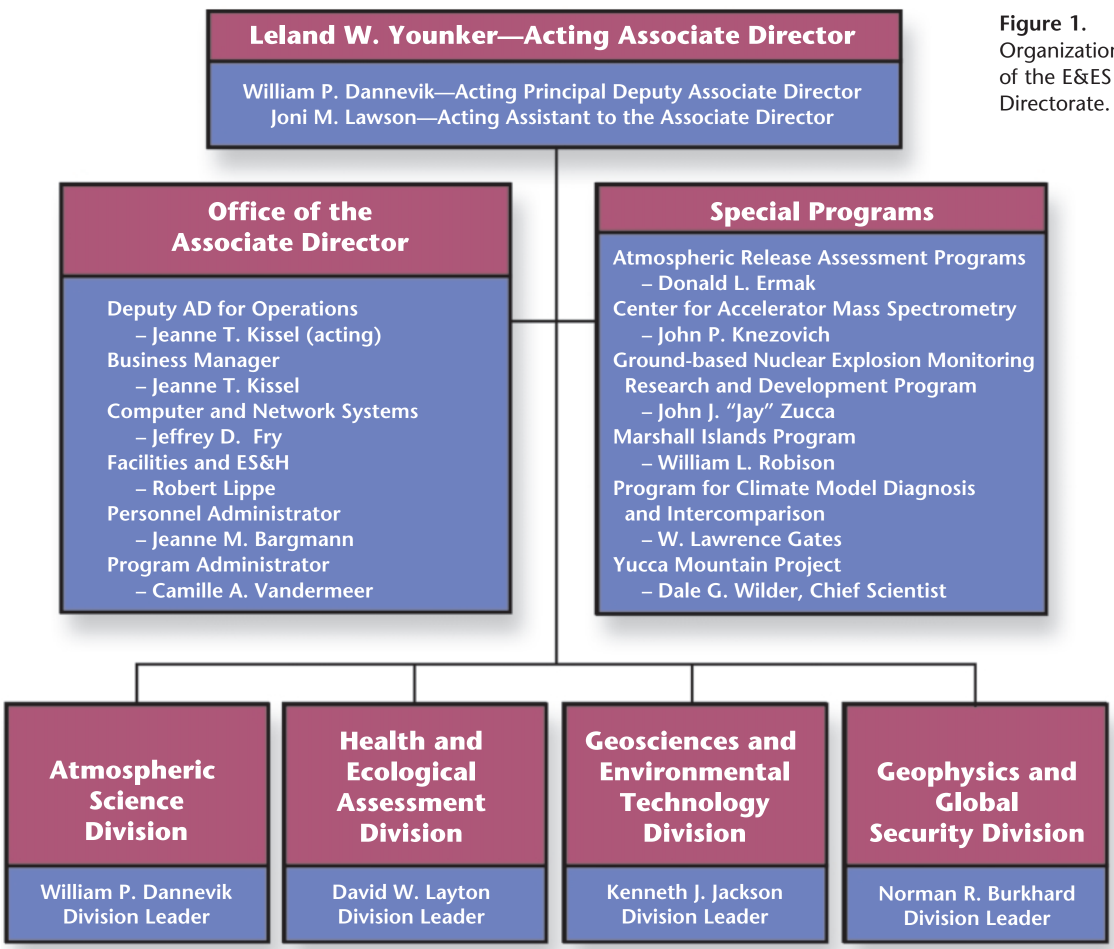


Figure 1. Organization of the E&ES Directorate.

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 2 and the breakdown of funding shown in Figure 4. The project organizations control a major fraction of the directorate's resources. The mission and capabilities of each division are described below.

Atmospheric Science Division

The mission of the Atmospheric Science Division is to expand scientific understanding of how the earth's atmosphere, oceans, and biosphere respond to anthropogenic and natural influences, and to predict and assess the impacts of hazardous materials released into the atmosphere. To meet these needs, the division maintains expertise in:

- Atmospheric climate, dynamics, aerosols, chemistry, and physics.
- Ocean dynamics, transport, and biogeochemistry.
- Mesoscale atmospheric prediction, transport, and dispersion.
- Global carbon cycle science and carbon sequestration methods.
- High-performance computing and computational physics.
- Advanced diagnostic software and database management systems.

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. We are working to advanced predictive modeling through integration of real-time observed data with high performance computing and communication systems. The Division provides the technical staff for several major programs, including the National Atmospheric Release Advisory Center, the Program for Climate Model Diagnosis and Intercomparison, the Chem-Bio Nonproliferation Program and NASA's Global Modeling Initiative.

For more information on the Atmospheric Science Division, contact the division leader, Bill Dannevik, at (925) 422-3132 (dannevik1@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.
- Inductively coupled plasma atomic emission spectrometry and 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, ^{10}Be, ^{26}Al) and various elements.

Our measurement technologies support and enable broad range of field and laboratory studies within the division, and the E&ES Directorate and the university community. 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, quantify their environmental fate and transport and develop methods for managing the risks they pose to humans and ecosystems—an example is our work 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 Health and Ecological Assessment, contact the division leader, Dave Layton, at (925) 422-0918 (layton1@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 Laboratory programs including Comprehensive Test Ban verification, 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 of national significance involving the geochemistry, geophysics, and hydrology of the earth's near-surface. The division's research is focused on five basic areas:

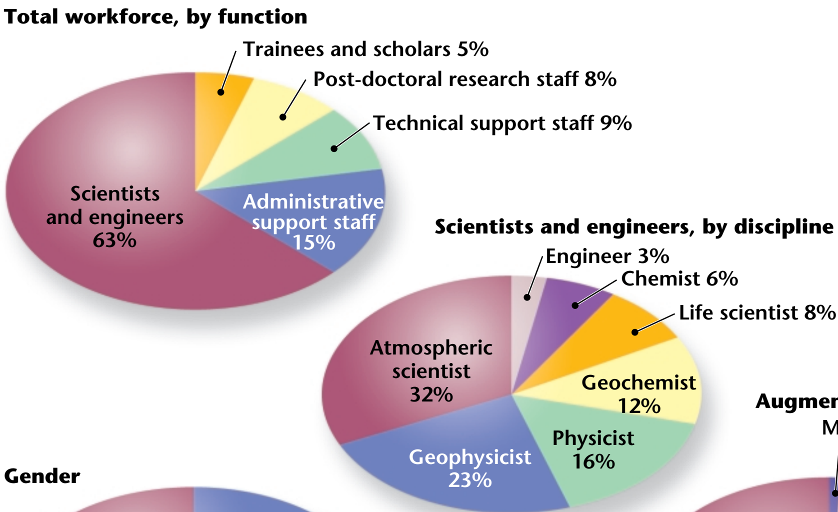
- Subsurface characterization, especially the development of new geophysical and electromagnetic methods for characterizing the physical and chemical properties in the shallow subsurface and for identifying and mapping contaminant plumes.
- Subsurface remediation, with emphasis on developing new assessment 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 nuclear waste forms after they are emplaced into a repository.
- Geologic sources of energy, including research on geothermal systems and the production of oil and gas resources.

We also have programs to study geologic aspects of CO_2 emissions and the ocean and deep geological sequestration of carbon dioxide.
- 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).

Workforce

Our directorate currently employs 285 people in 31 job series reflecting a wide range of employment categories supporting the directorate's mission (Figure 2). Of this total population, 71% are scientists, engineers, and



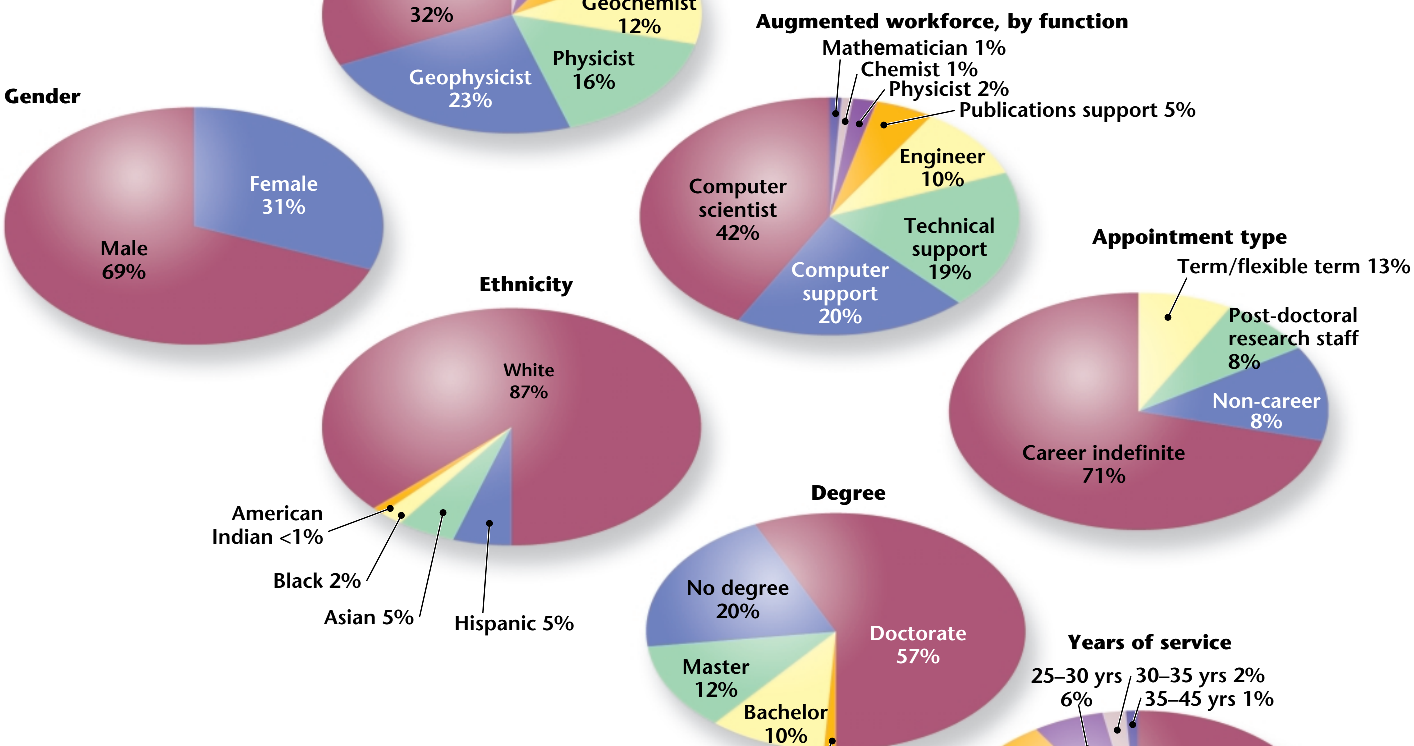
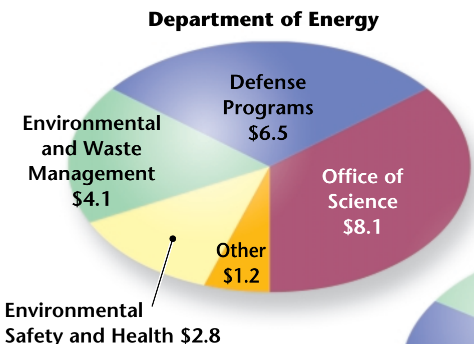


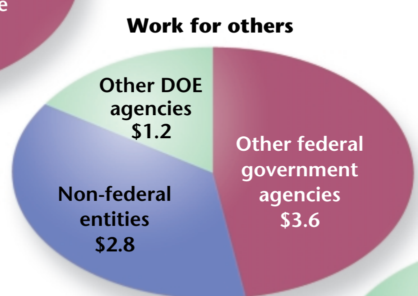
Figure 2. Workforce breakdown for E&ES by function, discipline (scientists and engineers), function (augmented workforce), appointment type, gender, ethnicity, educational degree, and years of service.

post-doctoral research staff members. Of note is the almost 50% increase in the post-doctoral research staff in 1999 to a total of 23 employed in all four divisions. A strength of the directorate is its diverse workforce with the skills and flexibility required to meet administrative and programmatic objectives. Approximately 80% of the workforce have advanced degrees reflecting a wide range of skills, knowledge, and abilities, which are listed in Table 1. Personnel from other Laboratory 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 Earth and Environmental Sciences makes it one of the largest environmental research organizations in the nation.

Funding

The E&ES Directorate provides scientific leadership, technical support, and management expertise to a diverse set of programs and projects (Figure 3). In fiscal year (FY) 1999 the total funding for E&ES programs from all sources was $62.6 million, including a $4.5 million allocation from Laboratory-Directed Research and Development. DOE directly funded E&ES Programs in Defense Programs,





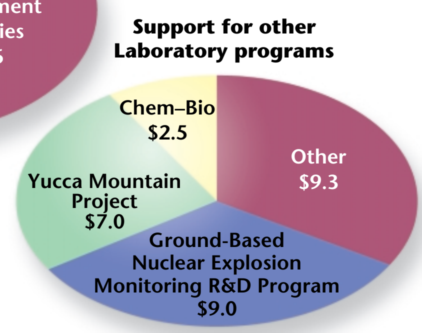


Figure 3. Breakdown of funding for E&ES in 1999 (in millions of dollars). Funding received directly from the Department of Energy totaled $62.6 million. Funding received in work for others totaled $7.6 million. Funding received to provide scientific expertise and program management for other Laboratory programs totaled $27.8 million.

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 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, atmospheric, 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.

Office of Science, Environmental Restoration and Waste Management (ERWM), Environmental Safety and Health, and others (International Affairs and Nuclear Reactors). The E&ES Directorate also received $7.6 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 FY99 our directorate received $27.8 million of funds through other Laboratory directorates. This represents programs for which our personnel provided scientific and program leadership and expertise. Continuing programs include the Ground-Based Nuclear Explosion Monitoring R&D (formerly Comprehensive Test Ban Treaty) Program, the proposed repository at Yucca Mountain, the Chem-Bio Program, 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 4 shows the breakdown of funding by project or program.

In FY99, we managed an indirect budget of $10.5 million to cover management and

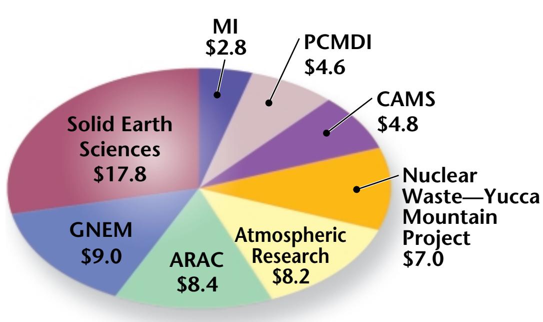


Figure 4. Breakdown of 1999 funding by major projects and programs. Amounts are in millions of dollars. ARAC = Atmospheric Release Advisory Capability, CAMS = Center for Accelerator Mass Spectrometry, GNEM = Ground-based Nuclear Explosion Monitoring R&D Program, MI = Marshall Islands, PCMDI = Project for Climate Model Diagnosis and Intercomparison (excludes $700,600 of work for others).

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 FY99 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, upgrade of laboratory space, and integration of long-term needs. The directorate, along with the Laboratory, continues to take every opportunity to monitor and control infrastructure cost expenditures to stay efficient and cost-effective.

Environmental Safety & Health (ES&H)

The E&ES Directorate is committed to performing work safely and in a manner that ensures protection of employees, the public, Laboratory assets, and the environment. E&ES's line management, its staff, matrixed personnel and guests are responsible and accountable for the safe performance of work, and will exert a reasonable degree of care and provide resources for the safe conduct of its operations. Research and development frequently involve working at the limits of technical understanding and can consequently generate unique risks. Our challenge is to properly identify and appropriately manage these risks. It is therefore essential that all individuals work proactively to anticipate hazards and manage risk so that experiments occur in a timely manner, at reasonable cost, and in compliance with health, safety, environmental, and waste minimization requirements.

To meet this commitment, E&ES has fully integrated ES&H into all Facilities Operations. The E&ES system is based on providing proactive ES&H technical support to our personnel, providing the information and tools they need to safely conduct their work, clear communication of ES&H responsibilities and expectations, feedback and continual improvement.

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 and focused facility management has greatly increased our use efficiency as well as the quality of our laboratory, computer, and office areas. From our 1994 total of 62 facilities, we have consolidated into 30 in 1999 by combining and consolidating assets and vacating obsolete buildings. This has served to greatly reduce our maintenance burden and operating costs, as well as those of the Laboratory.

Major facility management milestones realized in 1999 included the reconfiguration of a large portion of B292 to incorporate a significant portion of the Marshall Island's project laboratory work, greatly consolidating and improving their work areas. This allowed us to close down the legacy facility B412 and return it to the institution for decommissioning and eventual dismantlement. This relieved our directorate and the Laboratory of several million dollars of maintenance backlog. Also accomplished during this period was the refurbishment of T1404. This pilot project showed that we could successfully and efficiently refurbish a badly antiquated trailer complex at approximately 50% of the cost of replacement. Efforts are underway to continue this effort with the other 1400 area trailers housing a total of 150 or our employees. We are currently conducting a comprehensive review of all our facilities to further increase efficiency and ensure our long-term assets are used to their highest potential. We are committed to being one of the Laboratory's lead organizations in cost-effective research and programmatic operations without compromising capability.

The directorate's five primary facilities are described in Table 2.

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

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

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 environment encompasses a wide variety of computational effort. Scientific and engineering staff use high-performance UNIX workstations to develop the modeling codes, perform calculations locally, and to 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.

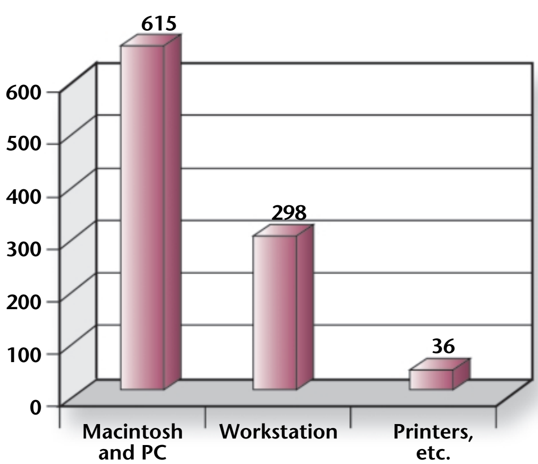


Figure 5. The directorate has more than 900 networked computers with applictions ranging from office computing to control of laboratory experiments to high-performance computing.

The Directorate has over 900 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 the Laboratory'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 the Laboratory and other institutions. In FY 1999, along with the institution, E&ES began to place a growing emphasis on computer security. The advanced complexities inherent in network connectivity have posed a challenge within government and industry to seek solutions to protect selected data. That the national laboratories need to protect national security information is evident and this has posed a challenge to the scientific community. The Laboratory and E&ES are working together to create an environment which will protect critical data and allow the continuation of scientific collaborations.

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 the Laboratory'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 which 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, which can help in many simulations including the prediction of dispersion of airborne contaminants.

In addition to ASCI, our researchers use supercomputers at Sandia National Laboratories, Lawrence Berkeley National Laboratory (LBNL), Los Alamos National Laboratory (LANL), and the National Aeronautics and Space Administration (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 of 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 codes developed at the Laboratory that are most widely used.

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 Laboratory's LODI dispersion model are integrated into our Atmospheric Release and Advisory Capability (ARAC) Program that provides information to emergency responders in the case of radioactive and other contaminant releases. These collaborative research and model development efforts are instrumental in carrying out programmatic goals as well as preparing 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 a specific geographic location.

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 scientific and computational expertise.

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

ADPIC/LODI	*Description:* 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 *Applications:* Modeling of local- and regional-scale atmospheric dispersion and surface deposition of toxic materials and air pollutants *Usage:* Laboratory research, emergency response system (ARAC), and chemical and biological weapons nonproliferation studies; various international groups for nuclear accident preparedness and response
Artificial Neural Network Analysis (ANN)	*Description:* Interpolate the output of large subsurface transport codes in groundwater or oil reservoir prediction problems *Applications:* Optimizing well locations for groundwater remediation and waterflood of an oil and gas reservoir *Usage:* Published in *Solving Problems in Environmental Engineering and the Geosciences with Artificial Neural Networks,* Farid U. Dowla and Leah L. Rogers (MIT Press, Cambridge, MA, 239 pp.)
CDAT	*Description:* A set software tools enabling climate scientists to access, organize, analyze, diagnosis, visualize, and carry out complex mathematical manipulations of climate observations and climate model simulation results *Applications:* Simulations and observered data analysis of global atmospheric general circulation models, ocean circulation models and coupled ocean-atmosphere models *Usage:* Academia, national laboratories, and industry across the national and international climate science community
EQ3/6	*Description:* 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 *Applications:* 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 *Usage:* Widely used in academia, national laboratories, and industry
FEM3C	*Description:* Three-dimensional CFD model for simulating local-scale atmospheric flow and dispersion of heavier-than-air gas releases *Applications:* Simulations of the atmospheric dispersion of heaver-than-air gas releases. Could also be used as an incompressible flow code for engineering problems *Usage:* Academia, national laboratories, and industry
GIMRT98/ OS3D98	*Description:* Simulates non-isothermal multicomponent multiphase reactive transport in porous media. Developed in part at the Laboratory *Applications:* Subsurface problems involving contaminant transport, biodegradation, chemical weathering, early diagenesis, acid mine drainage, disposal of nuclear waste, porosity and permeability change due to chemical reactions *Usage:* Used at some universities and national laboratories
IMPACT	*Description:* Models atmospheric chemical transport *Applications:* Effects of aircraft emissions in the atmosphere; effects of energy-related nitrous oxide and sulfur emissions on ozone *Usage:* 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
Livermore Ocean Biogeochemistry Model	*Description:* Models oceanic distribution of carbon, carbon isotopes, nutrients, chlorofluorocarbons (CFCs), and other ocean tracers *Applications:* Prediction of air/sea fluxes of carbon dioxide, CFCs, and other tracers, and to evaluate ocean general-circulation transport model *Usage:* Used as DOE's participation in the Ocean Carbon-Cycle Model Intercomparison Project
NUFT	*Description:* Simulates non-isothermal multi-phase flow and transport in porous media *Applications:* Subsurface problems in high-level nuclear waste storage, environmental remediation, and petroleum recovery; containment of underground nuclear explosions *Usage:* 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 the Laboratory
PARFLOW	*Description:* Simulates three-dimensional simulation of flow and transport in heterogeneous saturated or unsaturated hydrologic regimes using a parallelized architecture *Applications:* Modeling migration of contaminants from nuclear tests, transport of environmental contaminants, and aquifer management *Usage:* Laboratory research; interest expressed by other national laboratories and academia
SAC 2000	*Description:* Processes and analyzes seismic signals and other time series *Applications:* 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 *Usage:* 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
SUPCRT	*Description:* Calculates a set of internally consistent thermodynamic properties for organic and inorganic aqueous species, gases, and solids as a function of temperature and pressure *Applications:* Generation of a set of internally consistent thermodynamic parameters used as input for EQ3/6 and many other geochemical models *Usage:* Widely used in academia, national laboratories, and industry

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Awards

Recipient	Source	Name of Award	Research Topic	Purpose	Achievements and Contributions
Bill Dannevik Don Eliason Art Mirin Bruce Curtis Mark Duchaineau Dan Schikore Andris Dimits Ron Cohen	IEEE Computer Society	**Gordon Bell Award**	High-Performance Scientific Simulation	Best performance on a scientific or engineering application	Achieved a computational rate of over 1 trillion operations per second on a high-resolution turbulence simulation
Steve Carle	American Geophysical Union	**Editor's Citation for Excellence in Refereeing**		For outstanding services to the authors and readers of water resources research	Outstanding Reviewer Award for refereeing journal articles
Al Duba	Marshall University	**Distinguished Alumni of the Twentieth Century—Certificate of Outstanding Performance**	Applied and Basic Geophysics	Recognition for outstanding performance of alumni	Remote sensing applied to energy and environmental problems; measurement in the laboratory basic to planetary interiors and applied to energy and environmental problems; scientific leadership at the national and international levels
Michael Fiorino	U.S. Government	**Government Technical Leadership Award for WxMAP web site. Fleet Numerical Meteorology & Ocean Center**			
Mike MacCracken	American Association for the Advancement of Sciences	**Fellow**	Climate Modeling		Cited for "leadership of modeling of climate and air quality, for studies of natural and anthropogenic effects on climate, and for coordination of national and international research activities"
Carolin Middleton Paul Harding Camille Vandermeer	Society for Technical Communication—Northern California Chapter	**Touchstone 1998**		Annually recognizes excellence in communications materials in government, industry, and academia	Recognition of Excellence for 1996 Environmental Programs Annual Report, *Protecting Environment, National Security, and Health*
Robin Newmark Roger Aines	Environmental Protection Agency	**Outstanding Remediation Technology Award**	Hydrous Pyrolysis/ Oxidation Concept	Recognition for technical excellence in the development of innovative *in situ* thermal treatment technologies	For their work on dynamic underground stripping and hydrous pyrolysis/oxidation, technologies that heat soil and ground water to remove contaminants and destroy them in place

Patents

Edward J. Kansa Brian L. Anderson Ananda M. Wijesinghe Brian E. Viani	**Separation of Toxic Metal Ions, Hydrophilic Hydrocarbons, Hydrophobic Fuel, and Halogenated Hydrocarbons and Recovery of Ethanol from a Process Stream** U.S. Patent No. 5906748 May 25, 1999
Harley M. Buettner William D. Daily Roger D. Aines Robin L. Newmark	**Electrode Wells for Powerline-Frequency Electrical Heating of Soils** U.S. Patent No. 5907662 May 25, 1999
William D. Daily Abelardo L. Ramirez	**Electrical Resistance Tomography Using Steel Cased Boreholes as Electrodes** U.S. Patent No. 5914603 June 22, 1999
Charles R. Carrigan John J. Nitao	**Electro-Osmotic Infusion for Joule Heating Soil Remediation Techniques** U.S. Patent No. 5975799 November 2, 1999
Roger D. Aines Kent S. Udell Carol J. Bruton Charles R. Carrigan	**Chemical Tailoring of Steam to Remediate Underground Mixed Waste Contaminants** U.S. Patent No. 5986159 November 16, 1999

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