Protecting Environment, National Security, and Health

Earth and Environmental Sciences 1996 Annual Report

Lawrence Livermore
National Laboratory

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Protecting Environment, National Security, and Health

In 1994, Lawrence Livermore National Laboratory established a new directorate, called Environmental Programs, to form one organization combining most of the Laboratory's capabilities in the geosciences and ecological sciences with its supporting technologies in analytical areas such as molecular, radiation, and particle spectrometry; high-pressure physics; and bioscience applied to bioremediation. The directorate applies these capabilities to national problems in the environment, security, and health. In such applications, our work spans the full range from anticipating a problem, to providing a detailed understanding of the basic science underlying it, to developing response and recovery capabilities, which may vary from policy guidance and options to remediation technologies deployed at large scale in the field.

In addition to our ongoing research and development activities, the first three years of the directorate's operation included strategic planning, to coordinate our work with the shifting mission probabilities of the overall Laboratory, and intensive assessment of our structure and activities, to build a vital and flexible organization. As a result of these assessments, we changed the directorate's name to Earth and Environmental Sciences. This change was made to better represent the spread of disciplines within the directorate and to recognize that our work contributes to all of the Laboratory's mission areas: environment, national security, and health.

The staff of the directorate reflect this mission focus. We represent a mix of environmental and other scientific specialties and conduct research ranging from the most fundamental problems of climate processes to the most applied policy and technical tasks to meet national security needs such as treaty verification.

Today, the multidisciplinary teams in Earth and Environmental Sciences collaborate with other federal agencies not only to investi-

gate all facets of the environment—from deep within the Earth to the land surface and from groundwater to the upper reaches of the atmosphere—but also to support national security needs and to develop new insights for health protection. Current areas of research include

- Atmospheric radiative transfer, chemistry, dynamics, and climate processes.
- Physics of the atmospheric boundary layer and cloud processes.
- Seismic processes.
- Geochemistry and geophysics.
- Pathway, dosimetry, and risk analysis of radioactive and toxic substances.
- Isotopic and ion-beam sciences.
- Modeling of subsurface flow and transport.
- Subsurface imaging and characterization.
- *In situ* environmental remediation using natural and engineered processes.
- Design, analysis, and testing of advanced waste-treatment technologies.

Benefits to the Nation

Research in Earth and Environmental Sciences ranges from emergency response activities to national policy assessments. Seismic studies, derived in part from underground nuclear testing research, have led to better design criteria for reactors and other critical structures. Geoscience studies have led to novel site-remediation technologies. Working in teams with other Livermore programs and directorates, we have developed new methodologies for water purification, waste treatment, and dose assessment from radionuclide or toxic exposure. Atmospheric science studies have helped define international protocols for chemicals that are routinely released to the atmosphere. Other projects have led to the development of emergency-response capabilities for atmospheric releases of toxic materials.

This broad range of scientific and technical excellence, together with our ability to integrate those skills into multidisciplinary teams

working to solve national problems, provides an excellent resource for addressing complex environmental issues. Our achievements exemplify Livermore's hallmark ability of turning scientific concepts into working prototypes and problem solutions. Much of the work in Earth and Environmental Sciences is focused on determining and mitigating the risks and impacts of natural and manmade hazards and on remediating environmental damage. We also provide science and technology that supports the Laboratory's environmental compliance requirements. A number of our projects address environmental issues of global significance, and many of our scientists are participants on national and international science and policy committees.

1996 Accomplishments

The Earth and Environmental Sciences Directorate is funded almost equally by six branches of the Department of Energy, and our work spans a wide range of disciplines. We also collaborate with other government agencies (such as the Federal Aviation Administration, the National Aeronautics and Space Administration, and the U.S. Geological Survey) and with nongovernment entities such as universities and private industry. Hence, an annual report focused on either a principal customer or a disciplinary allegiance is not possible for us.

Instead, in this report, we describe a few of our significant accomplishments during 1996. These projects highlight the diverse nature of our research as well as technical expertise. For example, in 1996, we had major accomplishments in modeling carbon isotope distribution and transport in coupled atmospheric-ocean models and in detecting a human signature in climate change. We also demonstrated more cost-effective technologies for use in environmental remediation and played a major role in support of the Comprehensive Test Ban Treaty. In the Research Highlights section of this book, we describe several of the directorate's important project results for 1996.

In other national security areas, we conducted characterization activities at the

Nevada Test Site and in the Middle East, performed significant experiments to evaluate gas release from clandestine nuclear tests, and continued to contribute to site characterization and suitability studies for nuclear waste storage. In health-related areas, we continue to characterize the ecological consequences and related human dose at several sites worldwide where significant nuclear releases have occurred.

In 1996, we also relocated about half of the directorate into new office space and improved laboratory facilities and reduced our own indirect costs. Work in this area is described in the Resources section. As a result of these efforts, the directorate has been a leader in the Laboratory's overall effort to reduce cost and improve effectiveness and efficiency.

The broad role of environmental capabilities within a national security laboratory has become increasingly clear since this directorate was established. National security in the broad sense requires capabilities in geophysics and ecological sciences to avoid surprise, to respond to threats, and to meet economic challenge. Our multidisciplinary organizations must meet these needs with significant operational capabilities. Thus, a central management task for the directorate is to maintain the dynamic between large project or program organizations and the excellent, but smaller, disciplinary science activities, which provide the seeds for future projects and programs.

We believe that this mix of disciplinary divisions, whose individuals accomplish at the highest scientific standards, and project organizations, whose excellence and uniqueness are similarly validated by review, allow us to satisfy the directorate's mission. We find that, indeed, there is still a place for Ernest Lawrence's model: disciplinary excellence of individuals coupled into the team effort of a project environment.

The Search for a “Fingerprint” of Human Activities in Observed Climate Records

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The rapid increase in atmospheric carbon dioxide (CO₂) and other greenhouse gases over the past century has no direct analog in recent geologic history. Thus, we cannot use information on *past* relationships between changes in CO₂ and changes in climate to predict the rate and patterns of climate change that may occur over the next century. We must instead rely on complex numerical models of the Earth's climate system to make such predictions. According to climate models, if the level of atmospheric CO₂ continues to increase until it is double the level prior to the Industrial Revolution 200 years ago, then the global-mean temperature would eventually rise by between 1.5 and 4.5°C. A change of this size would significantly affect many areas of human endeavor, including the world's agriculture, energy and water resources, and human health.

But are model projections of future climate change realistic? These projections involve what has been called a “cascade of uncertainties”—uncertainties derived from many sources, such as assumptions regarding future energy use and how CO₂ is absorbed and released by the oceans and terrestrial biosphere. Current climate models are themselves inadequate, partly because we do not completely understand the complex physical processes, such as cloud formation and precipitation, that we are trying to model. Also, models represent the continuous, evolving climate in terms of discrete points in time and space, which requires numerical and computational simplifications.

Confidence in climate projections would be enhanced if scientists could demonstrate that model representations of present-day and historical climate agreed with observations. At the Program for Climate Model Diagnosis and Intercomparison (PCMDI) in Lawrence Livermore's Earth and Environmental Sciences Directorate, we are comparing the observed record to our model simulations, to determine if in fact there is a matching pattern, or a “fingerprint,” we can attribute to human-induced changes in atmospheric composition. Such a fingerprint would constitute a powerful form of model verification and thus could have far-reaching policy implications regarding future energy use.

What Causes Changes in Climate?

The Earth's climate changes—and will continue to change—for reasons that have nothing to do with human activities. Natural changes in climate result from processes internal to the climate system, such as the complex transfer of heat, moisture, and momentum between the atmosphere and ocean, and from changes in external “forcings” of climate, such as changes in the Sun's energy output or the amount of material injected into the upper atmosphere by a volcanic eruption. Any climate-change signal caused by human activities is thus superimposed on—and to some extent obscured by—the so-called noise of these natural climate fluctuations.

Studies that attempt to identify a human influence on climate usually consist of two parts: *detection* of an unusual change, and *attribution* of all or part of that change to a particular cause or causes. These concepts can be understood in terms of a simple medical analogy. Measurement of a body temperature of 40°C (104°F) “detects” the presence of some abnormal condition or symptom but does not in itself give the cause of the symptom. To attribute the symptom to an

underlying cause often requires additional, more complex tests, such as chemical analyses of the blood and urine or even x rays and magnetic resonance imaging scans.

Pattern analysis is the climatological equivalent of the more comprehensive medical tests. Just as it is unlikely that two different illnesses could yield an array of medical diagnostics that were identical in all respects, so it is unlikely that changes in the output of the Sun and changes in human-produced atmospheric pollutants could produce identical patterns of climate response. Thus, pattern studies help us attribute causes to the different changes.

Early work on climate-change detection examined changes in the global-mean temperature of the Earth over the last century. Most studies of this type concluded that the observed increase of about 0.5°C (0.9°F) was larger than would be expected from natural climate variability alone (Wigley et al., 1997a). However, using a single global-mean temperature series to estimate the relative contributions of numerous factors leads to a problem in which many combinations of factors could yield the same scenario of changes.

Since 1991, PCMDI has worked to address many shortcomings of this initial work. Research on the natural variability of climate has led to improved estimates of what constitutes “normal” behavior of the climate system, particularly on time scales of decades to centuries. We also have more complete estimates of the climate-change signal expected to result from past, present, and future human activities.

Another area of progress has been in applying pattern recognition techniques to the attribution problem. Rather than dealing with global-mean values, we are using the detailed information contained in complex *patterns* of change. For example, we can compare how well model predictions match the data for changes in near-surface temperature at many points on the Earth’s surface (Figure 1, Santer et al., 1995) and in the vertical structure of atmospheric temperature (Figure 2, Santer et al., 1996a). Patterns may also be defined for climate variables other than temperature, and

(a) Modeled near-surface temperature change: present-day CO_2 levels minus preindustrial CO_2 levels

(b) Modeled near-surface temperature change: present-day CO_2 and sulfate aerosols minus preindustrial levels

(c) Observed near-surface temperature change: 1988 data minus 1948 data

Figure 1. Changes in near-surface temperature. Model results are from experiments with (a) nominal present-day levels of atmospheric CO_2 and (b) present-day CO_2 and sulfur emissions (Taylor and Penner, 1994). Model changes are defined relative to a control run with a preindustrial level of atmospheric CO_2 and no anthropogenic sulfur emissions. (c) Observed changes represent the (smoothed) difference between 1988 and 1948 (Jones and Briffa, 1992). White indicates regions where data coverage was not continuous for this 40-year period. Results are for September, October, and November and are given in $^{\circ}\text{C}$.

Research Highlights

(a) Modeled changes in vertical structure of atmospheric temperature using present-day CO₂ levels

(b) Modeled changes in vertical structure of atmospheric temperature using present-day CO₂ and sulfur emission levels

(c) Observed changes in vertical structure of atmospheric temperature between May 1963 and April 1988

Figure 2. Changes in the vertical structure of atmospheric temperature. Model results (given in °C) are from experiments with (a) nominal present-day levels of atmospheric CO₂ and (b) present-day CO₂ and sulfur emissions. See Figure 1 for further details. The results in b also incorporate the effects of stratospheric ozone depletion from 1979 to 1990 (Ramaswamy et al., 1996). (c) Observed changes (given in °C per 25 years) are radiosonde-based temperature measurements (Oort and Liu, 1993) in the form of linear trends from May 1963 to April 1988. All results are for annually averaged data. Although the amplitude of modeled and observed changes is not strictly comparable, the patterns of change in b and c are highly similar.

they may have an explicit time dimension, such as a seasonal cycle or an evolution over many decades.

Finding a Pattern

In a typical pattern-based study, a signal pattern predicted by the model is compared with a sequence of observed patterns of temperature change. Some index of pattern similarity is used to quantify how closely the model prediction matches reality. If there is in fact a human effect on global climate, we might expect, from the historical increase in greenhouse gases and aerosol-producing emissions, that the statistical measure of pattern similarity would become larger over time, as the signal strength increases. Simply put, a sustained increase in the similarity statistic would indicate that the observations were becoming increasingly similar to the model prediction.

We do not expect the similarity statistic to follow a simple linear trend. Natural climate variability will be superimposed on any growing climate signal (Wigley et al., 1997b), and the pattern of the signal itself may change with time. Instead, we want to determine whether the overall changes in pattern similarity with time are larger than we might expect to result from natural variability alone, and whether such changes differ for different types of signal—for example, is there a “greenhouse only” signal and a signal due to combined greenhouse-gas and aerosol effects.

What the Patterns Reveal

In our pattern-based work, we use model signals caused by the individual and combined effects of greenhouse gases and aerosols. These signals were taken from experiments performed at Lawrence Livermore (Taylor and Penner, 1994) and from integrations carried out by our collaborators at the Hadley Centre for Climate Prediction and Research in the United Kingdom (Mitchell et al., 1995; Tett et al., 1996) and at the Geophysical Fluid Dynamics Laboratory in Princeton (Ramaswamy et al., 1996). We then compared these signals with instrumental records of near-surface temperature

change (Jones and Briffa, 1992) and with weather balloon (radiosonde) measurements of temperature change in the free atmosphere (Oort and Liu, 1993; Parker and Cox, 1995).

The near-surface comparisons indicate that model results most closely match reality for a combined greenhouse-gas and aerosol signal. To compare vertical patterns of change, we also incorporated the effects of stratospheric ozone depletion (Figure 2b). As shown in Figure 3, the degree of agreement between models and data generally increases over the last 25 to 50 years.

It is possible that such increasing correspondence could arise by chance as a result of natural climate variability on decadal and longer time scales. To assess the statistical significance of the signal trend shown in Figure 3b (roughly +1.4 correlation units in 25 years), we need some estimate of how often natural variability might yield a positive trend this large or larger.

The observational record is too short for this purpose. We therefore rely on multi-century simulations of coupled atmosphere-ocean models to provide us with information about climate variability. From such model output, we generated many sequences of “natural” patterns of climate fluctuations. The signal pattern in Figure 2b was then correlated with these natural patterns, thus yielding a time series that reflects the unforced behavior of the pattern statistic.

By fitting linear trends to many different 25-year chunks of this time series, we produced a distribution of noise trends. As Figure 4 illustrates, the pattern correspondence found between observations and model predictions of atmospheric temperature change is a highly unusual event, unlikely to occur through natural internal variability of the climate system (as simulated by this and other coupled models).

Could externally caused natural climate variability fully explain the observed climate changes? Our best answer to this question is “no.” Over the last several decades, radiosonde measurements of atmospheric temperature have revealed a distinctive pattern of stratospheric cooling and tropospheric warming. This

fingerprint is highly specific to increases in carbon dioxide and decreases in stratospheric ozone—both anthropogenic effects. The temperature-change patterns that we might expect to see for changes in the Sun’s output (no cooling of the lower stratosphere) or in the amount of volcanic dust in the stratosphere (stratospheric warming) are quite different from those resulting from human influences.

Clearly, the correspondences found between models and observations are caused by pattern similarities at large scales—for example, contrasts between the Northern and Southern Hemispheres or between the

Figure 3. Correlations between modeled and observed patterns of temperature change (a) at the Earth’s surface and (b) in the free atmosphere from about 2 to 20 km. These correlations were made by searching for the patterns predicted in Figures 1b and 2b in instrumental measurements of near-surface temperature change from 1910 to 1993 and in radiosonde-based measurements of temperature change from 1963 to 1988. The pattern similarity statistic shows a sustained positive trend, indicating that observations are becoming increasingly similar to the model predictions.

Figure 4. Relationship between “signal” and “noise” trends in pattern similarity. The red line shows the signal trend, which represents the 25-year linear trend in the statistic that measures the correlation between modeled and observed patterns of temperature change in the free atmosphere (see Figure 3b). The green curve shows a distribution of noise trends that we generated by correlating the signal pattern in Figure 2b with time-varying patterns of natural internal climate variability.

stratosphere and troposphere. It is at these large scales that we have the most confidence in model performance (Gates et al., 1996). More importantly, although detection and attribution studies are fundamentally statistical in nature, many of these results agree with our basic physical understanding of the climate system and do not depend on sophisticated numerical models or statistical techniques.

A Discernible Human Influence

Our work contributed to the conclusion that “the balance of evidence suggests a discernible human influence on global climate,” which was one of the primary findings of the Intergovernmental Panel on Climate Change (IPCC, Houghton et al., 1996; Santer et al., 1996b). This conclusion does not mean that the search for a human signal in observed climate records is now over. Rather, it means that the search is now beginning in earnest. The IPCC’s conclusion was accompanied by many caveats. These are primarily related to our imperfect knowledge of the “true” climate-change signal resulting from climatic variability against which this signal must be detected. Although these uncertainties will be reduced with time, they will never be removed entirely, so detection and attribution studies (like medical prognoses) will always be inherently probabilistic in nature.

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References

- Gates, W. L., A. Henderson-Sellers, G. J. Boer, C. K. Folland, A. Kitoh, B. J. McAvaney, F. Semazzi, N. Smith, A. J. Weaver, and Q.-C. Zeng (1996), “Climate Models—Evaluation,” in *Climate Change 1995: The Science of Climate Change*, J. T. Houghton et al., Eds. (Cambridge University Press, Cambridge), pp. 229–284.
- Jones, P. D., and K. R. Briffa (1992), “Global Surface Air Temperature Variations over the Twentieth Century. Part 1: Spatial, Temporal and Seasonal Scales,” *The Holocene* **2**, 165–179.
- Mitchell, J. F. B., T. C. Johns, J. M. Gregory, and S. Tett (1995), “Transient Climate Response to Increasing Sulfate Aerosols and Greenhouse Gases,” *Nature* **376**, 501–504.
- Oort, A. H., and H. Liu (1993), “Upper-Air Temperature Trends over the Globe, 1958–1989,” *J. Climate* **6**, 292–307.
- Parker, D. E., and D. I. Cox (1995), “Towards a Consistent Global Climatological Rawinsonde Database,” *Int. J. Climatol.* **15**, 473–496.
- Ramaswamy, V., M. D. Schwarzkopf, and W. J. Randel (1996), “Fingerprint of Ozone Depletion in the Spatial and Temporal Pattern of Recent Lower-Stratospheric Cooling,” *Nature* **382**, 616–618.
- Santer, B. D., K. E. Taylor, T. M. L. Wigley, J. E. Penner, P. D. Jones, and U. Cubasch (1995), “Towards the Detection and Attribution of an Anthropogenic Effect on Climate,” *Climate Dynamics* **12**, 77–100.
- Santer, B. D., K. E. Taylor, T. M. L. Wigley, T. C. Johns, P. D. Jones, D. J. Karoly, J. F. B. Mitchell, A. H. Oort, J. E. Penner, V. Ramaswamy, M. D. Schwarzkopf, R. J. Stouffer, and S. Tett, (1996a), “A Search for Human Influences on the Thermal Structure of the Atmosphere,” *Nature* **382**, 39–46.
- Santer, B. D., T. M. L. Wigley, T. P. Barnett, and E. Anyamba (1996c), “Detection of Climate Change, and Attribution of Causes,” in *Climate Change 1995: The Science of Climate Change*, J. T. Houghton et al., Eds. (Cambridge University Press, Cambridge), pp. 407–443.
- Taylor, K. E., and J. E. Penner (1994), “Anthropogenic Aerosols and Climate Change,” *Nature* **369**, 734–736.
- Tett, S. F. B., J. F. B. Mitchell, D. E. Parker, and M. R. Allen (1996), “Human Influence on the Atmospheric Vertical Temperature Structure: Detection and Observations,” *Science* **274**, 1170–1173.
- Wigley, T. M. L., P. D. Jones, and S. C. B. Raper (1997a), “The Observed Global Warming Record: What Does It Tell Us?” *Proc. National Academy of Sciences Colloquium on Carbon Dioxide and Climate Change*, Irvine, CA, November 1995.
- Wigley, T. M. L., P. J. Jaumann, B. D. Santer, and K. E. Taylor (1997b), “Relative Detectability of Greenhouse-Gas and Aerosol Climate Change Signals,” *Climate Dynamics* (in press).

Global Carbon Cycle Modeling

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During the past 200 years, the concentration of carbon dioxide (CO_2) in Earth's atmosphere increased about 30%. The increase, which continues at a rate of about 0.4% per year, is caused primarily by burning fossil fuels, but a substantial amount results from the destruction of plants and soil carbon stocks as a result of deforestation processes. This increase is of concern because it may be causing changes to the global climate. Perhaps the most important change is that it warms the climate. Because increasing atmospheric CO_2 is a potential driver of climatic change, we want to understand, in quantitative terms, the fate of CO_2 released to the atmosphere in fossil-fuel use and other processes. In particular, we want to determine how much CO_2 can be taken up by and stored in the plants and soils in terrestrial ecosystems and in the oceans.

Today, about half of the CO_2 released in fossil-fuel use is stored in oceans and on land in a process known as CO_2 uptake (Figure 1). The other half is causing the increase in atmospheric CO_2 . We can attempt to measure the current CO_2 uptake in oceans and on land, but to predict the future, we must use computer models. The goal of the carbon cycle modeling project at Lawrence Livermore is to develop and validate models that simulate the exchange of CO_2 between sea and air and between land and air at the global scale and thus reduce the uncertainty about future CO_2 levels and potential climatic changes.

Uptake of CO_2 on Land

When the concentration of CO_2 in the atmosphere increases, it generally stimulates plant growth—one positive aspect of the increase—and carbon storage in plants and soils in a process called CO_2 fertilization. Because this biotic response slows the increase in atmospheric CO_2 , it is a negative feedback on the system. In this project, we

want to determine whether this negative feedback is significantly slowing the present CO_2 increase and how much it will limit future levels. Our model of the terrestrial biosphere, which is similar in key respects to other models, indicates that plants assimilate in photosynthesis and growth about 10 to 15% more CO_2 globally each year than they did 200 years ago. Thus, the potential net terrestrial uptake, or land sink, of CO_2 is now about 5 billion tons of carbon each year, or about 80% of present fossil-fuel CO_2 releases. (Slightly more than 6 billion tons of carbon are now released to the atmosphere annually, a value that is accurately known.)

In calculating the land sink, we assume that the preindustrial terrestrial biosphere was in an approximate steady state with respect to carbon—that is, it was neither a net sink nor a net source of CO_2 to the

Figure 1. Carbon dioxide fluxes into and out of the atmosphere. The burning of fossil fuels adds CO_2 to the atmosphere (brown curve), but not all of it accumulates there (blue curve). Some is absorbed by the ocean (red curve), and some is absorbed by the terrestrial biosphere (green curve). Shown are results from an ocean biogeochemistry model calculation for oceanic CO_2 absorption. Inferred net uptake of CO_2 by the terrestrial biosphere since approximately 1950 is consistent with our understanding of forest regrowth and CO_2 fertilization of plant growth. (Except for oceanic uptake, all positive values are addition of CO_2 to the atmosphere.)

atmosphere. (This assumption is based on several lines of reasoning that are beyond the scope of this article; for example, see Bolin et al., 1979.) Much of the “additional” carbon assimilated by plants today (compared with preindustrial rates) is later released back to the atmosphere during plant respiration and the decomposition of organic matter in the soil. According to our models, about 2.0 to 2.5 billion tons of carbon are stored on land each year over and above the steady-state preindustrial carbon storage amounts.

This net storage of carbon on land is, however, transitory. That is, the CO₂ released in decomposition processes is quantitatively linked to the amount of CO₂ previously absorbed. Eventually, given some future stable concentration of atmospheric CO₂, the terrestrial biosphere will again approach a steady state with respect to annual CO₂ uptake and release, although the amount of carbon stored in the terrestrial biosphere will be greater than it is today.

The increased CO₂ assimilation on land does not include CO₂ transferred from land to the atmosphere as a result of deforestation and other human land-use changes. The most commonly cited estimates of the annual CO₂ flux from land-use changes are between 1.5 and 2.0 billion tons of carbon. If this amount is subtracted from the 2.0 to 2.5 billion tons of additional carbon stored annually in CO₂ fertilization, then only 0 to 1 billion tons of carbon are added to the terrestrial biosphere each year. This range is consistent with what seems to be occurring in nature based on the annual balance of CO₂ released in fossil-fuel burning, the CO₂ accumulating in the atmosphere (an amount that is determined accurately from direct measurements at several remote sites), and the amount of CO₂ that is thought to be taken up by the oceans. Indeed, our best estimate for the present net storage of carbon in the terrestrial biosphere, based on detailed ocean modeling, is about 0.5 billion tons of carbon a year (see Figure 1).

In addition to the negative feedback from CO₂ fertilization of the terrestrial biosphere, a potentially important positive feed-

back on future global warming might be mediated through the terrestrial biosphere's carbon cycle. In general, climatic warming speeds the decomposition processes and the release of CO₂ to the atmosphere from soils. Our models account for this effect, although knowledge of future temperature is limited. (Precipitation, or more specifically soil moisture, also affects the decomposition rate, and precipitation patterns may well be altered by climatic changes resulting from elevated atmospheric CO₂. However, the effects on decomposition may be either negative or positive and are difficult to predict. Moreover, predictions by climate models of future precipitation patterns are variable.)

The positive feedback might operate as follows: Increasing atmospheric CO₂ concentration causes some degree of global warming, which then stimulates the decomposition rate. The stimulated decomposition rate reduces the lifetime of carbon within soils and terrestrial ecosystems, resulting in a net release of CO₂ to the atmosphere. This CO₂ release enhances the atmospheric CO₂ increase and thus furthers global warming. The potential magnitude of such a scenario is large.

The process can be studied with models; however, of great use in our research have been the data concerning the effects of temperature on carbon residence time in soils. These data were collected in field research in California forests by scientists from the University of California at Irvine, in association with carbon isotope measurements at Lawrence Livermore's Center for Accelerator Mass Spectrometry (CAMS). The field research corroborates model predictions that soil carbon storage is reduced by high temperature.

Uptake of CO₂ by Oceans

The ocean component of our modeling efforts combines a three-dimensional ocean general circulation model (OGCM) with models of ocean-air CO₂ exchange, inorganic chemistry, and ocean biology. The isotopes of carbon ¹²C, ¹³C, and ¹⁴C react at somewhat different rates in various physical, chemical, and biological processes, which results in

carbon isotope ratio signatures in the ocean. (Such signatures also exist in terrestrial ecosystems and are due to fractionation processes associated with terrestrial photosynthesis.) Our ocean model includes a full treatment of carbon isotope fractionation processes. Because of the complex three-dimensional nature of this model, it was developed to run on Livermore's massively parallel computers. To our knowledge, it is the most complete and detailed global ocean biogeochemistry/circulation model (OBGCM) in use today.

In one study, the OBGCM successfully simulated ocean-air CO_2 exchange processes from the preindustrial period to the present (Figures 1 and 2). In 1996, we compared the OBGCM simulations to observations of the increase in atmospheric CO_2 and of the spatial and temporal distributions of oceanic ^{12}C , ^{13}C , and ^{14}C . The results convincingly showed that the model can calculate important carbon cycle processes in the ocean and that it will help reduce the uncertainty about future ocean-air CO_2 exchange rates and the atmospheric CO_2 concentration increase.

Also of interest to carbon cycle studies is the so-called spike of radiocarbon (that is, radioactive $^{14}\text{CO}_2$) that was added to the atmosphere during aboveground thermonuclear bomb testing in the 1950s and 1960s. By the time international test bans became effective, the tropospheric radiocarbon content was almost double the content prior to the tests. Present tropospheric radiocarbon levels are only 10 to 15% above prebomb levels, but since the half-life of radiocarbon is greater than 5000 years, we know it has not decayed to this value. Instead, the oceans and terrestrial biosphere are storing it.

This additional, or bomb, radiocarbon is an important tracer for atmospheric CO_2 and ocean and land carbon compounds that can be used to test our models. In 1996, we used models of Earth's ocean, stratosphere, and terrestrial biosphere to predict the course of this radiocarbon and thus assess our understanding of the present global carbon cycle. We then compared the model predictions to

the generally accurate measurements of $^{14}\text{CO}_2$ in the troposphere during the past several decades. Our model predictions agreed with the atmospheric measurements, indicating that the models conform to the actual carbon cycle.

In addition to measuring recent changes in atmospheric radiocarbon, we also can test our models by measuring the time course of changes in ^{12}C , ^{13}C , and ^{14}C at specific locations in the ocean. Our research demonstrated that models are best tested with measurements of ocean carbon isotopes at specific times and locations, rather than with whole-ocean carbon isotope mean values. As a result, our use of the OGCM and OBGCM significantly altered the methods used by the research community at large. We also developed several diagnostic tools to validate OGCMs based on carbon and other chemical tracers.

Interannual Variability in Atmospheric CO_2 Increase

Year-to-year changes in global fossil-fuel use are small, but in recent years, the interannual variability in atmospheric CO_2

Figure 2. Amount of CO_2 in the ocean per unit area (in moles per square meter of ocean surface), as calculated by our ocean biogeochemistry model. This calculation indicates the oceans absorb CO_2 most readily at high latitudes.

increase has been significant. Many researchers believe that interannual variability in temperature and precipitation may alter the terrestrial biosphere's ability to assimilate CO₂ enough to account for such variations. Little direct evidence is available to test this notion, however.

To increase our understanding of this issue, we used a sophisticated, geographically explicit (on a 1-degree latitude $\times$ 1-degree longitude grid) model of terrestrial photosynthesis and respiration. Our goal was to assess how observed changes in monthly mean temperature and precipitation (also on a 1-degree $\times$ 1-degree grid) affected the global land-air CO₂ exchange during each year of the 1980s. Our model predictions of interannual variability correlated positively with the observed interannual variability in the atmospheric CO₂ increase, and they are of the proper magnitude—in the range of ± 0.8 billion tons of carbon a year. This exercise demonstrated for the first time that present understanding of plant and soil responses to atmospheric CO₂ level, temperature, and precipitation can account for the observed interannual variability in atmospheric CO₂ increase.

Links to Field Ecology and Carbon Isotope Measurements

We can improve our knowledge of long-term CO₂ fertilization by studying carbon storage in soils and plants near natural CO₂ vents, such as those associated with many hot springs. Several CO₂ vents have been active for many centuries to millennia, which allows time for plant metabolism to adapt to elevated atmospheric CO₂, as might occur with increasing global atmospheric CO₂. Because the CO₂ released from these vents is of geologic origin, it contains no radiocarbon. Therefore, the radiocarbon content of soils and plants at various distances from the vents is a measure of the average CO₂ concentrations to which plants are exposed.

Perhaps the only way to assess the long-term effects of CO₂ fertilization on terrestrial ecosystem CO₂ uptake and carbon storage is

to determine the carbon storage per unit ground area as a function of long-term atmospheric CO₂ concentration near CO₂ vents. In collaboration with San Diego State University, we are initiating such measurements at the CAMS. This knowledge will help us predict the role of the terrestrial biosphere in the future global carbon cycle.

Measurements at CAMS are also reducing uncertainty in turnover times of deadwood in tropical forests. Researchers recently acknowledged that deadwood is a large item in the global terrestrial carbon budget. Changes in the deadwood turnover rate (the rate of decomposition and conversion of organic carbon to CO₂ released to the atmosphere) that result from increasing atmospheric CO₂ or climatic changes may noticeably affect the global land-air exchange rates in the future. The longevity of tropical trees is also important to carbon cycle dynamics. Collaborative work with the University of California at Santa Barbara has enhanced our understanding of the longevity of trees in tropical rainforests and the environmental factors regulating the decomposition of deadwood in the tropics and elsewhere. As a result of this work, we have improved the parameterizations in our models of carbon cycling in the terrestrial biosphere.

Future Work

In 1997, we are using our models, having incorporated improvements made in 1996 and earlier, to predict how fossil-fuel use will affect the global carbon cycle. These predictions will reduce uncertainty about future atmospheric CO₂ concentrations, which will in turn constrain predictions of future climate and the ecological and economic effects of climatic change.

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Reference

Bolin, B., E. T. Degens, S. Kempe, and P. Ketner, Eds. (1979), *The Global Carbon Cycle* (Wiley, Chichester).

Accelerated Cleanup: Combining Technologies for Groundwater Remediation

Richard B. Knapp, Roger Aines, Sally Bahowick, Richard Blake, Alan B. Copeland, Kenneth J. Jackson, Albert Lamarre, Robin Newmark, and Andrew F. B. Tompson

Contaminant plumes in underground water are a major national problem. The volume of contaminated groundwater approaches a trillion gallons, and the anticipated cleanup costs are in the hundreds of billions of dollars. The primary technology being used to remediate contaminant plumes is the pump-and-treat method, in which contaminant is extracted from the subsurface and treated before disposal. Although this technology is effective at plume boundaries, it cannot clean plume source regions. A faster and more effective approach would be to remediate groundwater *in situ*.

To help develop such an approach, Lawrence Livermore National Laboratory established a collaborative project between scientists in the Laboratory's Earth and Environmental Sciences Directorate and its Environmental Restoration Division. In laboratory experiments and computer simulations, we continued to evaluate a concept to rapidly destroy plume source regions while preventing the plume from expanding further. The core technology in this concept is hydrous pyrolysis/oxidation (HPO), combined with permeable microbial barriers and the traditional pump-and-treat method. Ultimately, our goal is to evaluate this concept in a large-scale field test of a 100-meter-diameter contaminated zone at Lawrence Livermore's main site.

The Accelerated Cleanup Concept

Hydrous pyrolysis/oxidation relies on a novel *in situ* thermal heating technique from injected steam to accelerate the contaminant breakdown and degradation processes

(Figure 1). We enhanced the HPO technology by placing permeable microbial barriers downstream, to intercept and destroy the contaminated groundwater displaced by steam injection, and adding traditional pump-and-treat well systems in perimeter areas, to contain the plume's flow.

Comparing the hypothetical time histories of different remediation techniques reveals that our approach may perform well (Figure 2). Contaminant mass removal by the pump-and-treat method alone may be initially rapid as the high-permeability regions are flushed, but the rate is reduced over time

Figure 1. Example of an accelerated cleanup system combining the hydrous pyrolysis/oxidation technology with *in situ* microbial filters. (a) A single pump-and-treat extraction well is placed downstream of a contaminant plume. Different colors denote ranges in contaminant concentrations. (b) The hydrous pyrolysis/oxidation technique is used to rapidly destroy contaminants in and around the source region. A biofilter is placed downstream to intercept and destroy contaminants that are displaced by steam injection but are not drawn back into the thermal destruction zone.

because contaminant transport from the low-permeability units to the high-permeability units is slow. Hydrous pyrolysis accelerates cleanup by rapidly destroying the source region—in both high- and low-permeability units—thereby eliminating the long pump-and-treat cleanup tail. *///*microbial filters amplify this acceleration by intercepting and destroying contaminated groundwater displaced during steam injection, thereby truncating part of the plume that comprises the pump-and-treat capture zone and reducing the overall cleanup time.

Hydrous Pyrolysis/Oxidation

The hydrous pyrolysis/oxidation technology proved to be effective in both high- and low-permeability units and for a wide range of concentrations. As shown in Figure 3a, when steam is injected into an aquifer in high-permeability units, it displaces the contaminated groundwater and builds a large thermal reaction zone. When the zone has the desired volume, steam injection is terminated, and the contaminant destruction phase begins. The shut-in well causes the steam to condense, which draws the contaminated fluid back into the thermal reaction zone. The fluids then heat up, causing the spontaneous oxidation of contaminant. If low-permeability clays and silts are also present, as in

Figure 2. Hypothetical time history of contaminant concentrations in groundwater withdrawn from a single extraction well.

Figure 3b, they are heated both by the conduction of heat from the thermal reaction in the high-permeability units and by the buoyant, advective rise of heat through vertical infiltration pathways.

In laboratory experiments, the thermal destruction reaction was effective, fast, and robust. We found that a wide range of aqueous contaminants can be degraded to innocuous products when heat is applied in the presence of at least stoichiometric amounts of oxygen. In these experiments, the oxidation reaction rate was fast and destroyed contaminants over a range of temperatures that can be easily achieved in the subsurface. In fact, the rate is so fast that the practical limiting factor is the rate at which the subsurface can be heated through steam injection. In 1997, we will conduct laboratory experiments to define how contaminant concentration, aqueous chemistry (such as pH), and coexisting gas phases affect the aqueous-phase oxidation rate.

Before HPO technology can be used in a field test, we must determine whether the chemistry of site sediments in the treatment zone will affect the process rate. Some effects can be positive; for example, the sediments might catalyze the reaction or provide additional oxide surface reaction sites. However, the sediments might also consume too much oxygen via oxidation of metals or sediment organic material. A series of laboratory experiments demonstrated that the chemistry of sediments at the Livermore site does not interfere with the contaminant destruction reaction, and that there is no excess consumption of oxygen.

Another concern is whether metals are released from the sediment during the steaming process. In laboratory experiments with sample sediments from the Livermore site, we found that metal release also was not a problem. In addition, a preliminary experiment with a manganese oxide mineral—a common sediment component—showed that it can participate in an oxidation-reduction coupled reaction with contaminants such as trichloroethene (TCE), thus enhancing the

contaminant oxidation reaction. Its presence thus increases our confidence that hydroous pyrolysis/oxidation can be used successfully in the subsurface.

In 1996, we began a series of fluid flow and transport simulations using Lawrence Livermore's NUFT simulator to explore issues related to the feasibility of the HPO process. For this simulation study, we focused attention on TCE contamination in a confined, high-permeability layer of the site's subsurface. These simulations are based on a simplified, two-dimensional conceptualization of radially symmetric flow and transport in a vertical plane that intersects a steam injection well. In this representation, saturated steam, or a mixture of saturated steam and oxygen, enters the formation through the wellbore, as a function of an applied well-head steam pressure.

Computer simulations showed that it is relatively simple to establish the necessary coincidence of dissolved contaminant, dissolved oxygen, and elevated temperatures for TCE degradation *in situ*. Nevertheless, care must be taken to avoid generating significant noncondensable gas phases in the thermal reaction zone, because these phases may reduce the chemical reaction rate. In our simulation, most of the reaction during steam injection occurs near the leading edge of the advancing steam front.

This result seems consistent with the argument that TCE is displaced by steam injection, so the reaction can occur only near the front because heat and dissolved oxygen diffuse into the native (contaminated) groundwater, or TCE diffuses back into the condensed water phase. Once the steam zone collapses and condenses, the reaction front recedes back toward the well, and more importantly, the reaction zone widens. Because heat remains in the formation, TCE-laden water is drawn back into the collapsing steam zone, and residual oxygen is regained in condensed water to the extent saturation limits allow. In this manner, the *in situ* operations approach a batch process in the thermal reaction zone.

In Situ Microbial Filter

With *in situ* microbial filter technology, permeable microbial destruction zones must be established in the subsurface through which contaminated groundwater flows and is microbially remediated. These zones are created by injecting into the subsurface harmless bacteria that can destroy the contaminants. Portions of the injected biomass attach to the sediment and form a fixed-bed bioreactor. In our accelerated cleanup concept, biofilters supplement the HPO process by intercepting contaminated groundwater displaced by the steam injection (Figure 4).

Before microbial filter technology can be used in a field test, we must evaluate several features regarding a site's geology, hydrology,

(a) Hydrous pyrolysis technology in high-permeability units

(b) Hydrous pyrolysis technology in low-permeability units

Figure 3. The hydrous pyrolysis/oxidation technology in (a) high-permeability units and (b) low-permeability clays and silts.

and chemistry. These features include the aquifer's saturation state, sediment pore size, groundwater chemistry, contaminant species and concentration, and ratio of dissolved oxygen to contaminant. In a series of laboratory tests with selected sediments and groundwater from the Livermore site, we found that all of these conditions are within acceptable ranges for the filter technology to work.

We also completed a set of treatability experiments to determine whether the microbial filter technique can be used as part of the accelerated cleanup effort at Lawrence Livermore. In laboratory experiments with groundwater from the Livermore site, bacteria degraded TCE for more than 50 days in the absence of growth substrates. Injected cells also attached to the site's sediment to a very high degree, giving substantial flexibility in establishing an effective filter in the subsur-

face. We also conducted an in-well test where contaminated groundwater was drawn through a biofilter established on a column of sediment from the Livermore site. This test showed that the bacteria can degrade the contaminants to below the concentrations levels required for groundwater cleanup.

The most expensive part of the *in situ* microbial filter approach is producing cells. The overall cost of producing biomass is strongly influenced by the density to which bacteria can be grown during commercial fermentation. Recent advances in the biomass generation process tripled the amount of biomass generated in a given bioreactor run. Also, TCE-degrading specific activity (degrading activity per unit biomass) was improved by about 30%, to about 85 nanomoles per milligram (dry weight) per minute. These improvements substantially reduced the cost of generating the bacteria needed for an *in situ* microbial filter and simultaneously improved performance.

Process Monitoring and Control

One objective of a field test is to quantify whether a technology, or a suite of technologies, can successfully destroy or degrade contaminants. The field program must also provide sufficient detail to calibrate models of contaminant destruction and to define the minimum controls required for future commercial application. An additional objective is to quantitatively measure the success of the remediation effort.

For successful demonstration of our accelerated cleanup approach, both physical and chemical parameters must be monitored. Although many techniques can be used to measure properties such as temperature, pressure, or contaminant concentration, the specific constraints on applying this concept require that many of these parameters be measured *in situ*, under high-temperature and high-pressure conditions. Spatial and temporal requirements pose additional challenges. At the same time, the methods used

Figure 4. *In situ* microbial filter technology. Steam injected into high-permeability units accelerates the displacement of contaminated groundwater from the source region. An *in situ* microbial filter emplaced downstream destroys or degrades this contaminant, prevents it from returning to the source region, and further accelerates cleanup.

to monitor the remediation process and assess its performance must be cost-effective and timely.

Thus, a major accomplishment for this project in 1996 was using cone penetrometry to successfully emplace monitoring points at depths greater than 50 meters in highly heterogeneous sediments. This method is not only inexpensive, but it also allows for dense emplacement of measuring devices such as the sensors used to record temperature and the electrical resistance tomography for determining the steam zone geometry.

In addition, we designed an extractive system for sampling fluids and measuring their chemistry under the extreme conditions expected during the steam injection phase of HPO. Initial tests on an advanced oxygen sensor indicate it can survive exposure to steam and make viable measurements at temperatures above 80°C. In 1997, we will design and test tracer application and analysis methods to track injectate and differentiate it from connate water. Fluid saturation will be measured using existing logging techniques.

Characterizing the Field Site

Site-specific investigations demonstrated that Lawrence Livermore's main site is a viable location for an initial pilot-scale field test. With data from a series of wells in the proposed test area, we defined the major

subsurface features that control the flow of fluids, including injected steam and displaced contaminated groundwater. This information is critical to establishing an efficient monitoring network and as input into process simulations. It also allows us to define the initial contaminant distribution in both low- and high-permeability units, against which the effectiveness of hydrous pyrolysis/oxidation will be measured. Similar data will be acquired across the contaminant plume, so the technologies can be quickly deployed once they are successfully demonstrated at the pilot scale.

Future Work

Field tests at the pilot scale are a key ingredient to achieve technology acceptance. These tests reduce uncertainties regarding technical performance and cost effectiveness. Our future efforts will be directed toward field demonstration of hydrous pyrolysis/oxidation, both individually and combined with the *in situ* microbial filter and pump-and-treat technologies. Following a successful field demonstration, these technologies will be phased into Lawrence Livermore's site cleanup activities.

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Evaluating Potential Designs of a Nuclear Waste Repository

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The U.S. Department of Energy (DOE) is investigating whether it is feasible to dispose of highly radioactive wastes, including spent nuclear fuel from electrical utilities and wastes stored at federal facilities, in a repository built in the unsaturated zone at Yucca Mountain, Nevada. For such a repository, the waste isolation system must limit the release of radionuclides from the waste packages and their transport to the accessible environment. As part of the DOE effort, scientists in Livermore's Earth and Environmental Sciences Directorate are developing computer models that trace how heat from the waste packages affects water flow in Yucca Mountain, particularly how water contacts waste containers and the waste itself.

The Repository Environment

A potential repository at Yucca Mountain would contain as many as 12,000 waste packages in a site that is nearly one kilometer underground and extends several kilometers horizontally. The radioactive waste to be stored in the waste packages consists of hotter commercial spent nuclear fuel, which ranges from about 3 to 18 kilowatts per waste package, and cooler defense high-level waste, which ranges from about 1 to 3 kilowatts per waste package. The types of spent-nuclear-fuel waste packages are those containing 12 or 21 fuel assemblies from a pressurized water reactor (PWR) and 44 assemblies from a boiling water reactor (BWR). The spent nuclear fuel ranges in age from 10 to more than 40 years (that is, time since it was removed from the reactor core). The defense high-level waste is from the Hanford and Savannah River sites and is in a glass waste (vitrified) form.

As long as the waste packages remain intact, radionuclides are not released. The primary threat to the containers is corrosion, which is caused by the presence of water. Therefore, how and when water contacts a waste package will affect its integrity. Water contact occurs in two ways: (1) gaseous flow (water vapor and air), where the condensation of water vapor then forms a liquid film on the waste package; and (2) liquid flow (water) in the underground environment. For both of these, changes in temperature, relative humidity, and liquid-phase flow affect how and when water contacts the waste containers.

Unfortunately, the environment in the unsaturated zone is corrosive for the metallic waste-package materials; the ambient relative humidity there is about 99%—high enough to form liquid films from condensation. However, the radioactive materials stored in the packages give off decay heat that will reduce the relative humidity to levels at which corrosion is minimal. Thus initially, when packages are emplaced in the repository, the relative humidity is reduced (although the magnitude and duration of this reduction depends on the repository design). Relative humidity then rises as the packages “cool”—that is, as the radioactive elements decay over time.

One of the goals in evaluating repository designs is to determine how long it takes for the relative humidity to rise to 65 to 95%—a range at which significant corrosion might begin. A lower value, such as 65%, pertains to the situation where hygroscopic salts are present on the waste package. A higher value, such as 95%, is more likely if the surface is free of salt. Thus, an important goal is to prevent liquid water from dripping on (and evaporating on) waste packages, thereby minimizing the buildup of salts.

The Challenge: Detailed Modeling in Three Dimensions

Modeling multiple-phase flow in an unsaturated, porous rock with varying temperature is itself a significant challenge. To evaluate a potential repository at Yucca Mountain, we must model 12,000 waste packages in a large, underground site. Yet, our simulations must show changes down to a centimeter level of detail. Also, to ensure the long-term performance of the repository, we must extend the simulations from the present to 10,000 years in the future. Obviously, a single calculation is not sufficient. Parametric studies require tens of calculations, and more than a thousand calculations have been performed.

Much of the early modeling work in repository design was performed in one or two dimensions. Where three dimensions were addressed, the calculations were simplified by modeling the heat as either a planar source or, in more recent calculations, an averaged line source. To better evaluate design alternatives, we used a three-dimensional code called NUFT (Nitao, 1992), which was developed at Livermore to simulate the coupled transport of water, vapor, air, and heat in fractured, porous media. The resulting NUFT-based models explicitly represent a realistic mixture of waste in individual packages and thus allow us to study how the relative placement of the hottest and coolest packages would affect the temperature and humidity of a repository.

Our Results: Evaluating Two Designs

In 1996, we used our three-dimensional model to compare two repository designs: point-load spacing and line-load spacing (Figure 1). The point-load design attempts to evenly distribute the decay heat over the repository area by placing the waste packages with nearly equal spacing on all sides. In the line-load design, decay heat from the waste packages is concentrated in a line by placing

Figure 1. Plan view of two waste-package layouts: (a) the point-load design and (b) the line-load design. Both designs result in an areal mass loading of 83.4 metric tons of uranium (MTU) per acre. Note: heat outputs are at the time the waste packages are emplaced. SNF = spent nuclear fuel; DHLW = defense high-level waste; 21-PWR = 21 pressurized-water-reactor assemblies; 44-BWR = 44 boiling-water-reactor assemblies; and kW = kilowatts.

the waste packages nearly end to end along more widely spaced drifts.

The thermal loading of the repository is constrained by both near-field and far-field effects. The far-field environment is affected by the average areal mass loading (AML, expressed in metric tons of uranium per acre, MTU/acre). The near-field environment is affected to a great degree by the geometry of emplacement. Because we are concerned with the details of repository design, we held the AML constant but varied the geometry of emplacement, as shown in Figure 1. Our detailed simulations showed that the temperature, relative humidity, and liquid-phase flux history of the waste-package surfaces—and hence the time before corrosion begins—

differed significantly in the two designs (Buscheck et al., 1996).

As shown in Figure 2, relative humidity will increase to 65% between 25 to 660 years with the point-load design and between 1540 and 1710 years with the line-load design. The coolest package in the line-load design is dry—that is, relative humidity is less than 65%—more than twice as long as the hottest package and 60 times as long as the coolest package in the point-load design. (For a detailed list of the temperature and humidity results for the design options we modeled, see Table 1 in Buscheck et al., 1996.) Only our recent modeling of individual waste packages reveals these ranges; earlier calculations would have given only an averaged time for each layout.

Figure 2. Temperature and relative humidity on the upper surface of the waste packages when no backfill is emplaced in the drifts. Curves are plotted for (a,c) the point-load design and (b,d) the line-load design.

Figure 2 addresses conditions when the drifts are left open (filled with air). Another option is to close in the repository with backfill material 100 years after the packages are emplaced. Figure 3 shows the results of our calculations for that option. The spread in temperature and relative humidity is pronounced for the point-load design because the backfill isolates these waste packages. For most waste packages in drifts with backfill and with line-load spacing, it does take longer (between 3550 to 4770 years) for relative humidity to rise to 65%. However, one package type in the point-load layout now exceeds the hottest line-load packages, which extends the time to reach 65% relative humidity to 12,250 years. However, results

for the cooler point-load packages are similar to those when no backfill is added.

Another problem we are concerned with is limiting large variations in local temperature at any given time throughout the repository. A wide variation in the temperature from one location in the repository to another will set up cold traps that concentrate moisture on the coolest packages. Because water can be driven from hotter packages to cooler packages, adding backfill in the point-load design will greatly extend the time during which water can be driven to the cooler packages and thus will adversely affect them. Also, to meet the DOE licensing requirements, we must test all materials to ensure they can withstand the conditions of a repository.

Figure 3. Temperature and relative humidity on the upper surface of the waste packages when backfill is emplaced at 100 years and the thermal conductivity is 0.6 watts per meter Celsius. Curves are plotted for (a,c) the point-load design and (b,d) the line-load design.

Thus, for a cost-effective licensing application process, we want to limit the range of temperatures in a repository to reduce the number of tests required.

In our previous simulations using averaged line loads, peak temperatures at the drift walls and the waste-package surfaces appeared to be limited to an acceptable range (Buscheck et al., 1995). However, when we used the updated model with individual package calculations, the peak temperature in the point-load layout is 540°C compared with 360°C for the line-load layout. Also, the large variation in the point-load temperatures throughout the repository sets up the cold traps we wanted to avoid.

Experimenting with the model, we found that with close spacing (0.1 meter) of waste packages, cooler waste packages act as thermal shunts, distributing the heat along the drift and approximating an averaged line load. This spacing eliminates the cold-trap effect and greatly improves the performance of the cooler packages. Such a design also allows us to make approximate calculations using an average line load, assuming that the hot and cool packages are interspersed—not grouped into cooler and hotter segments.

From this study, we found that the line-load design offers several advantages when compared with the point-load design. For example, the wide spacing of the drifts allows condensed water to drain through the rock pillars between the openings. The total length of the emplacement drifts is reduced up to 60%, which reduces the cost of building the repository. The line-load design uses significantly less backfill material—another cost saver—and because it results in a narrower range of temperature and relative humidity, fewer material tests are needed for licensing applications. In addition, heat and liquid-phase flow vary less throughout the repository, so performance analyses for licensing are less complicated than with the point-load design. All waste packages, including those

with cooler waste, benefit from the reduced relative humidity, and the probability of condensate flow entering the openings is decreased. Finally, the tendency for negative hydrothermal effects in certain overlying geologic units is decreased because of the water drainage, which also reduces the temperature near the ground surface.

Future Work

In 1997, we will focus on modeling the drift seepage potential at differing percolation flux. We also want to incorporate mountain-scale variability as well as drift-scale variabilities in the natural system. As a result of these and other modeling efforts, we will gain a better understanding of the performance of an engineered barrier system and its ability to contribute to the isolation of radioactive waste.

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References

- Buscheck, T. A. (1996), "Hydrothermal Modeling," Chapter 1 in D. G. Wilder, Ed., *Near-Field and Altered-Zone Environment Report*, Volume II, Lawrence Livermore National Laboratory, Livermore, CA, UCRL-JC-124998.
- Buscheck, T. A., J. J. Nitao, and L. D. Ramspott (1995), "Localized Dryout: An Approach for Managing the Thermal-Hydrological Effects of Decay Heat at Yucca Mountain," *Proceedings Materials Research Society XIX International Symposium on the Scientific Basis for Nuclear Waste Management* (Materials Research Society, Pittsburgh, PA, November 27–December 1, 1995). Also available from Lawrence Livermore National Laboratory, Livermore, CA, UCRL-JC-121232.
- Buscheck, T. A., J. J. Nitao, and L. D. Ramspott (1996), *Near-Field Thermal-Hydrological Behavior for Alternative Repository Designs at Yucca Mountain*, Lawrence Livermore National Laboratory, Livermore, CA, UCRL-JC-124629.
- Nitao, J. J. (1992), "The NUFT Code for Modeling Nonisothermal, Multiphase, Multicomponent Flow and Transport in Porous Media," *EOS, American Geophysical Union* 74(3), 3.

Update on the National Atmospheric Release Advisory Center

Thomas J. Sullivan

The National Atmospheric Release Advisory Center (NARAC) opened in February 1996 when Livermore's 22-year-old program, the Atmospheric Release Advisory Capability (ARAC), moved into its new, permanent facility. The NARAC facility, which also serves as headquarters for the Earth and Environmental Sciences Directorate, was designed to integrate all ARAC operations in an efficient and highly robust environment (Figure 1).

ARAC was originally established to help emergency managers in tracking the atmospheric dispersal of radiation from a nuclear test. Since then, the program has expanded to include atmospheric releases of many toxic materials. For example, ARAC supported emergency response efforts following the Three Mile Island and Chernobyl nuclear reactor accidents and during the Persian Gulf War.

Using our models, we can quickly assess the short-term consequences that toxic release would pose to the populations at risk, whether they be workers at an accident site or people living nearby. Such assessments help decision makers determine what early protective actions are needed, the size of the event, the area it will affect, and which of the many available measurement systems must be deployed to effectively monitor the event. ARAC models also can be used to estimate the quantity of radionuclides released, which helps to define boundaries on the scale of the event and thus on the size of the populations at risk and the potential economic impact.

Obviously, these actions must take place almost immediately, to minimize the dose or the health consequences to individuals. Thus, an ongoing part of ARAC's work is to

improve the timeliness and quality of initial assessments. This past year, 1996, was no exception. By combining a highly skilled operations staff with automated data-acquisition and consequence-modeling capabilities, ARAC typically delivers an initial assessment in graphical form in less than 30 minutes for any location in the world; the initial response for selected facilities operated by the U.S. Department of Energy (DOE) and the Department of Defense (DOD) is typically less than 15 minutes.

Expanding Our Capabilities

ARAC is in the midst of redesigning and upgrading its systems and models, with funding from the DOE's Defense Program, Office of Emergency Response. With this upgrade, the ARAC software system will be changed to a UNIX-based non-proprietary system environment that is vendor independent and can be readily adapted to high-performance processing. The new system incorporates the latest mature software tools and languages, improved graphical user interfaces, and three- and four-dimensional visualization graphics. It will be phased into the emergency operations center during 1997 and 1998.

Concurrent with this system upgrade, ARAC has incorporated modeling capabilities for assessing accidents that involve biological materials and toxic chemicals, both those from industrial accidents and those from possible chemical warfare. A basic technique for handling the so-called dense-gas simple physics required in such modeling was incorporated in the transport wind model interface used in our dispersion model. We also added scalable accident scenarios, such as pipe ruptures, evaporation pools, and tank vents. In support of this new capability, a substantial chemical properties and characteristics database was generated.

Several geophysical databases were updated to support the finer-scale requirements for modeling chemicals and biological agents. Refined topographic data were included in our global 500-meter emergency response database, and a 100-meter topographic database now covers a large fraction of the highly industrialized region of the world. Similarly, updated high-resolution digital map (Digital Chart of the World) features and TIGER data were added to ARAC's suite of mapping databases to provide greater detail and improve the accuracy across the spectrum of responses from local to global.

Meteorological data are the lifeblood of the ARAC real-time response. During 1996, we added data sources from the U.S. Navy and the National Oceanic and Atmospheric Administration, which greatly expanded the volume of global gridded data and improved our immediate response readiness. These data range in spatial resolution from 2.5 degrees $\times$ 2.5 degrees (latitude, longitude) to 1.0 degree $\times$ 1.0 degree and in temporal resolution from every 12 hours (2.5 degrees) to every 3 hours (1.0 degree) and eventually out to 72 hours in the future. These databases are updated every 12 hours. Finer-resolution gridded data—for example, 0.25 degrees for the North American region extending 48 to 60 hours into the future—are acquired every 12 hours. We also improved the database of international weather observations by adding a satellite-based international datafeed for redundancy and adapted our meteorological data decoder software to ingest a revised international data format.

A primary goal of the ARAC upgrade is to develop and validate a new class of diagnostic atmospheric flow and dispersion models. These models are being designed using numerical techniques that allow us to generate emergency assessments in any environment. The models can use all forms of

meteorological data, such as grids, observations, towers, and sounders, to formulate mass consistent flow fields in any geographic region, including highly complex terrain.

Variable meshing in the vertical and horizontal directions and a continuous surface representation preserve the essential detail near an emergency event. A new Lagrangian particle dispersion model that we coupled to the flow fields includes the identical terrain surface and gridding structure of an accident site, and incorporates random walk (and in the near future Langevin) diffusion physics. These two models significantly improve our capability to model short-term dispersal events with unsurpassed fidelity.

To address longer emergency events, we are acquiring a regional or mesoscale prognostic weather model. In 1997, we will test two models: the U.S. Navy Operational Regional Atmospheric Prediction System (NORAPS), which has been in operation for 10 years, and the Combined Ocean Atmosphere Mesoscale Prediction System (COAMPS), an evolutionary state-of-the-art physics model currently being tested by the Navy. NARAC's goal is to apply these models quickly, at very fine resolution any place in the world, so we can create 12-, 18-, and 24-hour emergency assessment projections for emergency response decision makers.

Great demands are placed on the ARAC modeling system for fast response times and continued model development. Thus, in 1996, we substantially increased the ARAC computer power and data storage capacity, an effort that will continue into 1998. Available processing cycles were increased by nearly an order of magnitude, and disk storage space was tripled. We also added capabilities for chemical accident response, improved graphic presentation to the workstations fielded at DOE and DOD facilities, and adapted the ARAC modeling system to a single workstation environment. In 1997, we

will evaluate a UNIX-based laptop system with cellular communications interface for field use.

Recent advances in the Internet offer new opportunities for emergency management information support. As a result, we submitted a proposal to DOE and the Federal Emergency Management Agency to create a NARAC-Internet interface, which would provide platform-independent access to our system for authorized emergency response agencies. With such a system, users could bypass the more costly and unique systems hardware requirements of ARAC's present onsite support architecture. This system also reduces the communication costs for emergency response, allows agencies to share platforms, and can be used with commercial technology.

Expanding the Scope

Because of the national concern regarding terrorism and the threat of nuclear proliferation, the ARAC operations staff is using our emergency response tools to support several projects in Livermore's National Security Programs, including the Nonproliferation, Arms Control, and International Security (NAI) Directorate. Many of the tools developed for industrial toxic chemical accidents are being adapted to address the threat of chemical weapons terrorism. Modeling the consequences from a release of biological agents presents new challenges, particularly regarding the form of the agent released and the atmospheric viability range of secondary conditions, such as temperature, moisture, and sunlight as well as each agent's deposition and attachment characteristics.

At present, the ARAC system is somewhat limited in terms of treating these secondary factors. Although such effects can be added to the current system, much of the work is classified, which imposes some constraints on where and how specific knowl-

edge can be incorporated. Consequently, in conjunction with the NAI Directorate, ARAC is developing a smaller, classified system for NAI's proliferation assessment program. This project is building on previous successes at Lawrence Livermore in developing workstation-based modeling systems, data-handling cluster architecture, geophysical databases, and integration of secure communications.

The Future at NARAC

The current upgrade of ARAC is providing the base to expand the emergency support that Lawrence Livermore can provide to other federal agencies, such as the Federal Emergency Management Agency, Environmental Protection Agency, Nuclear Regulatory Commission, and Department of Transportation. Under the National Response

Figure 1. The National Atmospheric Release Advisory Center. By combining a highly skilled operations staff with automated data-acquisition and consequence-modeling capabilities, NARAC is equipped to quickly assess the initial, short-term consequences of a toxic release to the atmosphere.

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Plan, each of these departments or agencies has basic responsibilities to minimize accident consequences and assist state and local governments in emergency management. In an effort to provide immediate technical assessment following an emergency, ARAC's goal is to deliver information through the Internet (or similar links) to all key agencies.

Because of our success, several international programs are interested in collaborating with ARAC to provide a system for exchanging information concerning nuclear power plant accidents. We are working with scientists from the Japan Atomic Energy

Research Institute, under the umbrella of a G-7 initiative entitled GEMINI—Global Emergency Management Information Network Initiative—to evaluate an Internet-based information exchange interface protocol. In addition, the Commission of the European Community has asked ARAC to collaborate in developing a nuclear accident decision support system. Other requests for international collaboration are being evaluated by the Department of Energy.

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Seismic Characterization of the Middle East and North Africa for Test Ban Monitoring

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The Comprehensive Test Ban Treaty (CTBT), recently signed by President Clinton and the leaders of most of the world's nations, will ban all nuclear explosions worldwide. Data for monitoring compliance with the treaty will be transmitted from automated stations all over the world to international and national data centers for analysis. Both international and national monitoring stations will be used. The U.S. Department of Energy has a major responsibility for conducting the research and development necessary for the U.S. National Data Center to meet the nation's monitoring goals.

Since seismic records are the most tell-tale signs of an underground explosion, a key component of the monitoring system will be a global network of seismic monitoring stations. For data to be interpreted correctly, the system must include a database of the normal seismic activity and the underlying geologic features of the region of interest. A team of geophysicists, geologists, and computer modeling experts from Lawrence Livermore's Earth and Environmental Sciences Directorate, supporting the Nonproliferation, Arms Control, and International Security Directorate, is collecting data and developing computer models to characterize these parameters for the region of the Middle East and North Africa.

The Monitoring Goal

Our goal is to provide the U.S. National Data Center with the necessary calibrations,

data, and models to reach the nation's goals for detecting, locating, and identifying seismic events originating in the Middle East and North Africa. First, researchers must be able to find an event in a stream of background noise and determine where that event occurred. Then they must be able to classify the event as an earthquake, as some other explainable phenomenon such as a mining explosion, or as a possible nuclear explosion.

Tests of large-yield nuclear weapons produce seismic signals that, when recorded, are easy to identify. However, under the CTBT, potential violators may try to evade detection by detonating a low-yield device, or they may attempt to alter the seismic signal by detonating a device in the center of an underground cavity to decouple it from the surrounding rock. Because the seismic energy produced from decoupled explosions is much less than the energy from explosions conducted non-evasively, the signals are harder to detect. These low-energy signals are detected only at so-called regional distances (less than 2000 kilometers from the source); they do not propagate well to teleseismic distances (more than 2000 kilometers).

Because so many mining events and earthquakes are similar in magnitude to a small nuclear explosion, a monitoring system designed to detect small events will be flooded with data. (More than 200,000 seismic events at these levels occur in the world every year.) To provide a means of picking out the possible nuclear explosions from all the other events, we are developing region-specific procedures for event analysis and discrimination so events can be located and identified with greater accuracy.

This *regionalization* research includes analyzing seismograms to determine how seismic waves travel and attenuate in a region, as well as how propagation through

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that region affects the relative strengths of various parts (phases) of the wave. Calibrations must be based on seismograms collected from events that have adequate ground-truth measurements—that is, events

for which the location, origin time, and source type are well known. Calibrations of signal travel time demand the most accurate ground-truth information, especially about an event's epicenter, depth, origin time, and type.

(a) Sonseca, Spain, station results

(b) Belbasi, Turkey, station results

Figure 1. Travel-time residuals for events recorded at stations (triangles) in (a) Sonseca, Spain, and (b) Belbasi, Turkey. These residuals indicate the need for point travel-time corrections. Some patterns emerge: here, *P* phases from events in the Greek Isles and the Aegean arrive earlier at the station array in Sonseca than at the station in Belbasi. Travel-time calibrations to correct for these differences are necessary for the location algorithms to be used by the treaty-monitoring data centers.

The Challenge

Seismic waves from the small events of interest to CTBT monitoring travel through the structurally complex crust and upper mantle of the earth. The calibration task in the Middle East and North Africa is complicated by the variety of geophysical structures within the area. These structures range from relatively simple, stable cratonic and platform regions in North Africa and Saudi Arabia to complex tectonic provinces—subduction (continental collision) zones in the Mediterranean, orogenic (mountain) belts in Iran, and major fault zones in Turkey.

The principal challenge in characterizing the area is the uneven distribution of seismic event data for calibration. The region divides into seismic and aseismic areas. The seismic belts—the tectonic regions—have an excess of events suitable for calibration, the aseismic areas virtually none. Announced nuclear explosions and mining explosions provide the best calibrations, but nuclear explosions are rare in the Middle East and North Africa. We also do not know whether the many mines in the area produce explosions that are large enough for the monitoring system to detect.

Not only does the distribution of seismic events pose a problem, but data collection is also a formidable challenge. The region has few accessible seismic stations (those from which data are readily available; other stations exist, but they belong to closed networks and the waveform data are nearly unobtainable).

To help meet this challenge, we are collecting data on large earthquakes (magnitude greater than 5) with estimates of depth, epicenter, and mechanism, largely from existing seismic catalogs. The total data available exceed 16,000 individual waveforms representing 1300 events. In seismically active

regions, these data form the basis for calibration, which is our initial focus.

Empirical Calibrations

Travel-Time Calibration. We are beginning with travel-time calibration of four proposed primary monitoring stations located at Sonseca, Spain; Belbasi, Turkey; Alibek, Turkmenistan; and Tehran, Iran. We are systematically timing the arrival of the P phases of seismic signals (the parts of the signal arising from compressional waves) recorded by stations in our study area to generate bulk station corrections, point corrections for specific source regions, and average velocity models for each station. Figure 1 shows the travel-time residuals (that is, the observed arrival time minus the arrival time predicted by a global model) for two monitoring stations. Note that signals from events in Greece and the Aegean arrive earlier at the station in Sonseca than at the station in Belbasi. These patterns must be determined station by station for each region of interest.

Once the principal phases are timed, we plan to automate measurements of phase amplitude, surface-wave dispersion, back-azimuth, incidence angle, and phase velocity. The objective is to develop corrections for these quantities so we can refine the calculations for phase identification, association, magnitude estimation, and discrimination. For example, a pilot study for the station array at Sonseca shows that corrections are needed for a pronounced azimuth bias (northward) for P waves arriving from the east and a slight bias (fast) for P phase velocity estimates.

Phase-Propagation Characterization. The simplest phase calibrations are maps of regions that block the propagation of a seismic signal's phases. Figure 2 shows blockage of the L_g phase, a segment of the signal arising from shear waves that propagate through multiple reflections in the earth's crust. The relative amplitude of the L_g phase to the P phase is one measure used to discriminate between earthquakes and underground nuclear tests. L_g waves generally fail to prop-

agate across the Mediterranean Sea, and severe L_g attenuation appears to correlate with the length of the path in oceanic crust. Loss of this phase poses a significant problem for identification and shows the need for reliable monitoring stations on the African continent to discriminate events in North Africa. Furthermore, L_g propagation through the African craton appears to be especially efficient, suggesting that fewer stations may be required there than in more tectonically active regions.

Calibrations Using Modeling

Numerical modeling clarifies where corrections are needed and allows us to extrapolate them into aseismic areas. For this approach to be successful, we need accurate geophysical and geological models of the regions. One method of obtaining a geophysical model of the large, mostly aseismic region

Figure 2. Path characterization in the study area showing significant L_g blockage for most paths crossing the Mediterranean Sea, which is a significant problem for monitoring. Yellow lines denote efficient L_g propagation, red lines poor propagation. Reliable stations will be needed on the African continent before we can identify seismic events in North Africa.

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Figure 3. Example of waveform modeling to estimate velocity structure in an aseismic region. (a) The magnitude-5.3 event (red circle) in Tunisia was recorded 1288 kilometers away at station TAM (black triangle) in Algeria. Synthetic seismograms were calculated for a series of simple four-layer velocity structures (such as the one in b) until (c) a reasonable match between synthetics and data was obtained. (Here, we use P_{nl} , Rayleigh, and Love waves, which are dispersive surface waves.) Once the velocity structure is known, waveform modeling can be used to refine the source mechanism, depth, and location of smaller events.

of North Africa is by inverse waveform modeling. Our general approach is to use large events with locations and source mechanisms that are well constrained by teleseismic networks. Once the source and location are known for a given event, the waveform at a given regional station is primarily a function of the velocity structure, which we solve for using a one-dimensional synthetic seismogram code to give a least-squares fit to the waveform.

Figure 3 shows an example of this procedure for a Tunisian earthquake recorded at a monitoring station in Algeria. We determined the crustal thickness to be 40 kilometers and characterized some detail on the velocity structure of the crust. With many such profiles, we can begin to obtain one estimate of the velocity structure of North Africa. When we combine this information with studies of other parameters (for example, surface-wave dispersion and gravity), we can begin to piece together a geophysical model. Then we can use this composite model as input to a synthetic seismogram code to compute travel-time curves and the other data needed for calibration.

Future Work

In 1996, we collected the data available for the Middle East and North Africa and began interpreting them to calibrate the regions around key monitoring stations. In the future, many other types of data (such as receiver functions and surface-wave group velocity) and innovative methods of tomography and structural inversion will be necessary to characterize the aseismic portions of the area. By deploying temporary stations and arrays, we may be able to acquire the data necessary for determining geophysical structure before permanent stations are installed.

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Measuring Chemical Uptake through the Skin

Garrett A. Keating, Kenneth T. Bogen, and John S. Vogel

In studies of environmental contamination, one area of concern is low levels of hazardous chemicals in the soil and groundwater. Scientists are trying to determine how humans are exposed to these agents and in what magnitude. The goal of these studies is to characterize the multiple pathways by which a chemical released into the environment can be transported into the human body. By comparing the estimated chemical dose to which humans are exposed with the doses that cause biological effects in animals, we can determine the risk these chemicals pose to the population at large.

Researchers have often considered consumption of contaminated water to be the dominant pathway by which groundwater contaminants enter the body. Recent studies, however, indicate that chemicals absorbed through the skin from household water usage may represent a major pathway for human uptake—in some cases, one that may exceed the amount of chemical ingested by drinking water. In light of these findings, a major review of regulatory guidelines for dermal absorption is under way. In the Earth and Environmental Sciences Directorate, we are contributing to this review by evaluating the accuracy of the prediction methods. We also are using Lawrence Livermore's expertise in accelerator mass spectrometry to refine the estimates of dermal uptake and thus help reduce the risks of exposure.

Skin Physiology and Structure

Our skin performs important respiratory, immunological, and metabolic functions for the body. As shown in the simple cross section in Figure 1, skin is composed of two layers: the epidermis and the dermis. The

epidermis, a nonvascular layer about 100 micrometers thick, is generated from the basal membrane that separates it from the dermis, a highly vascularized layer about 1000 to 3000 micrometers thick. Cells proliferate from this membrane and grow outward until they are ultimately shed at the skin surface. During this differentiation, epidermal cells extrude their contents and take on a flattened, densely packed morphology, forming a distinct cell layer at the surface of the epidermis known as the *stratum corneum*.

The structure of the *stratum corneum* can be likened to brick and mortar, consisting of a 10- to 20-micrometer layer of dead, flattened cells (the bricks), each surrounded by a lipid matrix (the mortar). This matrix is considered to be the layer that determines how quickly chemicals diffuse through the skin. Although

Figure 1. Cross section of human skin (Montagna et al., 1992). SC = *stratum corneum*, which is about 10 micrometers thick; E = epidermis (100 micrometers thick); D = dermis (200 micrometers thick); C = blood capillaries; HF = hair follicle; and SG = sebaceous gland. (Reprinted courtesy of Springer-Verlag, New York.)

the *stratum corneum* is no greater than 20 micrometers in thickness, the actual diffusion pathway through its lipid channels is thought to be about 400 micrometers (Guy and Hadgraft, 1988).

Traditional Measurement of Skin Permeability

Skin permeability is typically measured with either excised skin from animals or on human skin taken in an autopsy, using a two-chambered apparatus known as a diffusion cell. For such measurements, the tissue is positioned between the two chambers of the diffusion cell, and tissue culture media (a surrogate for perfused blood) is circulated underneath the exposed skin tissue. A high concentration of chemical is applied to the skin surface, and its appearance in the culture media is assayed over time. The chemical's permeability through skin is then determined at its steady state—that is, after its rate of diffusion into the tissue media is constant. A permeability coefficient (K_p , measured in centimeters per hour) is used to measure this constant rate of diffusion through skin. Typically, determination of K_p requires experiments that last several hours because sufficient time is required for the chemical concentration in the skin to reach equilibrium with that in the exposure solution.

Using this traditional approach to examine dermal uptake under true environmental conditions has some drawbacks. To achieve detectable levels of the chemical in the underlying media, we must apply compounds to the skin in high concentrations in a solvent (typically acetone) that facilitates chemical partitioning into skin. In the environment, however, skin is exposed to contaminants in soil or water at much lower concentrations. In particular, for a widespread class of environmental contaminants called volatile organic compounds (VOCs), skin permeability experiments are problem-

atic because these chemicals tend to vaporize from solution. Understanding the skin permeability of VOCs is important because many of them are suspected human carcinogens and are commonly found in groundwater and soil.

Use of Permeability Data in Risk Assessment

By using a chemical's K_p , its concentration in the environment, and the surface area and duration of dermal exposure, we can estimate the mass of chemical absorbed through the skin from the environment. For example, with this traditional approach, if K_p for trichloroethylene (TCE) is estimated at 0.016 centimeters per hour, an adult (with an average surface area of 20,000 square centimeters) who showers for 10 minutes in water containing 5 micrograms per liter of TCE would absorb 1.6 micrograms of TCE. For comparison, the same person drinking 2 liters of the same water would ingest 10 micrograms of TCE, assuming that 100% of the TCE is absorbed from the gastrointestinal tract.

Recent studies indicate that this approach may significantly underestimate the total exposure. Because skin permeability has been determined for only a few environmental contaminants, K_p values for these chemicals must be estimated from regression equations based on K_p values of other compounds. But K_p traditionally measures the rate of chemical transport through the skin only *after* chemical equilibrium is established between water and skin. Therefore, this method underestimates the total chemical uptake during the initial, non-steady-state period in which chemical is *both* entering the skin *and* exiting to underlying tissues. As a result, traditional K_p measurements do not account for chemical that has penetrated the skin but has not yet diffused into blood. This reservoir of chemical will ultimately enter the blood at some time after exposure has ended,

so permeability measurements that do not account for this absorption will underestimate total exposure.

A report from the U.S. Environmental Protection Agency (EPA, 1992) suggested that for certain contaminants this underestimation may be substantial, particularly for exposures that are relatively short, such as bathing in contaminated water. Thus, the EPA proposed a new method for estimating dermal absorption. Using the EPA's proposed approach, we would expect chemical doses absorbed through the skin to exceed the dose ingested by drinking 2 liters of water only for those chemicals whose K_p values exceed 0.1 centimeters per hour.

A great deal of uncertainty surrounds this new approach because few experimental measurements are available to address the issue of short-term dermal absorption into skin. In a recent analysis, permeability estimates for nine chemicals based on *in vivo* data from the few studies that used live animals or human volunteers were compared to corresponding estimates derived from equations developed by the EPA from a larger set of traditional K_p measurements obtained using diffusion cells (Bogen, 1994). This study revealed that the *in vivo* K_p estimates were all greater, by about fivefold, than corresponding estimates obtained using the EPA's proposed approach (Bogen, 1994). This discrepancy highlights the importance of resolving fundamental uncertainties concerning dermal uptake of environmental chemicals.

Skin Uptake Measurements at LLNL

In research at Livermore's Health and Ecological Assessment Division, we are trying to measure dermal uptake at experimental conditions more relevant to human exposure. In one of our studies, we measured the chemical loss from dilute solutions of carbon-14 (^{14}C) radiolabeled TCE, perchloroethylene, and chloroform, into which hairless

guinea pigs had been partially submerged for 1 hour (Bogen et al., 1992). The implied K_p values for all three compounds exceeded 0.1 centimeters per hour and were a factor of 10 to 20 greater than corresponding traditional K_p estimates.

We also found that chemicals may be absorbed into skin more quickly than previously expected (Bogen et al., 1992, 1994). Therefore, in 1996, we expanded our research to examine skin absorption at even lower concentrations and for shorter exposure times (Bogen et al., 1996). For this study, we used accelerator mass spectrometry (AMS), a highly sensitive analytical method for which many environmental and biomedical applications have been invented and developed at the Laboratory.

Figure 2. Uptake of dilute (about 5 parts per billion) aqueous ^{14}C -radiolabeled trichloroethylene into full-thickness human skin obtained within 48 hours of surgery, as a function of exposure time. Fits to these data are shown for our physiologically based pharmacokinetic model of skin (LLNL) and for a model of dermal uptake for short-term exposure developed by the U.S. Environmental Protection Agency (EPA).

AMS is an isotope-ratio mass-spectrometry method for quantifying radioisotopes independent of their decay times. For ^{14}C , AMS has a sensitivity in the range of one part in 10^{12} to 10^{15} . With this unique capability, researchers have examined dermal exposures as brief as 1 minute with chemical concentrations between 1 and 5 parts per billion (ppb). Using human skin freshly obtained from surgery, we measured the dermal uptake of ^{14}C -labeled TCE at 5 ppb (or 5 micrograms per liter) at intervals ranging from 1 to 60 minutes. Chemical uptake was determined by taking small cores from the skin and analyzing for ^{14}C with AMS.

Our results indicate that TCE uptake exhibits simple "first-order kinetics," by which uptake initially occurs at an approximately constant rate and then declines in an apparently exponential way (Figure 2). The K_p value estimated from these results (the initial linear slope in Figure 2) is 0.28 centimeters per hour, essentially the same as that measured in the *in vivo* guinea pig study (0.23 centimeters per hour, Bogen et al., 1992). In contrast, our measured uptakes were significantly greater than values predicted by the EPA's proposed model. After 10-minute exposures (corresponding, for example, to the exposure from a typical shower), the EPA model underpredicts the measured *in vitro* uptakes of TCE into human skin by a factor of about 5.

Additional *in vitro* and *in vivo* studies with other compounds are clearly needed to determine whether these models adequately predict human dermal exposures to a wide range of water contaminants. In related work supported by the EPA, we are conducting additional AMS-based studies on dermal uptake of several contaminants from soil and dust at environmentally relevant conditions. AMS sensitivity will allow experiments with soil contaminants at actual skin soil levels measured in humans (between 0.1 and

1 milligram per square centimeter) and with multiple soil contacts, analogous to the daily exposure with contaminated soil that occurs in the environment.

Conclusion

An important consequence of these findings is that current dermal risk assessments may underpredict the amount of daily dermal intake from low-level exposures to environmental contaminants, in some cases by a substantial amount. Our research indicates that AMS measurement of chemical uptake may provide a reliable, and relatively inexpensive, way to obtain permeability measurements that can be used to assess exposure and risk. In addition, AMS can be used to evaluate the low-dose toxicity of environmental contaminants, another large source of uncertainty in risk assessment.

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References

- Bogen, K. T. (1994), "Models Based on Steady-State *In Vitro* Permeability Data Underestimate Short-Term Dermal Exposures *In Vivo*," *J. Expos. Assess. Environ. Epidemiol.* **4**, 457-476.
- Bogen, K. T., B. W. Colston, and L. K. Machicao (1992), "Dermal Absorption of Dilute Aqueous Chloroform, Trichloroethylene, and Tetrachloroethylene in Hairless Guinea Pigs," *Fund. Appl. Toxicol.* **18**, 30-39.
- Bogen, K. T., G. A. Keating, S. Meissner, and J. S. Vogel (1996), *Non-Steady-State In Vitro Kinetics for Uptake of Dilute Aqueous Chloroform and Trichloroethylene into Human Skin*, Lawrence Livermore National Laboratory, Livermore, CA, UCRL-JC-125647.
- Guy, R. H., and J. Hadgraft (1988), "Physicochemical Aspects of Percutaneous Penetration and Its Enhancement," *Pharmaceutical Res.* **5**, 753-758.
- Montagna, W., A. M. Kligman, and K. S. Carlisle (1992), *Atlas of Normal Human Skin* (Springer-Verlag, New York), p. 4.
- U.S. Environmental Protection Agency (EPA) (1992), *Dermal Exposure Assessment: Principles and Applications*, U.S. EPA Office of Environmental Assessment, Washington, DC., EPA/600/8-91/011B.

Resources: An Overview of the Earth and Environmental Sciences Directorate

In establishing the Earth and Environmental Sciences Directorate, Lawrence Livermore provided a focus for ongoing research programs and enabled a strategy to address new Laboratory missions. Specifically, the directorate's mission is to assess and mitigate environmental and human risk from natural and manmade hazards and to develop and demonstrate new tools and technologies for environmental restoration. To achieve these goals, the management team for Earth and Environmental Sciences assessed the best use of existing facilities and funding to support the sustaining missions under our responsibility and the credible missions we could develop. The directorate's success is

directly related to our primary resources: talented scientists and engineers working in high-quality research facilities.

Workforce

Our directorate employs nearly 300 people (Figure 1). Of this total population, about 70% are scientists and engineers with a wide range of specialties, which are listed in Table 1. In addition, this workforce is complemented by personnel from other Livermore organizations, such as Engineering and Computation, who are assigned to support the directorate's mission. The total number of people working within Earth and Environmental Sciences makes this one of the largest environmental research organizations in the nation.

(a) Total workforce for Earth and Environmental Sciences

(b) Scientists and engineers in Earth and Environmental Sciences

Figure 1. Workforce breakdown for Earth and Environmental Sciences. (a) Total workforce is about 300 employees, of which (b) about 200 are scientists and engineers.

Table 1. Discipline specialties within the Earth and Environmental Sciences Directorate.

Discipline	Research specialties
Physics	Accelerator applications, astrophysics, atomic, computational, theoretical, materials, biophysics, and geophysics. Staff also include specialists in meteorology, atmospheric science, seismology, hydrology, geology, climatology, and oceanography.
Chemistry	Isotope, theoretical, nuclear, organic, biochemistry, and geochemistry. Staff also include specialists in marine chemistry and chemical ecology.
Life sciences	Environmental science, environmental health, forestry, biology, plant science, toxicology, water resources, wildlife and fishery biology, and zoology. Staff also include a medical doctor, an environmental lawyer, a geographer, and an economist.
Engineering	Mechanical, geological, geotechnical, electrical, environmental, and chemical engineers. Staff also include specialists in mining, applied science, and cybernetics systems.

Funding

The directorate's workforce supports a diverse set of programs and projects (Figure 2). In 1996, the total budget from all funding sources was \$71.5 million, including a \$4.0 million allocation from the Laboratory Directed and Research Development Program and a \$1.5 million allocation for General and Administrative (G&A) costs. Several programs at the U.S. Department of Energy sponsor our projects directly, with \$28.4 million in 1996. These programs include Environmental Restoration and Waste Management, Energy Research, Defense Programs, Environmental Safety and Health, International Affairs, and Nuclear Reactors. We also received about \$10.5 million in support of Work for Others, including funding from Department of Energy field offices and integrated contractors; from other federal agencies, such as the U.S. Navy, Air Force, and Department of Defense and the National Aeronautics and Space Administration

(NASA); and from private industry and universities, such as California State University. In addition to direct funding to this directorate, in 1996, we received \$27.1 million from the Department of Energy through other Livermore directorates for work on such projects as Treaty Verification and the proposed repository at Yucca Mountain, Nevada.

Listing the funding sources for Earth and Environmental Sciences does not describe the diverse nature of our research. Thus, in Figure 3, we show the breakdown of funding by project or program.

In recent years, Livermore has streamlined its management and financial practices to reduce infrastructure costs and make procedures less cumbersome. The Laboratory also has revised its procurement practices to expedite purchasing and reduce costs. In a review by Livermore's Cost-Cutting Initiative Team, the infrastructure for the Earth and Environmental Sciences Directorate was found to be efficient and cost effective. Our commitment to reducing infrastructure costs has led to decreases in G&A spending, procurement charges, and overhead costs and rates.

Facilities

When this directorate was formed in 1994, the inherited facilities were delegated along organizational lines, a plan that was

Figure 2. Breakdown of funding for Earth and Environmental Sciences in 1996 (in millions of dollars). (a) Funding received directly from the Department of Energy totaled \$28.4 million. (b) Funding received in work for others totaled about \$10.5 million. (c) Funding received to support other Lawrence Livermore programs totaled \$27.1 million.

not only inefficient but also offered little room for growth. The challenge we faced in consolidating space was how to balance the available funds for facilities with plans for the future operations of the directorate. Thus, our goal was to consolidate these facilities to improve the directorate's operations and its programmatic capabilities while minimizing one-time moving expenses and recurring overhead costs.

In 1996, we reached a significant milestone toward this goal, when the directorate headquarters relocated into the new facility commissioned for the National Atmospheric Release Advisory Center. As a result of our improved facilities management, we reduced overhead space-charge costs for this directorate from \$1.8 million to \$1.2 million. We also improved our use of the available space and thus the efficiency of our operations, and by vacating obsolete buildings, we reduced the directorate's maintenance burden. Figure 4 shows our 1994–1996 accomplishments in reconfiguring and optimizing the directorate's facilities. In both office space and net space per person housed, we are below the Laboratory averages. The directorate's six primary facilities are described in Table 2.

In the future, we plan to complete the consolidation process and release any remaining underused or low-quality space. We also plan to improve the capabilities of key facilities to enhance programmatic success. As a result, we hope to continue to be one of Livermore's lead organizations in cost control and efficient business operations.

Organization

Figure 5 shows the organization of Earth and Environmental Sciences. The major components are the four divisions, which contain the scientific and support staff and have principal responsibility for the execution and maintenance of disciplinary science; the project organizations, which execute focused missions for this directorate and others at Lawrence Livermore; and the infrastructure activities, which we execute as stewards of a research organization. Each of these three

Figure 3. Breakdown of 1996 funding by program or project. Amounts are in millions of dollars. ARAC = Atmospheric Release Advisory Capability, PCMDI = Program for Climate Model Diagnosis and Intercomparison, and CAMS = Center for Accelerator Mass Spectrometry.

Figure 4. Consolidation of facilities in Earth and Environmental Sciences between 1994 (green) and 1996 (purple). We are now at acceptable norms for the directorate to function smoothly, and our office and laboratory space per employee are below the Laboratory averages.

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 other geographically separate facilities
 Includes both wet and dry chemistry, laser, and high-pressure laboratories and support space

Expedited Technology Demonstration Project, Building 292

3,500-square-foot facility
 Currently under construction in a previously underused portion of Building 292
 Used to study performance of an integrated molten salt oxidation (MSO) system including primary unit, offgas, and salt recycle subsystems
 Construction completion and subsequent startup scheduled for May 1997

Geoscience Technologies Laboratories, Building 243

18,000-square-foot facility
 Includes both wet and dry chemistry, laser, and high-pressure laboratories, as well as 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, the Environmental Technology program, 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
 Integral technology to the Accelerated Site Cleanup project

Figure 5. Organization of the Environmental Programs Directorate.

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 safe, cost-effective, and agile in the current climate of national science and technology. A point particularly worth noting is the correlation between Figure 5 and the breakdown of funding shown in Figure 3. The project organizations control a major fraction of the directorate's resources. The mission and capabilities of each division are described on the following pages.

Atmospheric Science Division

The mission of the Atmospheric Science Division is to expand scientific understanding of how Earth's atmosphere, oceans, and bio-

sphere respond to the anthropogenic and natural disturbances that contribute to environmental risk. To meet the demands of contemporary environmental problems, the division maintains expertise in:

- Atmospheric dynamics, chemistry, and physics.
- Ocean dynamics, transport, and biogeochemistry.
- Mesoscale atmospheric prediction, transport, and dispersion.
- Hydrology and terrestrial ecology.
- High-performance computing and computational physics.

This expertise is combined with the best available environmental simulation models, observational and real-time datasets, and computing resources to examine a range of

problems. For example, our studies include the transport and dispersion of hazardous 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 regional-scale variations in hydrological processes. The division also provides the technical staff for two major programs: the Atmospheric Release and Advisory Capability, and the Program for Climate Model Diagnosis and Intercomparison.

For more information on Atmospheric Science, contact the division leader Bill Dannevik (510) 422-3132 (dannevik1@llnl.gov).

Health and Ecological Assessment Division

The mission of the Health and Ecological Assessment Division is to perform research in the health, ecological, and measurement sciences that supports assessments of toxic and radioactive substances released to the environment. An important asset of this division is a unique set of research facilities, which include

- Laboratories for processing soil and vegetation samples for subsequent analysis.
- Alpha and gamma spectrometry for determining low levels of radionuclides in environmental media.
- Gas chromatography and high-performance liquid chromatography for measuring various organic compounds in different media.
- Atomic absorption spectrometry for analyzing metals.
- Accelerator mass spectrometry and proton-induced x-ray fluorescence for quantifying selected nuclides (such as ^{14}C , ^{129}I , ^{36}Cl , ^{59}Ni) and elemental distributions.
- Three-dimensional imaging capabilities for determining the transport processes that occur at microscopic scales in porous media.

In addition to these research facilities, we offer expertise in various disciplines and can

augment our work through collaborative relationships with researchers at other institutions. In our research, we have developed risk models to assess how and when humans are exposed to radionuclides and to chemical and organic pollutants. We can determine what risk these pollutants pose to humankind as well as how organ and cellular systems will respond to them. We also perform detailed studies of ecological risk assessment and environmental toxicology, and we can develop remediation plans for cleaning up organic contaminants. We are equipped to characterize pollutant-transport processes and to measure the resuspension of contaminants deposited on soil. We also offer an expertise at conducting large-scale field programs, developing remote-sensing technology, and developing environmental databases and geographic information systems.

For more information on Health and Ecological Assessment, contact the division leader Dave Layton (510) 422-0918 (layton1@llnl.gov).

Geosciences and Environmental Technology Division

The mission of the Geosciences and Environmental Technology Division is to conduct basic and applied research to solve problems involving the geochemistry, geophysics, and flow and transport properties of the Earth's near-surface and to develop or improve the nation's waste-disposal and waste-processing technologies. The division's research is focused in five basic areas:

- Subsurface characterization, which includes developing new geophysical and electromagnetic methods for characterizing the physical and chemical properties of the shallow subsurface, and identifying and mapping contaminant plumes.
- Subsurface remediation, including novel techniques developed for the accelerated *in situ* cleanup of subsurface contaminants as well as integrated assessment and cleanup strategies.

- Nuclear waste disposal, including characterization and modeling of the thermally perturbed geochemistry, hydrology, and transport mechanisms of high-level nuclear waste repositories. We also design and test different disposal plans and model how various nuclear waste forms will react once placed in a repository.

- Waste processing technologies to develop and test systems that provide alternatives to incineration for treating and stabilizing mixed, hazardous, and nuclear wastes.

- Basic geosciences, such as studying the dissolution kinetics of minerals and glasses and the thermodynamic and transport properties of aqueous geochemical systems; modeling the kinetics of oil and gas formation; developing geologic information systems; and applying cosmogenic isotopes as tracers and age-dating tools.

For more information on Geosciences and Environmental Technology, contact the division leader Ken Jackson (510) 422-6053 (jackson8@llnl.gov).

Geophysics and Global Security Division

The mission of the Geophysics and Global Security Division is to conduct basic and applied research and development to characterize the physical and chemical properties within the solid Earth and to describe how these properties affect the environment, national security, public health and safety, and industrial needs. We then apply these results to address significant problems both for the nation and the State of California. This division offers a wide range of discipline strengths and resources that allow us to make major contributions both to the work of the Environmental Programs Directorate and to that of the Laboratory at large. The division's primary areas of research are

- Seismology, including regional and teleseismic seismology, signal processing for verification activities in support of comprehensive test ban, and wave propagation codes.

- Computational physics, including shock physics, computer modeling, information sciences, weapons physics, and theoretical and applied mechanics.

- Experimental geophysics, including synthesis of materials, rock mechanics, porous flow, physical and chemical properties of rocks and cementitious materials, high-pressure and high-temperature measurement capabilities, and experimental design.

- Geophysical site characterization, including theoretical and applied geophysics, geomechanics, engineering, containment science, field programs, earthquake hazards, and instrumentation.

For more information on Geophysics and Global Security, contact the division leader Jim Hannon (510) 422-3921 (hannon2@llnl.gov).

Outreach and Collaboration

Research and development in the earth and environmental sciences is broadly spread across both sponsoring federal agencies and the academic, industrial, and national laboratory organizations working in this area. Unlike the weapons and nuclear-related energy programs, no one agency or organization dominates this area, and expertise is widely distributed. Thus, to access expertise outside this directorate and to leverage our own capabilities, we actively seek collaborations. This exposure to the large outside community also serves to validate our excellence and expose our weaknesses, to teach us the strengths of other groups at the earliest stages of their development, and to similarly reveal our strengths to those who might not have inferred them from more formal activities such as publication and workforce proceedings.

Major components of outreach in 1996 include the following:

- Participation in approximately 170 ongoing and new collaborations with external researchers.

- Visits to this site by more than 60 faculty and student visitors for stays of over a week and similar visits by 74 non-academic visitors.

Resources

- Work on this site by nearly 60 students in eight work-study programs.
- Organization or hosting of about 37 conferences or workshops.
- Tours of our facilities, predominantly ARAC and CAMS, given to 170 groups.
- Participation by more than 100 directorate employees on major committees and review panels, in visiting lecturer appointments, and as journal associate editors and reviewers.

Although the directorate does not establish specific measures for employee participation or performance in these areas, such participation is considered when evaluating an employee's professional development and contribution to public and peer understanding of the Laboratory's missions and capabilities. Communicating our strengths and values is essential for the continued growth of the directorate, as are our efforts to absorb external views and to pursue developments for renewal and change.

Publications

- Aminzadeh, F., N. R. Burkhard, J. Long, T. Kunz, and P. Duclos (1996), "Three Dimensional SEG/EAGE Models—An Update," *Leading Edge* (February), pp. 131–134.
- Amthor, J. S. (1996), "Global Carbon-Cycle Modeling," *Int. J. Environmentally Conscious Design Manufacturing* 5(3–4), 123–128.
- Amthor, J. S. (1996), *A Model of Tree-Leaf Stomatal Conductance*, Lawrence Livermore National Laboratory, Livermore, CA, UCRL-AR-125338.
- Amthor, J. S. (1996), *Models of Plant Growth Costs and Their Application to Trees in Walker Branch Watershed*, Lawrence Livermore National Laboratory, Livermore, CA, UCRL-AR-125547.
- Amthor, J. S. (1996), *Models of Solar Elevation, Daylength, and Above-Forest Radiation Applied to Walker Branch Watershed*, Lawrence Livermore National Laboratory, Livermore, CA, UCRL-AR-125629.
- Amthor, J. S. (1996), *Predictive Models of Crop Responses to Temperature and CO₂ Concentration: Respiration and Photosynthesis, Including Acclimation*, Lawrence Livermore National Laboratory, Livermore, CA, UCRL-JC-123721.
- Amthor, J. S., and G. W. Koch (1996), "Biota Growth Factor β : Stimulation of Terrestrial Ecosystem Net Primary Production by Elevated Atmospheric CO₂," in *Carbon Dioxide and Terrestrial Ecosystems*, G. W. Koch, and H. A. Mooney, Eds. (Academic Press, Inc., New York), pp. 399–414.
- Amthor, J. S., and R. S. Loomis (1996), "Integrating Knowledge of Crop Responses to Elevated CO₂ and Temperature with Mechanistic Simulation Models: Model Components and Research Needs," in *Carbon Dioxide and Terrestrial Ecosystems*, G. W. Koch, and H. A. Mooney, Eds. (Academic Press, Inc., New York), pp. 317–345.
- Anspaugh, L., and J. I. Daniels (1996), "Bases for Secondary Standards for Residual Radionuclides in Soil and Some Recommendations for Cost-Effective Operational Implementation," *Health Phys.* 70, 722–734.
- Anspaugh, L. R., D. Hickman, J. Lucas, I. Proctor, T. Sullivan, T. Straume, and W. Robison (1996), "Assessing Exposure to Radiation," in *Science and Technology Review*, Lawrence Livermore National Laboratory, Livermore, CA, UCRL-52000-97-1/2, pp. 14–21.
- Barnett, T. P., B. D. Santer, P. D. Jones, R. S. Bradley, and K. R. Briffa (1996), "Estimates of Low-Frequency Natural Variability in Near-Surface Air Temperature," *The Holocene* 6, 255–263.
- Barnett, T. P., B. D. Santer, and K. E. Taylor (1996), *The Potential Effect of GCM Uncertainties on Greenhouse Signal Detection*, Scripps Institution of Oceanography Reference Series No. 96-7.
- Beck, S. L., G. Zandt, S. C. Myers, T. C. Wallace, P. G. Silver, and L. Drake (1996), "Crystal Thickness Variations in the Central Andes," *Geology* 24, 407–410.
- Bergmann, D. J. (1996), *A Comparison of Lagrangian vs. Eulerian Advection in an Atmospheric Chemical Transport Model*, Lawrence Livermore National Laboratory, Livermore, CA, UCRL-ID-124997.
- Berryman, J. G., and D. Elata (1996), "Contact Force-Displacement Laws and the Mechanical Behavior of Random Packs of Identical Spheres," *Mech. Materials* 24, 229–240.
- Blair, S. C., P. A. Berge, and H. F. Wang (1996), *Geomechanical Analysis of the Large Block Test*, Lawrence Livermore National Laboratory, Livermore, CA, UCRL-ID-122898.
- Blair, S. C., J. Kelly, O. Pine, P. A. Berge, and J. Roberts (1996), *Effect of Radiation on the Mechanical Properties of Topopah Spring Tuff*, Lawrence Livermore National Laboratory, Livermore, CA, UCRL-ID-122899.
- Bogen, K. T. (1996), *A Cytodynamic Two-Stage Model That Predicts Radon Hormesis (Decreased, Then Increased Lung-Cancer Risk vs. Exposure)*, Lawrence Livermore National Laboratory, Livermore, CA, UCRL-JC-123219.
- Bogen, K. T., C. L. Conrado, and W. L. Robison (1996), *Uncertainty and Variability in Updated Estimates of Potential Dose and Risk at a U.S. Nuclear Test Site—Bikini Atoll*, Lawrence Livermore National Laboratory, Livermore, CA, UCRL-JC-122616.
- Bonner, B. P. (1996), *Frequency Domain Observations of Small Motions at Concrete/Steel Interfaces*, Lawrence Livermore National Laboratory, Livermore, CA, UCRL-ID-124224.
- Bowen, B. M. (1996), "Example of Reduced Turbulence during Thunderstorm Outflow," *J. Appl. Meteorology* 35, 1028–1032.
- Bowen, B. M. (1996), "Rainfall and Climate Variation over a Sloping New Mexico Plateau during the North American Monsoon," *J. Climate* 9, 3432–3442.
- Bowen, B. M., and B. M. Pobanz (1996), *Atmospheric Dispersion Modeling for the Worst-Case Detonation Accident at the Proposed Advanced Hydrotest Facility*, Lawrence Livermore National Laboratory, Livermore, CA, UCRL-JC-125913.
- Boyle, J. (1996), *Atmospheric Ozone Climatology for Use in General Circulation Models*, Lawrence Livermore National Laboratory, Livermore, CA, UCRL-MI-125650, <http://www-pcmdi.llnl.gov/amip2/ozone2/o3wangdoc.html>.
- Boyle, J. (1996), *Intercomparison of the Seasonal Cycle in 200 hPa Kinetic Energy in AMIP GCM Simulations*, Lawrence Livermore National Laboratory, Livermore, CA, UCRL-ID-125556.
- Brenan, J. M., H. F. Shaw, F. J. Ryerson, and D. L. Phinney (1996), "Experimental Determination of Trace-Element Partitioning between Pargasite and a Synthetic Hydrous Andesitic Melt," *Earth Planet. Sci. Lett.* 140, 1.
- Caffee, M., M. L. Roberts, G. S. Bench, T. A. Brown, R. C. Finkel, S. Freeman, L. J. Hainsworth, M. Kashgarian, M. McAninch, J. E. Proctor, I. D. Southon, and J. S. Vogel (1996), *The LLNL AMS Facility*, Lawrence Livermore National Laboratory, Livermore, CA, UCRL-JC-123254.
- Caffee, M., M. L. Roberts, and I. D. Proctor (1996), *¹²⁹I Interlaboratory Comparison*, Lawrence Livermore National Laboratory, Livermore, CA, UCRL-ID-123253.
- Carrigan, C. R., and A. R. McBirney (1996), *Thermal Conductivity Controversy*, Lawrence Livermore National Laboratory, Livermore, CA, UCRL-JC-123628.
- Carrigan, C. R., R. A. Heinle, G. B. Hudson, J. J. Nitao, et al. (1996), "Trace Gas Emissions on Geological Faults as Indicators of Underground Nuclear Testing," *Nature* 382, 528–531.
- Chang, B. (1996), *FY95 Final Report for 94-LW-046: Compact De-Noxer for Automotive Exhaust*, Lawrence Livermore National Laboratory, Livermore, CA, UCRL-ID-124332.
- Chang, B. (1996), *NO_x Production from Lightning*, Lawrence Livermore National Laboratory, Livermore, CA, UCRL-ID-125003.
- Chen, C.-I., and M. A. Reinsel (1996), "Characterization of Microbial Souring in Berea-Sand Porous Media with a North Sea Oil Field Inoculum," *Biofouling* 9, 175–186.
- Connell, P. S. (1996), *Local and Global Effects on Ozone from Titan Rocket Exhaust and Deorbiting Spacecraft Debris*, Lawrence Livermore National Laboratory, Livermore, CA, UCRL-ID-124313.
- Covey, C. (1996), *The Coupled Model Intercomparison Project*, Lawrence Livermore National Laboratory, Livermore, CA, UCRL-MI-126100, <http://www-pcmdi.llnl.gov/covey/cmip/cmiphome.html>.
- Degteva, M. O., E. Drozhko, L. R. Anspaugh, B. A. Napier, A. C. Bouville, and C. Miller (1996), *Development of an Improved Dose*

Publications

- Reconstruction System for the General Population Affected by the Operation of the Mayak Production Association, Office of International Health Programs*, U.S. Department of Energy, Lawrence Livermore National Laboratory, Livermore, CA, UCRL-PROP-126084.
- Degteva, M. O., E. Drozhko, L. R. Anspaugh, B. A. Napier, A. C. Bouville, and C. W. Miller (1996), *Dose Reconstruction for the Urals Population, Urals Research Center for Radiation Medicine*, Lawrence Livermore National Laboratory, Livermore, CA, UCRL-ID-123713, UCRL-ID-123713Add.1, and UCRL-PROP-123713.
- Degteva, M. O., V. P. Kozheurov, M. I. Vorobyova, D. S. Burmistrov, V. V. Khokhryakov, L. R. Anspaugh, B. A. Napier, and A. Bouville (1996), "Population Exposure Dose Reconstruction for the Urals Region," in *Where Science Comes to Life, M. S. Strauss*, Ed. (American Association for the Advancement of Science, Washington, DC), p. A-7.
- Dowla, F. (1996), *Calibration of the Sonseca Array with Large Magnitude Regional and Teleseismic Events*, Lawrence Livermore National Laboratory, Livermore, CA, UCRL-ID-125023.
- Dowla, F. U. (1996), "Neural Networks in Seismic Discrimination," *Monitoring a Comprehensive Test Ban Treaty* **303**, 777-789.
- Dowla, F. U., and L. L. Rogers (1995), *Solving Problems in Environmental Engineering and Geosciences with Artificial Neural Networks* (MIT Press, Cambridge, MA).
- Durham, W. B., L. A. Stern, and S. H. Kirby (1996), "Rheology of Water Ices V and VI," *J. Geophys. Res.* **101**, 2989-3001.
- Duba, A. G., K. J. Jackson, M. C. Jovanovich, R. B. Knapp, R. T. Taylor, C. O. Boro, M. Evans, M. L. Hanna, W. E. Ralph, and N. N. Shah (1996), "TCE Remediation Using In Situ, Resting-State Bioaugmentation," *Environ. Sci. Technol.* **30**, 1982-1989.
- Elata, D., and J. Dvorkin (1996), *Pressure Sensitivity of Cemented Granular Materials*, Lawrence Livermore National Laboratory, Livermore, CA, UCRL-JC-121535.
- Elata, M. B., M. B. Rubin, and A. V. Attia (1996), *Modeling Added Compressibility of Porosity and the Thermomechanical Response of Wet Porous Rock with Application to Mt. Helen Tuff*, Lawrence Livermore National Laboratory, Livermore, CA, UCRL-JC-121535.
- Finkel, R. C., D. E. Granger, and J. W. Kirchner (1996), "Spatially Averaged Long-Term Erosion Rates Measured from *In Situ* Produced Cosmogenic Nuclides in Alluvial Sediment," *J. Geology* **104**, 249-257.
- Finkel, R. C., J. Klein, and C. P. Kohl (1996), "Cosmogenic Production of ^7Be and ^{10}Be in Water Targets," *J. Geophys. Res.* **101**, 22,225-22,232.
- Gleckler, P. J. (1996), *AMIP II Experimental Design*, Lawrence Livermore National Laboratory, Livermore, CA, UCRL-MI-125581, <http://www-pcmdi.llnl.gov/amip2/reqrec.html>.
- Gleckler, P. J. (1996), *AMIP II Sea Surface Temperature and Sea Ice: Observational and Boundary Condition Data Sets*, Lawrence Livermore National Laboratory, Livermore, CA, UCRL-MI-125597, <http://www-pcmdi.llnl.gov/amip2/bcs/bcsintro.html>.
- Gleckler, P. J. (1996), *New AMIP Information on the World Wide Web*, Lawrence Livermore National Laboratory, Livermore, CA, UCRL-MI-125932, <http://www-pcmdi.llnl.gov/amip2/temp/output/outintro.html>.
- Gleckler, P. J. (1996), *The Library of AMIP Data Transmission Standards—LATs*, Lawrence Livermore National Laboratory, Livermore, CA, UCRL-MI-125598, <http://www-pcmdi.llnl.gov/amip2/lats/latsintro.html>.
- Goldstein, P. (1996), *Computer Simulation of Regional Seismic Signals*, Lawrence Livermore National Laboratory, Livermore, CA, UCRL-MI-123960.
- Gouveia, F. J., and R. L. Baskett (1996), *Comparison of Data from Co-Located Sensor Packages and Implications for Dispersion Modeling: An In Situ Case Study of Rugged Versus Low-Threshold Anemometers and Natural Versus Forced-Ventilation Solar Shields*, Lawrence Livermore National Laboratory, Livermore, CA, UCRL-JC-123717.
- Granger, D. E., J. W. Kirchner, and R. Finkel (1996), "Spatially Averaged Long-Term Erosion Rates Measured from *In Situ*-Produced Cosmogenic Nuclides in Alluvial Sediment," *J. Geology* **104**, 249-257.
- Gu, Z. Y., D. Lal, T. S. Liu, J. Southon, M. W. Caffee, Z. T. Guo, and M. Y. Chen (1996), "Five Million Year ^{10}Be Record in Chinese Loess and Red Clay: Climate and Weathering Relationships," *Earth Planet. Sci. Lett.* **144**, 273-287.
- Guo, L., P. H. Santschi, L. A. Cifuentes, S. E. Trumbore, and J. R. Southon (1996), "Cycling of High-Molecular-Weight Dissolved Organic Matter in the Middle Atlantic Bight as Revealed by Carbon Isotopic (^{13}C and ^{14}C) Signatures," *Limnol. Oceanogr.* **41**(6), 1242-1252.
- Hegerl, G. C., H. von Storch, K. Hasselmann, B. D. Santer, U. Cubasch, and P. D. Jones, (1996), "Detecting Anthropogenic Climate Change with an Optimal Fingerprint Method," *J. Climate* **9**, 2281-2306.
- Heuze, F. E. (1996), *LLNL's Partnership with Selected U.S. Mines for CTBT Verification: A Pictorial and Some Reflections*, Lawrence Livermore National Laboratory, Livermore, CA, UCRL-ID-122577.
- Heuze, F. E., W. Maurer, W. Deskins, W. McDonald, and J. Cohen (1996), *Rapid Deployment Drilling System for On-Site Inspections under a Comprehensive Test Ban*, Lawrence Livermore National Laboratory, Livermore, CA, UCRL-CR-125259.
- Hobard, D. E. (1996), *Estimates of the Solubilities of Waste Element Radionuclides in Waste Isolation Pilot Plant Brines: A Report by the Expert Panel on the Source Term*, Sandia National Laboratory, Albuquerque, NM.
- Hsu, P. C., Z. Chiba, B. J. Schumacher, L. C. Murguia, and M. G. Adamson (1996), *Bench Scale Silver Recovery Unit for the MEO System*, Lawrence Livermore National Laboratory, Livermore, CA, UCRL-ID-123602.
- Hsu, P. C., Z. Chiba, B. J. Schumacher, L. C. Murguia, and M. G. Adamson (1996), *Recovery of Silver from Waste Silver Chloride for the MEO System*, Lawrence Livermore National Laboratory, Livermore, CA, UCRL-ID-123603.
- Hutchings, L. J., S. P. Jarpe, P. W. Kasameyer, and W. Foxall (1996), *Synthetic Strong Ground Motions for Engineering Design Utilizing Empirical Green's Functions*, Lawrence Livermore National Laboratory, Livermore, CA, UCRL-JC-123762.
- Ispenkov, E. A., Y. E. Kenigsberg, V. F. Minenko, M. I. Balonov, Y. I. Gavrilin, A. E. Kondrashov, M. N. Savkin, V. G. Skvortsov, F. F. Stepanenko, I. A. Zvonova, V. V. Chumak, L. N. Kovgan, I. A. Likhtarev, I. P. Los', V. S. Repin, B. G. Sobolev, W. Burkart, K. D. Martignoni, L. R. Anspaugh, R. Mould, and G. N. Souchevitch (1996), "Dose Reconstruction Project Protocol," in *International Programme on the Health Effects of the Chernobyl Accident* (World Health Organization, Geneva, Switzerland), p. 35.
- Jarpe, S., B. Moran, P. Goldstein, and L. Glenn (1996), *Implications of Mining Practices in an Open-Pit Gold Mine for Monitoring of a Comprehensive Test-Ban Treaty*, Lawrence Livermore National Laboratory, Livermore, CA, UCRL-ID-123017.
- Johnson, V. M. and L. L. Rogers (1995), "Location Analysis in Ground-Water Remediation Using Neural Networks," *Ground Water* **33**, 749-758.
- Keating, G. A., K. T. Bogen, and Vogel, J. S. (1996), "Human Skin Uptake of Trichloroethylene from Short-Term Aqueous Exposure," in

- Advances in the Biology of the Skin: Pharmacology and Toxicology* (Environmental and Occupational Health Sciences Institute, Rutgers University, NJ).
- Kim, J., and N. L. Miller (1996), "Simulating Winds and Floods: Regional Weather-River Prediction and Regional Climate Research," *IEEE Potentials* **15**(4), 17–20.
- Kinnison, D. E., and P. S. Connell (1996), *Evaluating the Importance of Innovative Heterogeneous Chemistry to Explain Observed Stratospheric Ozone Depletion*, Lawrence Livermore National Laboratory, Livermore, CA, UCRL-ID-123607.
- Kirchner, T. B., F. W. Whicker, L. R. Anspaugh, and Y. C. Ng (1996), "Estimating Internal Dose Due to Ingestion of Radionuclides from Nevada Test Site Fallout," *Health Phys.* **71**, 487–501.
- Knezovich, J. P., D. J. Steichen, J. A. Jelinski, and S. L. Anderson (1996), "Sulfide Tolerance of Four Marine Species Used to Evaluate Sediment and Pore-Water Toxicity," *Bull. Environ. Contam. Toxicol.* **57**, 450–457.
- Labolle, E. M., G. E. Fogg, and A. F. B. Tompson (1996), "Random-Walk Simulation of Transport in Heterogeneous Porous Media—Local Mass-Conservation Problem and Implementation Methods," *Water Resources Res.* **32**, 583–593.
- Labrecque, D. J., A. L. Ramirez, W. D. Daily, A. M. Binley, et al. (1996), "ERT Monitoring on Environmental Remediation Processes," *Measure. Sci. Technol.* **7**, 375–383.
- Ladd, A. J. C. (1996), *Sedimentation of Homogeneous Suspensions of Non-Brownian Spheres*, Lawrence Livermore National Laboratory, Livermore, CA, UCRL-JC-125165.
- Ladd, A., J. Kinney, and T. Breunig (1996), *Deformation and Failure in Cellular Materials*, Lawrence Livermore National Laboratory, Livermore, CA, UCRL-JC-124331.
- Ladd, A. J. C., J. Kinney, T. Breunig, and D. Haupt (1996), *Elastic Constants of Cellular Structures*, Lawrence Livermore National Laboratory, Livermore, CA, UCRL-JC-125166.
- Leger, A., E. A. Mathez, A. Duba, F. Pineau, et al. (1996), "Carbonaceous Material in Metamorphosed Carbonate Rocks from the Waits River Formation, NE Vermont, and Its Effect on Electrical Conductivity," *J. Geophys. Res.* **101**, 22,203–22,214.
- Leith, C. E. (1996), "Stochastic Models of Chaotic Systems," *Physica D* **98**, 481–491.
- Likhtarev, I. A., L. N. Kovgan, S. E. Vavilov, R. R. Gluvchinsky, O. N. Perevoznikov, L. N. Litvinets, L. R. Anspaugh, J. R. Kercher, and A. Bouville (1996), "Internal Exposure from the Ingestion of Foods Contaminated by ^{137}Cs after the Chernobyl Accident," *Health Phys.* **70**(3), 297–317.
- Likhtarev, I. A., L. N. Kovgan, S. E. Vavilov, R. R. Gluvchinsky, O. N. Perevoznikov, L. N. Litvinets, L. R. Anspaugh, J. R. Kercher, and A. Bouville (1996), "Response to Muller and Prohl," *Health Phys.* **71**(5), 798–799.
- Lioussie, C., J. E. Penner, C. Chuang, J. J. Walton, and H. Eddleman (1996), "A Global Three-Dimensional Model Study of Carbonaceous Aerosols," *J. Geophys. Res.* **101**, 19,411–19,432.
- Lucas, J., F. S. Hill, C. E. Burk, A. B. Cox, and T. Straume (1996), "Stability of the Translocation Frequency Following Whole-Body Irradiation Measured in Rhesus Monkeys," *Natl. J. Radiat. Biology* **70**, 309–318.
- MacCracken, M., J. Penner, and J. Dignon (1996), *LDRD Program Final Report*, Lawrence Livermore National Laboratory, Livermore, CA, UCRL-JC-124221.
- Marchetti, A. A., and T. Straume (1996), "A Search for Neutron Reactions That May Be Useful for Hiroshima Dose Reconstruction," *Appl. Radiat. Isotopes* **47**, 97–103.
- McNamara, D. (1996), *Regional Waveform Modeling and Phase Propagation in North America*, Lawrence Livermore National Laboratory, Livermore, CA, UCRL-MI-122059.
- McNamara, D. E., T. J. Owens, and W. R. Walter (1996), "Observations of Regional Phase Propagation across the Tibetan Plateau," *J. Geophys. Res.* **100**, 22,215–22,230.
- McNamara, D. E., T. J. Owens, and W. R. Walter (1996), "Propagation Characteristics of Lg across the Tibetan Plateau," *Bull. Seismol. Soc. Am.* **86**, 457–469.
- Measures, C. I., T. L. Ku, S. Luo, J. R. Southon, X. Xu, and M. Kusakabe (1996), "The Distribution of ^{10}Be and ^9Be in the South Atlantic," *Deep-Sea Res.* **143**(7), 987–1009.
- Miller, D. G., R. Sartorio, L. Paduano, J. A. Rard, and J. G. Albright (1996), "Effects of Different Sized Concentration Differences across Free Diffusion Boundaries and Comparison of Gouy and Rayleigh Diffusion Measurements Using $\text{NaCl-KCl-H}_2\text{O}$," *J. Solut. Chem.* **25**, 1185–1211.
- Miller, N. L., and J. Kim (1996), "Numerical Prediction of Precipitation and River Flow over the Russian River Watershed during the January 1995 California Storms," *Bull. Am. Meteorol. Soc.* **77**(1), 101–105.
- Minarik, W. (1996), *Textural Controls on the Formation of the Earth's Core*, Lawrence Livermore National Laboratory, Livermore, CA, UCRL-MI-124306.
- Minarik, W. G., F. J. Ryerson, and E. B. Watson (1996), "Textural Entrapment of Core-Forming Melts: Implication for Siderophile Element Abundances," *Science* **272**, 530–533.
- Mirin, A., and M. Wehner (1996), "Climate System Modeling in High-Performance Computing Systems, with an Application to Modeling the Atmosphere," *NERSC Buffer* **20**(1), 1–5.
- Moss, W., and V. Simonenko (1996), "Single-Bubble Sonoluminescence: Physical Model Development and Computational Study," in *Proposal for Civilian Research and Development Foundation (CRDF)*, Arlington, VA, Lawrence Livermore National Laboratory, Livermore, CA, UCRL-PROP-123350.
- Nishiizumi, K., M. W. Caffee, A. J. T. Jull, and R. C. Reedy (1996), "Exposure History of Lunar Meteorites Queen Alexandra Range 93069 and 94269," *Meteor. Planet. Sci.* **31**, 893–896.
- Nishiizumi, K., R. C. Finkel, J. Klein, and C. P. Kohl (1996), "Cosmogenic Production of ^7Be and ^{10}Be in Water Targets," *J. Geophys. Res.* **101**, 22,225–22,232.
- Nitao, J. J., and J. Bear (1996), "Potentials and Their Role in Transport in Porous Media," *Water Resources Res.* **32**(2), 225–250.
- Oversby, O., and C. McPheeters (1996), *Plutonium Destruction in a Non-Fertile, ZrO_2 -Based Fuel—A Reactor Option for Disposition of Surplus Plutonium*, Lawrence Livermore National Laboratory, Livermore, CA, UCRL-ID-123613.
- Penner, J. E., and T. Novakov (1996), "Carbonaceous Particles in the Atmosphere: A Historical Perspective to the Fifth International Conference on Carbonaceous Particles in the Atmosphere," *J. Geophys. Res.* **101**, 19,372–19,378.
- Perry, G., P. B. Duffy, and N. Miller (1996), "An Extended Dataset of River Discharges for Validation of Climate Models," *J. Geophys. Res.* **101**, 21,339–21,349.
- Phillips, T. J. (1996), "Atmospheric Model Documentation Available Online—Part 1," *EOS, Trans. Am. Geophys. Union* **77**(27), 253.

- Phillips, T. J. (1996), "Atmospheric Model Documentation Available Online—Part 2," *EOS Electronic Suppl.* Internet URL: http://www.agu.org/eos_elec/96069e.html.
- Phillips, T. J. (1996), "Documentation of the AMIP Models on the World Wide Web," *Bull. Am. Meteorol. Soc.* **77**, 1191–1196.
- Proctor, I. D., M. L. Roberts, J. E. McAninch, and G. S. Bench (1996), *Proof-of-Concept Development of PXAMS (Projectile X-Ray Accelerator Mass Spectrometry)*, Lawrence Livermore National Laboratory, Livermore, CA, UCRL-ID-123620.
- Ramirez, A. L. (1996), *Electrical Resistivity Monitoring of the Thermomechanical Heater Test in Yucca Mountain*, Lawrence Livermore National Laboratory, Livermore, CA, UCRL-JC-126011.
- Ramirez, A. L., and W. D. Daily (1996), *Detection of Leaks in Underground Storage Tanks Using Electrical Resistance Methods: 1996 Results, 96/4*, Lawrence Livermore National Laboratory, Livermore, CA, UCRL-ID-125918.
- Rard, J. A. (1996), "Isopiestic Determination of the Osmotic Coefficients of $\text{Lu}_2(\text{SO}_4)_3(\text{aq})$ and $\text{H}_2\text{SO}_4(\text{aq})$ at the Temperature $T = 298.15$ K, and Review and Revision of the Thermodynamic Properties of $\text{Lu}_2(\text{SO}_4)_3(\text{aq})$," *J. Chem. Thermodyn.* **28**, 83–110.
- Rard, J. A., J. G. Albright, D. G. Miller, and M. E. Zeidler (1996), "Ternary Mutual Diffusion Coefficients and Densities of the System $\{\text{z}_1\text{NaCl} + (1-\text{z}_1)\text{Na}_2\text{SO}_4\}(\text{aq})$ at 298.15 K and a Total Molarity of 0.5000 mol dm^{-3} ," *J. Chem. Soc. Faraday Trans.* **92**, 4187–4197.
- Rashidi, M., and L. Cole (1996), *An Evaluation of In Situ Bioremediation Processes*, Lawrence Livermore National Laboratory, Livermore, CA, UCRL-ID-125046.
- Rashidi, M., L. Peurrung, A. F. B. Thompson, and T. J. Kulp (1996), "Experimental Analysis of Pore-Scale Flow and Transport in Porous Media," *Adv. Water Resources* **19**, 163–180.
- Rashidi, M., A. Thompson, T. Kulp, and L. Peurrung (1996), "3-D Microscopic Measurement and Analysis of Chemical Flow and Transport in Porous Media," *J. Fluids Eng. Trans. Am. Soc. Mech. Eng.* **118**, 470–480.
- Roberts, M. L., M. W. Caffee, and I. D. Proctor (1996), *Preliminary Report on SG126 Task 3: ¹²⁹I Interlaboratory Comparison*, Lawrence Livermore National Laboratory, Livermore, CA, UCRL-ID-123642.
- Robison, W. L., and C. L. Conrado (1996), *Radiological Conditions at Naen, Yugui, Lomiulal, Kabelle, and Mellu Islands in the Northern Half of Rongelap Atoll*, Lawrence Livermore National Laboratory, Livermore, CA, UCRL-ID-123374.
- Robison, W. L., and C. L. Conrado (1996), *Radiological Conditions at the Southern Islands of Rongelap Atoll*, Lawrence Livermore National Laboratory, Livermore, CA, UCRL-ID-123375.
- Ryerson, F. J., T. M. Harrison, A. Yin, and M. Murphy (1996), *The Gandese and Renbu-Zedong Thrust Systems: Lateral Extent and Thrust History*, Lawrence Livermore National Laboratory, Livermore, CA, UCRL-JC-125168.
- Ryerson, F. J., R. Quidelleur, O. Lovera, M. T. Harrison, and A. Yin (1996), *The Thermal Evolution and Slip History of the Renbu Zedong Thrust, Southeastern Tibet*, Lawrence Livermore National Laboratory, Livermore, CA, UCRL-JC-125169.
- Ryerson, F. J., and G. Zandt (1996), *Anomalous Crust of the Bolivian Altiplano, Central Andes*, Lawrence Livermore National Laboratory, Livermore, CA, UCRL-JC-125168.
- Ryerson, F. J., and G. Zandt (1996), *Convective Thermal Instabilities in the Wake of the Migrating Mendocino Triple Junction*, California, Lawrence Livermore National Laboratory, Livermore, CA, UCRL-JC-125169.
- Santer, B. D., K. E. Taylor, T. M. L. Wigley, T. C. Johns, P. D. Jones, D. J. Karoly, J. F. B. Mitchell, A. H. Oort, J. E. Penner, V. Ramaswamy, M. D. Schwarzkopf, R. J. Stouffer, and S. Tett (1996), "A Search for Human Influences on the Thermal Structure of the Atmosphere," *Nature* **382**, 39–46.
- Santer, B. D., K. E. Taylor, T. M. L. Wigley, T. C. Johns, P. D. Jones, D. J. Karoly, J. F. B. Mitchell, A. H. Oort, J. E. Penner, V. Ramaswamy, M. D. Schwarzkopf, R. J. Stouffer, S. Tett, J. S. Boyle, and D. E. Parker (1996), "Human Effect on Global Climate?" *Nature* **384**, 523–524.
- Santer, B. D., T. M. L. Wigley, T. P. Barnett, and E. Anyamba (1996), "Detection of Climate Change, and Attribution of Causes," in *Climate Change 1995: The Science of Climate Change*, J. T. Houghton, L. G. Meira Filho, B. A. Callander, N. Harris, A. Kattenberg, and K. Maskell, Eds. (Cambridge University Press, Cambridge), pp. 407–443.
- Shalk, W. W. III (1996), *Modeling SF6 Plume Dispersion in Complex Terrain and Meteorology with a Limited Data Set*, Lawrence Livermore National Laboratory, Livermore, CA, UCRL-ID-125646.
- Schultz, C. A., M. N. Toksoz, T. J. Owens, and C. J. Ammon (1996), "Experimental Study of Enhanced Backscattering from a Highly Irregular Acoustic-Elastic Interface," *Acoust. Soc. Am.* **99**, 880–892.
- Shah, N. N., M. L. Hanna, J. K. Veir, and R. T. Taylor (1996), "Batch Cultivation of *Methylinus trichosporium* OB3b: V. Characterization of Poly- β -Hydroxybutyrate Production under Methane-Dependent Growth Conditions," *Biotechnol. Bioeng.* **40**, 161–171.
- Shinn, J. H., C. O. Fry, and J. S. Johnson (1996), *Monitored Plutonium Aerosols at a Soil Cleanup Site on Johnston Atoll*, Lawrence Livermore National Laboratory, Livermore, CA, UCRL-ID-124059.
- Slingo, J. M., K. R. Sperber, J. S. Boyle, J.-P. Ceron, M. Dix, B. Dugas, W. Ebisuzaki, J. Fyfe, D. Gregory, J.-F. Guerey, J. Hack, A. Harzallah, P. Inness, A. Kitoh, W. K.-M. Lau, B. McAvaney, R. Madden, A. Matthews, T. N. Palmer, C.-K. Park, D. Randall, and N. Renno (1996), "Intraseasonal Oscillations in 15 Atmospheric General Circulation Models: Results from an AMIP Diagnostic Subproject," *Climate Dynamics* **12**, 325–357.
- Sperber, K. R., and T. N. Palmer (1996), "Interannual Tropical Rainfall Variability in General Circulation Model Simulations Associated with the Atmospheric Model Intercomparison Project," *J. Climate* **9**, 2727–2750.
- Steig, E. J., P. J. Polissar, M. Stuiver, P. M. Grootes, and R. C. Finkel (1996), "Large Amplitude Solar Modulation Cycles of ¹⁰Be in Antarctica: Implications for Atmospheric Mixing Processes and Interpretation of the Ice Core Record," *Geophys. Res. Lett.* **23**, 523–526.
- Straume, T. (1996), "Risk Implications of the Neutron Discrepancy in the Hiroshima DS86 Dosimetry System," *Radiation Protection Dosimetry* **67**, 9–12.
- Straume, T., A. A. Marchetti, L. R. Anspaugh, V. T. Khrouch, Y. I. Gavrilin, S. M. Shinkarev, V. V. Drozdovitch, A. V. Ulanovsky, S. V. Korneev, M. K. Brekeshev, E. S. Leonov, G. Voigt, S. V. Panchenko, and V. F. Minenko (1996), "The Feasibility of Using ¹²⁹I to Reconstruct ¹³¹I Deposition from the Chernobyl Reactor Accident," *Health Phys.* **71**(5), 733–740.
- Straume, T., A. A. Marchetti, and J. E. McAninch (1996), "New Analytical Capability May Provide Solution to the Neutron Dosimetry Problem in Hiroshima," *Radiat. Protect. Dosimetry* **67**(1), 5–8.
- Straume, T., O. G. Raabe, K. J. Walsh, and L. M. Wiley (1996), "Mouse Immature Oocytes Irradiated *In Vivo* at 14 days of Age and

- Evaluated for Transmitted Effects Using the Aggregation Embryo Chimera Assay," *Mutation Res.* **356**, 269–273.
- Sullivan, T. J. (1996), *The Atmospheric Release Advisory Capability (ARAC)*, Lawrence Livermore National Laboratory, Livermore, CA, UCRL-TB-123645.
- Tompson, A. F. B., and K. J. Jackson (1996), "Reactive Transport in Heterogeneous Systems: An Overview," in *Reactive Transport in Porous Media*, P. C. Lichtner, C. I. Steefel, and E. H. Oelkers, Eds., *Rev. Mineral.* **34**, 269–310.
- Tompson, A. F. B., A. L. Schafer, and R. W. Smith (1996), "Impacts of Physical and Chemical Heterogeneity on Cocontaminant Transport in a Sandy Porous Medium," *Water Resources Res.* **32**, 801–818.
- Tyburczy, J. A., and J. J. Roberts (in press), "Impedance Spectroscopy of Upper Mantle Earth Materials in Electrically Based Microstructural Characterization," *Proc. Mater. Res. Soc. Symp.* **41** (Materials Research Society).
- Vandegriff, J., G. Raimann, R. N. Boyd, M. Caffee, et al. (1996), "A Search for Stable Strange Quark Matter Nuggets in Helium," *Phys. Lett. B* **365**, 418–422.
- Van Konynenburg, R. A., R. W. Hopper, J. A. Rard, F. J. Ryerson, D. L. Phinney, I. D. Hutcheon, and P. G. Curtis (1996), "Ceramic Waste Form for Residues from Molten Salt Oxidation of Mixed Wastes," *Proc. Mater. Res. Soc. Symp.*, D. Knecht and W. M. Murphy, Eds. (Materials Research Society), pp. 321–328.
- Van Konynenburg, R. A., R. W. Hopper, J. A. Rard, F. J. Ryerson, D. L. Phinney, I. D. Hutcheon, and P. G. Curtis (1996), "Scientific Basis for Radioactive Waste Management XIX," *Proc. Mater. Res. Soc. Symp.* (Materials Research Society), pp. 321–328.
- Voigt, G., H. G. Paretzke, L. R. Anspaugh, and A. C. Bouville (1996), "Scientific Recommendations for the Reconstruction of Radiation Doses Due to the Reactor Accident at Chernobyl," *Radiat. Environ. Biophys.* **35**, 1–9.
- Walter, W. (1996), *Identifying Clandestine Underground Nuclear Tests by Their Seismic Signatures*, Lawrence Livermore National Laboratory, Livermore, CA, UCRL-MI-123958.
- Walter, W., S. Hunter, and L. Glenn (1996), *Preliminary Report on LLNL Mine Seismicity Deployment at the Twentymile Coal Mine*, Lawrence Livermore National Laboratory, Livermore, CA, UCRL-ID-122800.
- Wang, L., T. L. Ku, S. Luo, M. R. Southon, and M. Kusakabe (1996), "²⁶Al–¹⁰Be Systematics in Deep-Sea Sediments," *Geochim. Cosmochim. Acta* **60**(1), 109–119.
- Wehner, M. F., W. P. Dannevik, P. G. Eltgroth, A. A. Mirin, P. B. Duffy, C. Covey, and H. Wang (1996), "Coupled Oceanic–Atmospheric General Circulation Modeling at Lawrence Livermore National Laboratory," in *Research Activities in Atmospheric and Oceanic Modeling*, WMO Report 23, p. 9.28. Available from Lawrence Livermore National Laboratory, Livermore, CA, UCRL-ID-124203.
- Whicker, F. W., T. B. Kirchner, L. R. Anspaugh, and Y. C. Ng (1996), "Ingestion of Nevada Test Site Fallout: Internal Dose Estimates," *Health Phys.* **71**, 477–486.
- Wilder, D. G. (1996), *Volume II: Near-Field and Altered-Zone Environmental Report*, Lawrence Livermore National Laboratory, Livermore, CA.
- Wilt, M., K. H. Lee, A. Becker, B. Spies, and B. Wang (1996), *Crosshole EM in Steel-Cased Boreholes*, Lawrence Livermore National Laboratory, Livermore, CA, UCRL-JC-124210.
- Wilt, M., C. Schenkel, M. Wratcher, I. Lambert, C. Torres-Verdi, and H.-W. Tseng (1996), *Crosshole EM for Oil Field Characterization and EOR Monitoring: Field Examples from Lost Hills*, California, Lawrence Livermore National Laboratory, Livermore, CA, UCRL-ID-123893.
- Yow, J. L. (1996), "Suggested Method for Deformability Determination Using a Stiff Dilatometer," *Int. J. Rock Mechanics Mining Sciences* **33**.

Patents and Awards

Patents

Patent issued to	Patent title, number, and date of issue	Summary of disclosure
William D. Daily Abelardo L. Ramirez* Robin L. Newmark* Kent Udell Harley M. Buettner Roger D. Aines*	Dynamic Underground Stripping: Steam and Electric Heating for In Situ Decontamination of Soils and Groundwater U.S. Patent 5,449,251 September 12, 1995	A process for removing localized underground contamination of volatile organic compounds by heating a contaminated area using steam injection and electric currents to vaporize the contaminants, and then removing the migrating subsurface fluids and vapor by vacuum extraction and liquid pumping. Injection and extraction wells are constructed within or around the periphery of the contaminated area.
Daniel A. Seligmann, William C. Moss* Theodore C. Valk Alan D. Conder	Compact Self-Contained Electrical-to-Optical Converter/Transmitter U.S. Patent 5,469,442 November 21, 1995	A signal-conditioning circuit with elements electrically coupled to a transducer and optically coupled to a receiver/processor. The circuit elements receive from the transducer, generate a linear reference signal, and mix the analog and reference signals to form a calibrated output signal that is converted to an optical signal.
Margaret L. Carman Kenneth J. Jackson* Richard B. Knapp* John P. Knezovich* Nilesh N. Shah* Robert T. Taylor	Methods for Microbial Filtration of Fluids U.S. Patent 5,487,834 January 30, 1996	A method for purifying contaminated subsurface groundwater by contacting the contaminated subsurface groundwater with resting state methanotrophic or heterotrophic microorganisms that produce long lifetime contaminant-degrading enzymes. The micro-organisms are derived from surface cultures and are injected into the ground to act as a biofilter. The contaminants include organic or metallic materials and radionuclides.
Richard R. Leach* Farid U. Dowla*	Real-Time Neural Network Earthquake Profile Predictor U.S. Patent 5,490,062 February 6, 1996	A network that uses first-arrival energy to predict the characteristics of impending earthquake seismograph signals. The neural network produces a profile of the complete earthquake signal using data from the first seconds of the signal.
Abelardo L. Ramirez* John F. Cooper William D. Daily	Using Electrokinetic Phenomena and Electrical Resistance Tomography to Characterize the Movement of Subsurface Fluids U.S. Patent 5,495,175 February 27, 1996	A method using electrokinetic transport to enhance the ability of electrical resistance tomography (ERT) to detect position and movement of subsurface contaminant liquids, particles, or ions, and for subsurface imaging of soil and rock properties.

*Earth and Environmental Sciences employee.

Awards

Alfred G. Duba was elected a Fellow of the American Geophysical Union.

Frederick J. Ryerson received the Associated Western Universities Distinguished Lectureship Award.

Andrew Tompson received the Computation Directorate Distinguished Achievement Award, for extraordinary programmatic contribution.

The National Atmospheric Release Advisory Center, Building 170 at Lawrence Livermore National Laboratory, received a Distinguished Projects Award in architectural design from the Western Council of Construction Consumers.

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