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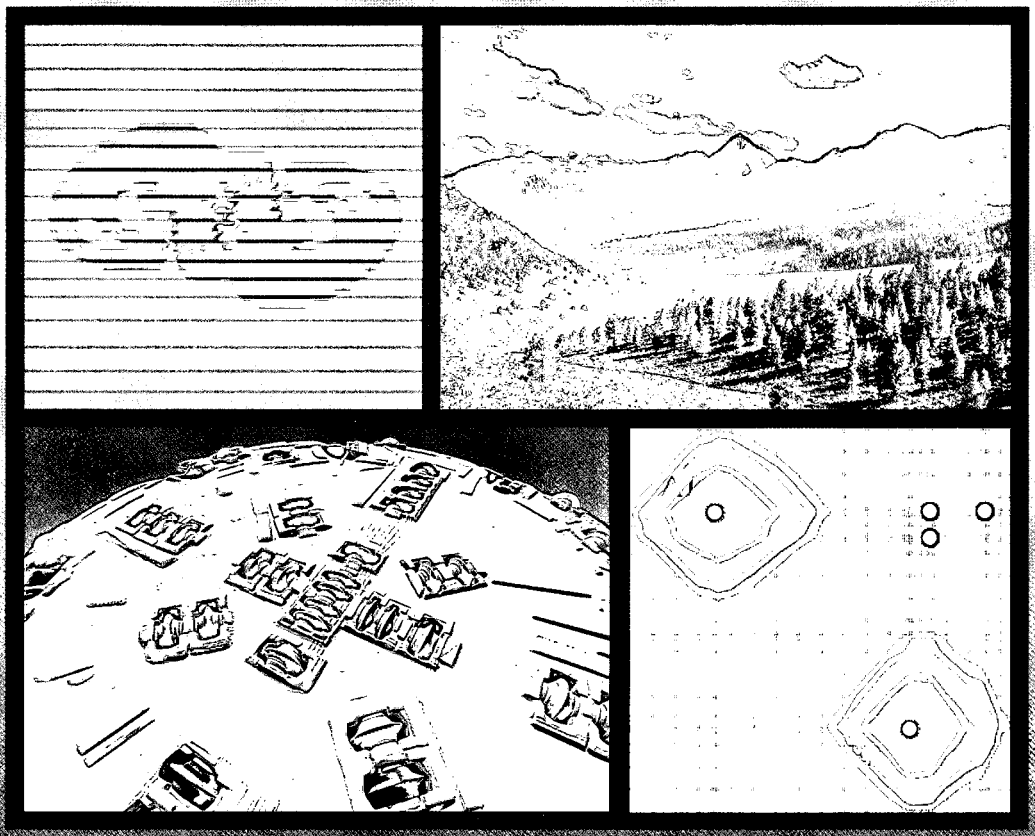

ANNUAL REPORT

EARTH SCIENCES DIVISION

2000-2001

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EARTH SCIENCES DIVISION ANNUAL REPORT

2000–2001

ERNEST ORLANDO LAWRENCE
BERKELEY NATIONAL LABORATORY

UNIVERSITY OF CALIFORNIA
BERKELEY, CALIFORNIA 94720

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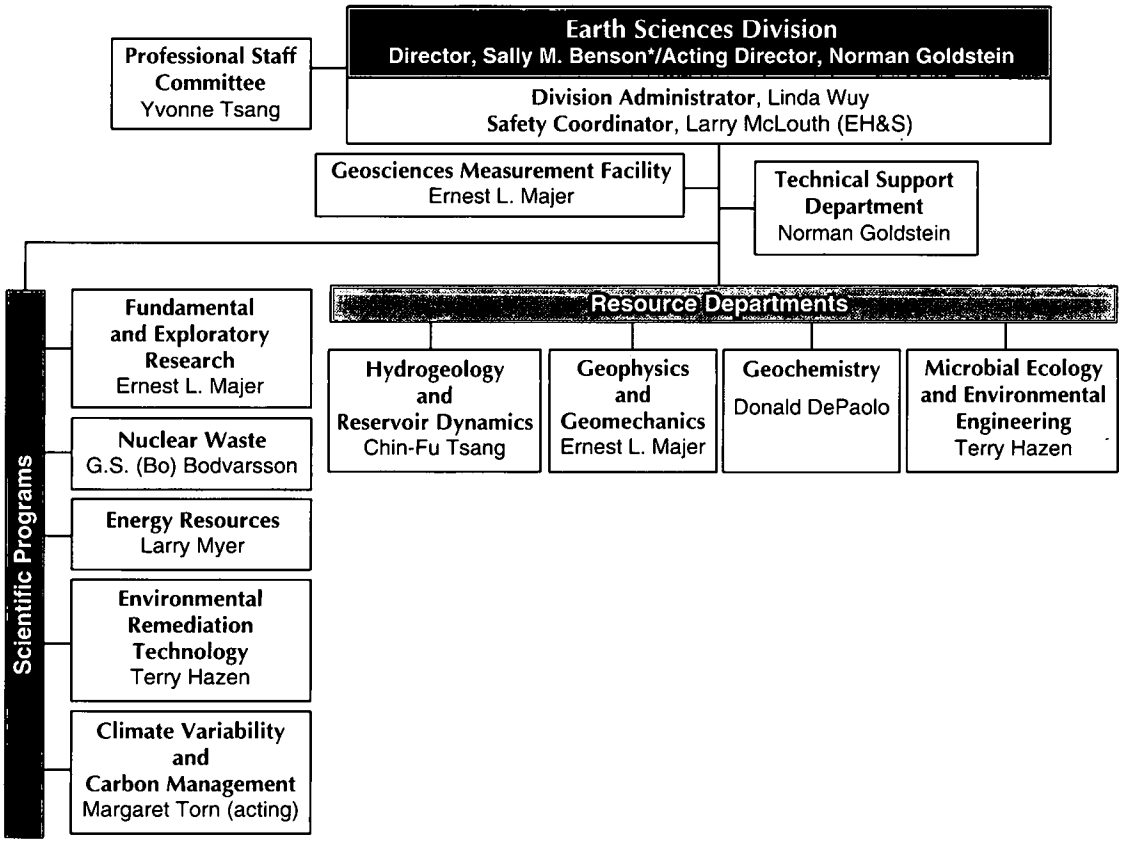
ESD Organization Chart



*Sally M. Benson was Earth Sciences Division Director through March 2001.

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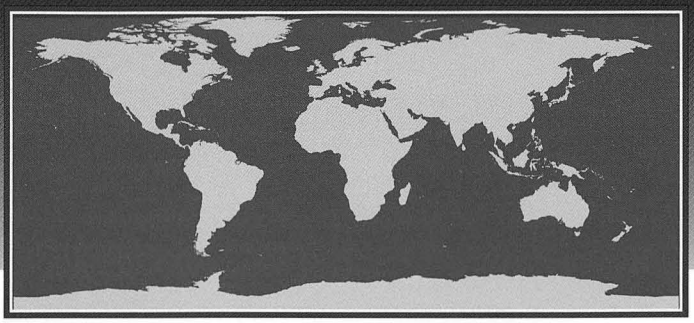

ERNEST ORLANDO LAWRENCE BERKELEY NATIONAL LABORATORY

EARTH SCIENCES DIVISION

ANNUAL REPORT 2000-2001

A PERSPECTIVE FROM THE DIVISION DIRECTOR

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Global population growth and increased industrialization are placing stronger demands on our earth's energy, mineral, and water resources, and are adding to concerns about whether we, as a global society, will be able to sustain economic growth and maintain a clean and safe environment for future generations. Not surprisingly, the importance of the earth and ecosystem sciences in shaping our future grows larger than ever. Not only must earth scientists continue to address the issues that were so pressing during the past century—secure and plentiful energy and water resources, remediation of contaminated ground and surface waters, and prediction of natural geologic hazards—but now we must face the challenges of the 21st century. Growing concentrations of greenhouse gases in the atmosphere and the need for safe and secure nuclear waste management have emerged as two important concerns faced by our nation and others around the world. As one of the U.S. Department of Energy's national laboratories, it is the mission of Ernest Orlando Lawrence Berkeley National Laboratory (Berkeley Lab) to provide a robust scientific foundation to better understand and identify solutions to these pressing issues.

Our long-standing scientific strengths and fundamental research in hydrogeology and reservoir engineering, geophysics and geomechanics, geochemistry, microbial ecology, and environmental engineering provide the foundation for all of our programs. Building on this scientific foundation, we perform applied earth science research and technology development to support the Department of Energy in a number of its program areas, namely:

- Nuclear Waste Management—theoretical, experimental and simulation studies of the unsaturated zone at Yucca Mountain, Nevada
- Energy Resources—collaborative projects with industry to develop or improve technologies for the exploration and production of oil, gas, and geothermal reservoirs
- Environmental Remediation Technology—innovative technologies for containing and remediating metals, radionuclides, chlorinated solvents, and energy-related contaminants in soils and groundwaters
- Climate Change and Carbon Management—geologic sequestration of carbon dioxide, carbon cycling in the oceans and terrestrial biosphere, and regional climate modeling, which are the cornerstones of a major new divisional research thrust related to understanding and mitigating the effects of increased greenhouse gas concentrations in the atmosphere

This year has been another exciting and productive one for our division. During the reporting period, we have made great strides in all our ongoing research programs, particularly in the newer areas of regional climate change and its impact on surface and groundwater, and the sequestration of carbon dioxide in geologic, terrestrial, and oceanic systems.

In this report, we present summaries of many of our current research projects. While it is not a complete accounting, it is representative of the nature and breadth of our research effort. We hope that you will be as excited about our research as we are.

ORGANIZATION OF THIS REPORT

This report is divided into five sections that correspond to the major research programs in the Earth Sciences Division:

- Fundamental and Exploratory Research
- Nuclear Waste
- Energy Resources
- Environmental Remediation Technology
- Climate Variability and Carbon Management

These programs draw from each of our disciplinary departments: Microbial Ecology and Environmental Engineering, Geophysics and Geomechanics, Geochemistry, and Hydrogeology and Reservoir Dynamics. Short descriptions of these departments are provided as introductory material. A list of publications for the period June 2000 to June 2001, along with a listing of our personnel, are appended to the end of this report.

ACKNOWLEDGMENTS

The Earth Sciences Division consists of 60 scientists and engineers, another 25 faculty scientists with joint Berkeley Lab-UC Berkeley appointments, and approximately 50 scientific and technical support persons. We gratefully acknowledge the support of our major sponsors in the Department of Energy, which include the Office of Science, the Office of Fossil Energy, the Office of Energy Efficiency and Renewable Energy, the Office of Civilian Radioactive Waste Management, and the Office of Environmental Management. We also appreciate the support received from other federal agencies such as the Bureau of Reclamation, the Department of Defense, the Environmental Protection Agency, and NASA. Lastly, we must also acknowledge and thank our industrial collaborators who provide both financial and in-kind support through various partnership projects, and who bring additional ideas, data, and experience to our division.

Resource Departments

Hydrogeology and Reservoir Dynamics

Geophysics and Geomechanics

Geochemistry

Microbial Ecology and Environmental Engineering

RESOURCE DEPARTMENT

HYDROGEOLOGY AND RESERVOIR DYNAMICS

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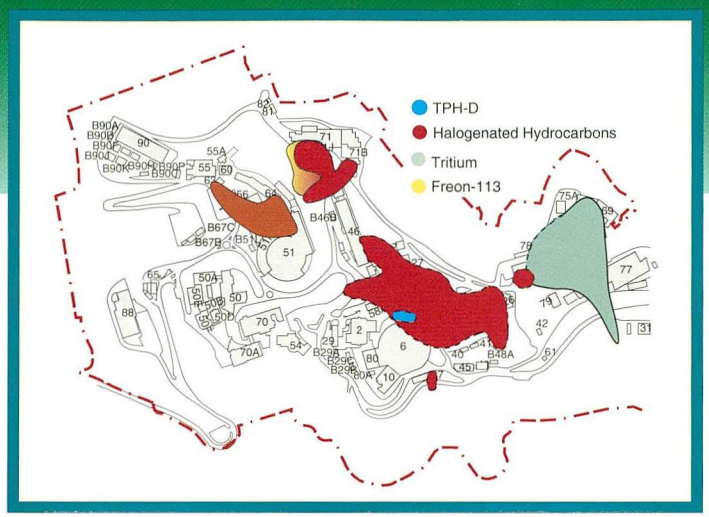

The Hydrogeology and Reservoir Dynamics Department (HRD) is one of the world's most active research groups in the fields of hydrogeology and reservoir engineering. Specific research areas include the following:

CONTAMINANT HYDROLOGY

Work conducted in this area covers various theoretical, experimental, and field studies, including a detailed evaluation and remediation of subsurface contamination at Berkeley Lab. In this multiyear program, the geologic and hydrogeologic structure of the site was characterized in detail. Plumes of groundwater contamination were identified, and the extent and sources of contamination were determined. Various technologies, both established and emerging, are being tested to determine their remediative effectiveness for the Berkeley Lab site. The presence of dense nonaqueous-phase liquids in fine-grained, low-permeability material makes aquifer cleanup at Berkeley Lab a very challenging task. The work involves geologists, hydrogeologists, geophysicists, and hydrogeochemists in a multidisciplinary effort, characteristic of many HRD research projects.

Other efforts in this area include understanding some of the conceptual issues governing tracer transport in heterogeneous media (with particular emphasis on the effect of variable saturation regimes), developing advanced numerical and semi-analytical models for transport studies of solutes and colloids in porous and fractured complex geologic media, and advancing well-test techniques and borehole-measurement methods to identify and estimate formation parameter values. Another subject in which HRD has considerable experience is the emplacement of *in situ* barriers using a new generation of materials (such as gels) to contain the contaminant plume. This experience manifests itself both in the choice of barrier materials and the optimization of emplacement strategy.

UNSATURATED ZONE HYDROLOGY

While the majority of research in HRD in unsaturated zone hydrology is stimulated by the need to understand flow and transport in the unsaturated zone at Yucca Mountain, Nevada, efforts are also underway to study flow and transport in unconventional unsaturated zones. Field measurements from active flow experiments along with monitoring of ambient conditions in the Exploratory Studies Facility (ESF) at Yucca Mountain remain the primary focal point for research in HRD. Results from the broad field campaign of testing in the ESF are the object of analysis by advanced theoretical and numerical approaches, including chaotic-flow models. In addition, observations in the field have inspired new laboratory work to be carried out at Berkeley Lab on rock samples from the ESF. We are also increasingly active in studies of contaminant migration and remediation in the unsaturated zone of the Hanford site. As for unconventional unsaturated zones, HRD is investigating the flow and transport of CO_2 in deep geologic formations such as depleted natural-gas reservoirs, as well as flow, transport, and biodegradation in landfills, a man-made unsaturated zone.

FRACTURE AND STOCHASTIC HYDROLOGY

For more than two decades, HRD has been active in the field of fracture hydrology, being one of the first groups to develop a fracture-network model and a channeling model of flow through variable-aperture fracture systems, and to apply annealing modeling to fracture hydrology. Our work is characterized by close interaction between modeling and field data evaluation, with complementary laboratory studies. This work continues and has been further generalized to research into strongly heterogeneous media, including studies with stochastic-continuum and double-permeability models. Work in HRD demonstrated flow-channeling phenomena in both 3D saturated and unsaturated media. Furthermore, new field meas-

urement techniques are being developed to measure strongly varying permeabilities in boreholes and along underground tunnels. The former includes the further advancement of the dynamic borehole fluid-logging method developed at Berkeley Lab some years ago. The latter includes so-called systematic testing, which is a repeated set of experiments at regularly spaced distances along an underground tunnel to provide unbiased data for stochastic modeling.

FLOW AND TRANSPORT MODELING

HRD has a long history in numerical modeling of flow and transport in geologic media. A suite of numerical models using finite-element, finite-difference, and integrated finite-difference methods has been developed. The most well-tested and applied computer code is the TOUGH family of simulators, which calculates flow and transport of multiphase, multicomponent fluids in complex fractured porous media under isothermal and nonisothermal conditions. A number of equation-of-state packages have been developed for different fluids appropriate for environmental, nuclear waste disposal, oil and gas, and geothermal reservoir applications. Associated with these codes are the iTOUGH codes, which perform inverse calculations of parameter estimation for such complex systems.

Current development involves a new code that implements reactive chemistry into the TOUGH codes. This includes both homogeneous reactions, such as aqueous complexation and redox reactions, and heterogeneous reactions, such as ion exchange, adsorption, mineral dissolution and precipitation, and gas dissolution and exsolution. The new code is called TOUGHREACT, which has already been applied to analyze several sets of real field data with success. Work is also underway on a new code called TMVOC, which enhances T2VOC for multicomponent mixtures of volatile organic chemicals.

The coupling of mechanical stress and temperature effects of permeability in fractured rock is important for injection testing, stimulation of oil and gas reservoirs as well as geothermal reservoirs, and nuclear waste repository performance. HRD's work involves the development of a coupled thermal-hydrologic-mechanical (THM) simulator for modeling of fully coupled HM processes in saturated and unsaturated media. Another effort has involved the coupling of two powerful existing codes, TOUGH2 and the industry-standard code FLAC3D. The latter calculates mechanical and THM processes in soil and rock mechanics. The joining of these two codes into one, named TOUGH-FLAC, gives us a new capability for addressing these coupled THM problems. So far, we have applied the TOUGH-FLAC code to THM problems related to the potential radioactive waste repository at Yucca Mountain and to CO_2 injection into deep brine aquifers.

RESERVOIR ENGINEERING

HRD is also very active in the study of oil and gas reservoirs as well as geothermal reservoirs. This includes optimization and control theory to maximize fluid production through a hydrofracturing process, using injection wells. Advanced and unconventional well-test methods to determine and characterize production zones have been developed. Quasi-static and dynamic pore-network simulators are being implemented to understand drainage and imbibition processes in reservoir rocks during flooding operations. Depositional models are being constructed and studied using distinct-element methods. Micromechanical models of rock damage under compaction are studied and calibrated with experimental results, while the dynamics of nonequilibrium co- and countercurrent imbibition are also being studied.

An interesting application for these studies is diatomaceous fields, which represent potentially billions of barrels of high-quality oil. However, production from the diatomites requires a secondary recovery process because of their low permeability, even though they have high porosity. As a result, research into rock damage in primary production and flooding is being conducted to explore optimal production strategies. Joint inversions of 3D electromagnetic geophysical data and reservoir data are performed. We are also developing stabilized finite-element methods for modeling multiphase flow in fractured porous media. A novel treatment of the unresolved subgrid scales was required for better numerical solutions of difficult problems that involve shock and boundary-layer formation.

FUNDING

Funding for HRD comes primarily from the U.S. Department of Energy, including: Office of Science, Office of Basic Energy Science, Geosciences Research Program; Office of Biological and Environmental Research; Assistant Secretary for Energy Efficiency and Renewable Energy, Office of Wind and Geothermal Technologies; Office of Civilian Radioactive Waste Management; and the Assistant Secretary for Environmental Management. The department also receives funding support from the U.S. Environmental Protection Agency. Other funding is provided through the Laboratory Directed Research and Development Program at Berkeley Lab.

RESOURCE DEPARTMENT

GEOPHYSICS AND GEOMECHANICS

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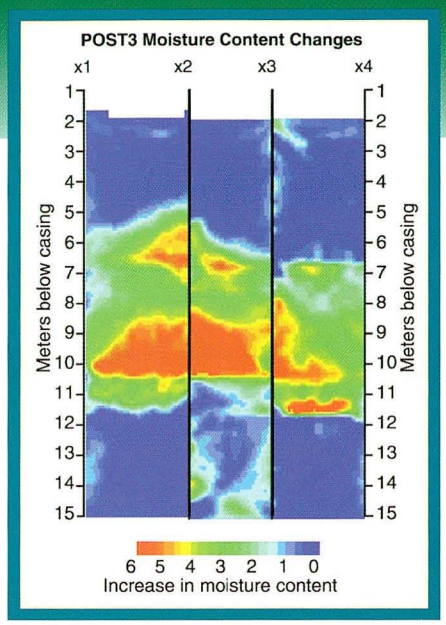

The Geophysics and Geomechanics Department performs a wide variety of work, ranging from fundamental to applied research.

SCIENTIFIC THRUSTS

The department is organized into three different research areas:

- Seismology (including the Center for Computational Seismology)
- Electrical and Potential Methods
- Rock and Soil Physics

These groups work closely together to address issues in subsurface imaging over a wide range of scales. The scientific thrusts have been in joint inversion, wave propagation in complex media (seismic and electromagnetic), coupled-process definition, and heterogeneity definition. New areas of research are in fluid imaging and "smart" reservoir exploitation. Much of the work focuses on developing and applying high-resolution geophysical methods to derive physical, chemical, and biological properties affecting flow and transport in heterogeneous media. A prime example is the work funded by the Department of Energy's Natural and Accelerated Bioremediation Research (NABIR) program for bacterial injection work. Another primary thrust involves using geophysical methods for fracture quantification. This thrust is evident in the range of studies (from fundamental to applied) that we carry out for DOE's Fossil Energy, Environmental Restoration, Nuclear Waste, and Geothermal programs.

The Geophysics and Geomechanics Department is unique within the national laboratory and academic communities in having equally strong theoretical, modeling, lab, field/data acquisition, and processing/interpretation capabilities. The department also works very closely with industrial partners in oil and gas and geothermal applications. This both strengthens the applied work and provides feedback into the fundamental studies.

INTEGRATED APPROACH TO FUTURE WORK

The future thrusts of the department are to continue to develop, test, and apply high-resolution geophysical methods not only for characterizing static properties of the subsurface, but for estimating dynamic properties as well. We plan to accomplish this through an integrated effort of theoretical, laboratory, and field programs. A specific thrust will be in the joint use of seismic and electrical methods for subsurface imaging and fluid-properties characterization. We have found that to address complex issues such as site remediation, flow and transport in fracture systems, vadose zone transport, CO_2 sequestration, and reservoir stimulation, we must use an integrated approach to geophysics and geomechanics.

FUNDING

The work of the Geophysics and Geomechanics Department is derived from a variety of U.S. Department of Energy and Work For Others sources. The primary sources of funding are the DOE's Office of Science (Basic Energy Sciences/Chemical Sciences and Office of Biological and Environmental Research), Office of Fossil Energy. Other funding sources include the U.S. Environmental Protection Agency, U.S. Air Force Office of Scientific Research, and the U.S. Geological Survey's Earthquake Hazard Reduction Program. Support has also been received from a variety of oil and service companies, including BP, Chevron, Conoco, Exxon, Schlumberger, and Shell Oil.

RESOURCE DEPARTMENT

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The Earth Sciences Division's Geochemistry Department combines expertise in chemical and isotopic analysis, molecular environmental science, mineralogy, and multiscale data-gathering methodology to enable geochemical characterization of earth systems from the macroscopic to the molecular. The department comprises four groups with complementary interests and capabilities.

AQUEOUS GEOCHEMISTRY

Studies in this group address issues of contaminant sequestration and migration in the environment, mineral-fluid reactions, and various aspects of aqueous solutions. Recent work includes characterization of the selenium speciation, transport, and reaction rates within soil horizons at the Kesterson Reservoir, a site where national attention is focused as a result of selenium poisoning of wildlife related to agricultural runoff. Related investigations examine arsenic transport and redox reactions in soils, and microbial effects on the speciation of selenium in hydrologic systems. The important but overlooked effects of the vadose zone air-water interface on the transport of colloids has been identified and quantified by department scientists.

Fundamental studies on the nature of the aqueous solution/mineral interface and on the structure of near-aqueous solvated ions and colloids are also being performed. The aim of these studies is to provide improved modeling capability for contaminant migration, weathering, sediment transfer, ion exchange, and nutrient cycles. Current work includes: molecular-dynamics modeling of the interlayer-solvated cations in clays; studies of the solvation environment of contaminant and nutrient molecules in aqueous solution; determination of the molecular identity of initial iron oxide precipitates on quartz surfaces; and characterization of environmentally important minerals via simulation, x-ray scattering, and x-ray spectroscopy methods. Many of these efforts involve newly developed capabilities utilizing synchrotron x-ray sources. Important new work on the aqueous behavior of humic and fulvic acids, hydroxyl speciation near cations in water, and the nature of organic contaminants on mineral surfaces has been carried out recently at Berkeley Lab's Advanced Light Source.

ISOTOPE GEOCHEMISTRY

The Isotope Geochemistry group operates the Center for Isotope Geochemistry, which was established in 1988 and includes six important analytical facilities: stable isotope and noble gas isotope laboratories; a soil carbon laboratory; an analytical chemistry laboratory; the Inductively Coupled Plasma Multi-Collector Magnetic Sector mass spectrometry laboratory, and a thermal-ionization mass spectrometry laboratory located on the UC Berkeley campus. We also have an affiliation with the cosmogenic isotope laboratory in UC Berkeley's Space Sciences Laboratory. These facilities provide state-of-the-art characterization of all types of earth materials for research throughout the department and elsewhere in the division. Further, they support the Center's goals of finding new ways to utilize isotopic ratio methods to study earth processes, and applying isotopic and chemical analysis procedures to specific environmental and energy problems of national interest.

Current research programs include: (1) the development of models that use isotopic composition data from element pairs in fluids to constrain fluid flow rates, water-mineral reaction rates, and the geometry and spacing of fractures in rock matrices; (2) the development and application of noble gas isotopes as natural tracers for injectate return in geothermal reservoirs and as natural tracers for fluid source and movement in hydrocarbon and geothermal systems; (3) the geochemical monitoring and analysis of large-scale experiments simulating the effects of nuclear waste heat generation within the nuclear repository in Yucca Mountain, Nevada; (4) the application of helium and neodymium isotopes to determine magma-chamber recharge rates in areas having possible volcanic hazards or the potential for geothermal energy extraction; (5) the development of C, N, and O isotope techniques for quantifying *in situ* bioremediation and environmental restoration; and (6) the use of carbon isotopes to quantify rates of organic carbon cycling and storage efficiency in soils, the impact of climate change on carbon cycling, and linkages between carbon, water, and nitrogen cycles. A new program is underway to study Fe isotope variations as a tracer in the oceanic and terrestrial Fe cycles.

ATMOSPHERE AND OCEAN SCIENCES

The focus of this group is on the characterization of conditions and chemical components in the oceans and atmosphere, and the development of process models using these inputs combined with other hydrospheric data to explain and predict climatic change. The group operates the NASA-sponsored California Water Resources Research and Applications Center and the DOE Center for Research on Ocean Carbon Sequestration. Both of these centers have made significant progress in program development in the ESD Geochemistry Department.

The California Water Resources Research and Applications Center has maintained a suite of research and operational tools for weather forecasts, climate prediction, and basic research. The

core hydroclimate and impacts team has expanded, with new projects from the California Energy Commission, CALFED, and the DOE Water Cycle Initiative. Numerous ongoing collaborations include: streamflow simulations with the National Oceanic & Atmospheric Administration's California Nevada River Forecast Center; runoff contaminant monitoring and management with the U.S. Bureau of Reclamation; development of landslide-hazard prediction models with faculty at UC Berkeley; development of snow-cover and snow-water equivalent maps for California with UC Santa Barbara; and development of a shared information distribution system with the U.S. Department of Energy's Accelerated Climate Prediction Initiative (DOE/ACPI) collaborators. Outreach activities for this year have included a scientific exchange program with AmazonTech.

Ocean-carbon cycle science has grown significantly at Berkeley Lab in the last year, with major new initiatives in the laboratory and at sea. Last year, the DOE Center for Research on Ocean Carbon Sequestration (DOCS) was established here, with co-hosting at Lawrence Livermore National Laboratory. The center's mission is to provide answers to scientific questions needed to evaluate the feasibility, effectiveness, and environmental/geochemical consequences of proposed methods to enhance the transfer of CO_2 from fossil fuel combustion into the ocean. DOCS collaborators include scientists from Massachusetts Institute of Technology, Rutgers University, Scripps Institution of Oceanography, Moss Landing Marine Laboratories, Monterey Bay Aquarium Research Institute, and the Pacific International Center for High Technology Research.

Berkeley Lab is now an ocean-going institution. In the past year, Lab scientists led several cruises from Scripps Institution of Oceanography in San Diego to test new optical carbon sensors and low-power, long-lived, robotic profiling floats for long-term carbon cycle monitoring. The robot floats and related platforms that can glide through seawater (or navigate) are designed to fill a major gap in at-sea observations of the ocean's biological systems and how they respond to natural and human perturbations. In April this year, the program realized a stunning operational success when it deployed the first pair of robotic profiling observers instrumented with carbon biomass sensors in the stormy North Pacific Ocean 1,000 miles west of Seattle. The floats, which cycle between the surface and depths as great as 1,000 m three times every two days, are still operating and are relaying their data in real time to Berkeley Lab. In the near future, the team will participate in SoFeX, an NSF-DOE-funded experiment to evaluate the biotic and carbon system response of the nutrient-rich Antarctic Circumpolar Current to iron addition.

GEOCHEMICAL TRANSPORT

A major effort of this group is the simulation and study of coupled mineral-water-gas reactive transport in unsaturated porous media—particularly in fractured rock under boiling conditions. This work has focused mostly on predicting thermally driven processes accompanying the potential emplacement of high-level nuclear waste at Yucca Mountain, Nevada, and on the understanding of the evolution of the natural hydrogeochemical system and such controlling factors as water infiltration and water-rock interaction. Collaboration among others in the division brings together essential pieces of the problem, including hydrological processes in the unsaturated zone, thermodynamics and kinetics of geochemical processes, and isotopic effects.

Current projects include:

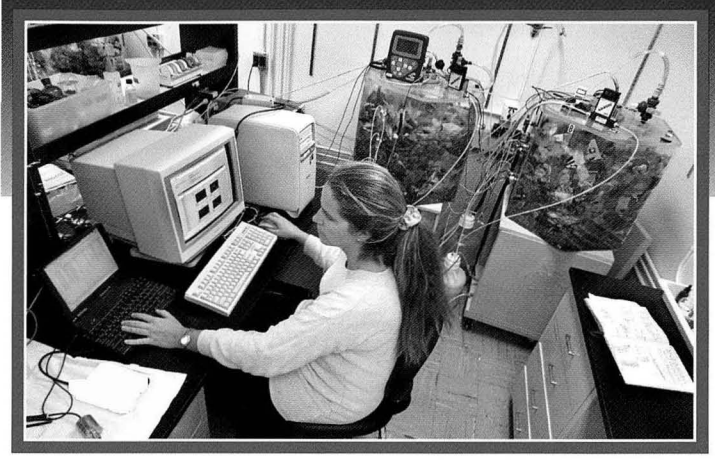
1. Simulation and analysis of an ongoing large-scale underground thermal test. Planning and design of future underground thermal testing and sample collection.
2. Prediction of the coupled thermal-hydrological-chemical processes around potential waste-emplacement tunnels and concomitant changes in water and gas chemistry, mineralogy, and flow.
3. Analysis of geochemical data from Yucca Mountain to constrain models of flow and transport in the unsaturated zone.
4. Development of models for reactive-transport in unsaturated systems and improvements in the reactive-transport code TOUGHREACT developed at Berkeley Lab.
5. Evaluation and development of improved thermodynamic and kinetic databases for water-rock interaction modeling.
6. Research on natural analogue sites, including (a) analysis of continuously cored intervals from the Yellowstone geothermal system to assess effects of mineral alteration on fracture and matrix permeability, (b) study of flow, transport, and secondary mineralization at Peña Blanca, Mexico, (c) anthropogenic analogues, such as those at the Idaho National Engineering and Environmental Laboratory. A comprehensive review of natural analogues is also underway.
7. Simulation and analysis of lab experiments of boiling in fractured tuff.
8. Modeling of CO_2 sequestration.
9. Evaluation of solvent extraction using room-temperature ionic liquids to strip and recover hazardous organic contaminants dissolved in ground and surface waters.

FUNDING

Funding for the Geochemistry Department comes from a variety of sources, including: the U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences, Divisions of Materials Sciences, and Engineering and Geosciences; DOE Office of Environmental Management, Office of Science and Technology; Office of Energy Efficiency and Renewable Energy, Office of Utility Technologies, Office of Geothermal Technologies; Office of Biological and Environmental Research; DOE Office of Civilian Radioactive Waste Management; U.S. Environmental Protection Agency; U.S. Navy; National Aeronautics and Space Administration, Office of Space Science and NASA Earth Enterprise; National Science Foundation, Office of Polar Programs; the University of California Campus-Laboratory Collaboration Hydrology Project; National Oceanographic Partnership Program (administered by the Office of Naval Research); National Oceanic and Atmospheric Administration, Office of Global Programs of the U.S. Department of Commerce, and the Laboratory-Directed Research and Development Program at Berkeley Lab.

RESOURCE DEPARTMENT

MICROBIAL ECOLOGY AND ENVIRONMENTAL ENGINEERING



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SCIENTIFIC FOCUS AREAS

The Microbial Ecology and Environmental Engineering Department (MEEED) maintains the highest quality and highest visibility for its research and development in two areas:

1. Real-time direct environmental assessment
2. Biological treatment, bioremediation, and natural attenuation

These two R&D areas are largely integrated, but contain some domains that are not inclusive. These two areas are considered MEEED's core competencies. (Note: MEEED is also increasingly interested in adding bioprocessing as another research focus area in the near future.)

REAL-TIME DIRECT ENVIRONMENTAL ASSESSMENT

The last decade has seen a revolution in information technology and in the power of microprocessors. It has also seen a quantum leap in the use of physical, chemical, and biological sensors, as ever-more-sensitive detection techniques have been married to these powerful data processing engines. The field of environmental assessment has only recently awakened to the potential that these new sensors offer. It has also become painfully obvious over the past decade that the dynamics and true understanding of functional biogeochemical processes in all types of environments cannot be fully understood without direct physical, chemical, and biological measurements. Indeed, what goes on in the sampling device and sample bottle after collection may have nothing to do with the functional dynamics of the original environment that the sample was taken from, thereby affecting our fundamental understanding of that environment and how to characterize, monitor, and control it. Hence, real-time direct environmental assessment is an area in which MEEED—with its unique facilities in the Center for Environmental Biotechnology, engineering, molecular biology, chemistry facilities, and access to the Advanced Light Source and the Center for Isotope Geochemistry—can demonstrate unique R&D capability.

Berkeley Lab has long provided scientific leadership in the disciplines of experimental physics, physical chemistry, geology, hydrology, geochemistry, molecular biology, modeling, and (more recently) natural attenuation and bioremediation technologies. Hence, MEEED is well situated to capitalize on the Lab's strengths while advancing the science in real-time direct environmental assessment. Specific focus areas include: real-time field sampling and monitoring, field sampling technologies, environmental sensors, environmental modeling and decision support systems, biogeochemical analysis (sample collection; microbial physiology; molecular-level analyses including DNA sequencing and terminal restriction-fragment-length polymorphism [T-RFLP] analysis; fatty-acid methyl ester analysis; signature lipid biomarker analysis; synchrotron-based x-ray, Fourier Transform infrared [FTIR], and x-ray spectromicroscopy techniques; stable isotopic analysis), and environmental risk assessment.

BIOLOGICAL TREATMENT, BIOREMEDIATION, AND NATURAL ATTENUATION

Biological treatment, bioremediation, and natural attenuation has been a rapidly growing area of science over the past decade. The acceptance of natural attenuation as a solution for cleaning up contaminated sites, and DOE's recognition that they will have long-term stewardship issues that they must address at the most contaminated sites, has greatly increased the urgency for basic and applied research related to microbial ecology and biogeochemistry. This type of research is truly enabling for natural attenuation, since characterization, predictions, and verification monitoring require a strong scientific basis. Natural attenuation is viewed as the best solution for cleaning up many waste sites and will save billions of dollars in cleanup costs. Bioremediation, both *in situ* and *ex situ*, have also enjoyed strong scientific growth, in part due to the increased use of natural attenuation, since most natural attenuation results from biodegradation. Bioremediation and natural attenuation

are also seen as a solution for emerging contaminant problems (e.g., methyl-*tert*-butyl ether [MTBE], endocrine disrupters, landfill stabilization, mixed waste biotreatment, and biological carbon sequestration).

MEEED scientists and engineers are recognized leaders in the field of biological treatment, bioremediation, and natural attenuation. The Center for Environmental Biotechnology provides the primary facilities used by MEEED, including state-of-the-art equipment for microbiology and environmental engineering. MEEED investigators have extensive experience in both water treatment and bioremediation, especially co-metabolic biodegradation and the treatment of inhibitory compounds. In addition to basic research, MEEED investigators have been involved in various aspects of more than 60 field demonstrations and deployments, and have five patents in this area that are licensed to more than 30 companies. The types of contaminants in which MEEED investigators have expertise include chlorinated solvents, petroleum hydrocarbons, polynuclear aromatic hydrocarbons, ketones, MTBE, TNT, inorganic nitrogen (NO_3, NH_4), tritium, Pu, Np, Cr, and U. The Biotreatment, Bioremediation and Natural Attenuation area has both basic research and field application foci for the MEEED. The basic research foci are co-metabolism, biotreatability, biotransformation kinetics, and modeling of biogeochemical processes. Field-application foci are co-metabolic techniques, biogeochemical assessment techniques, and modeling of attenuation and environmental fate.

FUNDING

MEEED personnel are funded by DOE Programs in (1) the Office of Science, Office of Biological and Environmental Research (OBER) (Natural and Accelerated Bioremediation Research Program); (2) the Office of Environmental Management, Offices of Science and Technology (EM50) (Subsurface Contaminants Focus Area) and Environmental Restoration Program (EM40); (3) the Office of Fossil Research, the Petroleum Environmental Research Forum, and (4) the National Nuclear Security Administration, Office of Nonproliferation Research and Engineering (NN20). In addition, support is obtained from the Department of Defense, U.S. Army Corps of Engineers, for the Bioremediation Education Science and Technology (BEST) Program; the Department of the Interior, Bureau of Land Management, and Bureau of Reclamation under the CALFED program, for bioreactor treatment of groundwater containing MTBE obtained from a remediation company, as well as several projects with remediation companies using DOE-patented technologies for *in situ* bioremediation. MEEED personnel are also funded by Berkeley Lab's Laboratory Directed Research and Development Program in the area of aerobic bioreactor studies of landfills.

Fundamental and Exploratory Research

Nuclear Waste

Energy Resources

Environmental Remediation Technology

Climate Variability and Carbon Management

RESEARCH PROGRAM

FUNDAMENTAL AND EXPLORATORY RESEARCH

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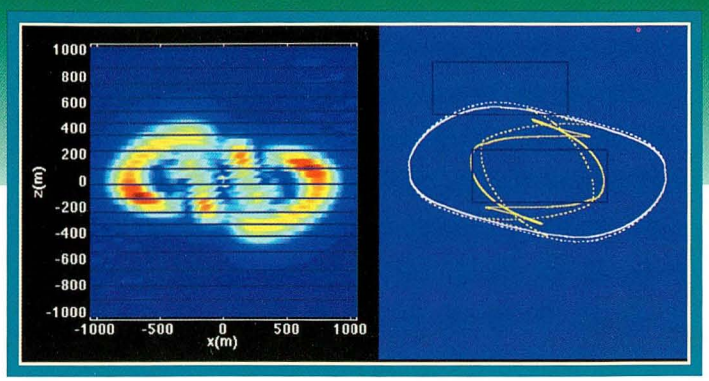

The Fundamental and Exploratory Research Program (FERP) covers fundamental earth sciences research conducted in support of the Department of Energy's science mission. This mission includes research in the natural sciences to provide a basis for new and improved energy technologies and for understanding and mitigating the environmental impacts of energy development and use. FERP also includes exploratory research in important new energy and environmental topics conducted under the Laboratory Directed Research and Development (LDRD) program. The scientific insights and breakthroughs achieved in FERP often become the underpinnings for projects that support DOE's applied research and development program offices.

Over the years, the basic earth sciences research program at Berkeley Lab has focused on three broad earth sciences problems:

1. Fundamental studies of chemical and mass transport in geologic media, with special reference to predictive modeling of multiphase, multicomponent, nonisothermal fluid flow in saturated and unsaturated fractured rocks
2. The development of new isotopic techniques for understanding the nature of a broad range of global processes—from the relatively short-term effects of natural fluid migration in the crust to longer-term (i.e., 10–20 thousand years) global climate variations
3. Fundamental studies in the propagation of seismic/acoustic and broadband electromagnetic waves through geologic media, with emphasis on new computational techniques for high-resolution imaging of near-surface and crustal structures (such as possible fracture flow paths) and for inferring the types of fluids present in pores and fractures

Results from these research endeavors have had a major impact on applied energy, environmental, and radioactive waste management programs. Current research projects are briefly described here.

CHEMICAL AND MASS TRANSPORT INVESTIGATIONS

Current research in this area is focused on colloid transport in unsaturated porous media and rock fractures, chemical transport in structured porous media, unsaturated fast flow in fractured rock, and production and evaluation of coupled processes for CO_2 in aquifers. Our recent colloid research has been focused on quantifying the partitioning of surface-active colloids at the air-water interfaces. Much effort has been devoted to characterizing surface accumulations of colloids. We have recently developed a simple dynamic method to quantify colloid-surface excesses at air-water interfaces without requiring assumptions concerning the thickness of interfacial regions.

The studies of chemical transport in structured porous media have focused on Cr(VI) diffusion and reduction to Cr (III) within natural soil aggregates, to test the validity of our previously reported results from synthetic soil aggregates. Experiments were conducted on intact aggregates of Altamont clay. Work on unsaturated fast flow in fractured rock concerns water films on fracture surfaces under near-zero (negative) matric potentials and examines the possibility of fast, unsaturated flow under "tension." We showed that at matric potentials greater than that needed to saturate the rock matrix, transmissive water films can develop on fracture surfaces.

In the work on prediction and evaluation of coupled processes for CO_2 disposal in aquifers, the accuracy of published data and correlations for thermophysical properties of CO_2 (density, viscosity, enthalpy) is being evaluated for the range of pressure and temperature conditions of interest in aquifer disposal. Suitable correlations are being implemented in our multipurpose simulator TOUGH2. Pre-existing models for CO_2 dissolution in aqueous fluids are being enhanced by incorporating salinity and fugacity effects. Special techniques are also being developed for describing the movement of sharp CO_2-water interfaces during immiscible displacement of saline brines by CO_2.

ISOTOPE GEOCHEMISTRY

The Center for Isotope Geochemistry (CIG) is a state-of-the-art analytical facility established in 1988 to measure the concentrations and isotopic compositions of elements in rocks, minerals, and fluids in the earth's crust, atmosphere, and oceans. Fundamental research conducted at this center is directed at finding new ways to use isotopic information to study earth processes, such as long-term climate changes, and at predicting the chemical transport of mantle-derived or deep crustal fluids as they move through the crust.

One of the major problems being studied at CIG is how to estimate fluid-solid reaction rates in natural-groundwater higher-temperature geothermal conditions, particularly as these rates affect mineral dissolution and secondary mineral precipitation. ESD researchers are developing novel ways of estimating reaction rates by using isotopic tracers (primarily Sr, but also U and Nd) to determine solid-fluid exchange rates in various natural situations. Scientists are able to derive the "reaction length," a parameter that depends on the ratio of isotope transport by diffusion and advection to the reaction rate. The ultimate objective is to understand the microscopic (as well as pore-scale and mesoscale) characteristics of natural systems that have been characterized in terms of "field scale" reaction-rate measures. An intermediate goal is to establish empirically the natural range of fluid-solid reaction rates.

ADVANCED COMPUTATION FOR EARTH IMAGING

The Center for Computational Seismology (CCS) was created in 1983 as the Berkeley Lab and UC Berkeley nucleus for seismic research related to data processing, advanced imaging, and visualization. In recent years, a great deal of cross-fertilization between seismologists and other geophysicists and hydrogeologists has developed within the division, resulting in collaborations on a wide variety of fundamental imaging problems. A primary thrust in this research has been to jointly develop seismic and electrical methods for understanding fluid flow and properties within the subsurface. In addition, fundamental studies on improved inversion and modeling of complex media in 3D are being carried out to analyze such effects as matrix hetergeneity fluid flow and anisotropy. Applications range from small-scale environmental problems to oil and gas reservoirs.

ROCK PHYSICS

A variety of rock and soil science experiments are being conducted through ESD's Geoscience Measurements Facility, which supports both field and laboratory work. In one new laboratory project, researchers are studying the compaction and fracturing of weakly cemented granular rocks. This study examines the effect of micromechanical properties of weak granular rock on macroscopic properties such as load-displacement response, ultimate strength, and failure mode. In a second study, a fundamental investigation of scattering and intrinsic attenuation of seismic waves in rock with heterogeneous distributions of fluids and gas is being conducted. This research represents a departure from past rock-physics studies on seismic attenuation, in that the emphasis here is not a detailed study of a specific attenuation mechanism, but rather to investigate theoretical and laboratory methods for obtaining separate estimates of scattering and intrinsic attenuation in rock with heterogeneous pore-fluid distributions.

FUNDING

Funding for research in FERP comes from a variety of sources. These include (primarily) the U.S. Department of Energy's Office of Science, Office of Basic Energy Sciences, Division of Chemical Sciences, Geosciences, and Biosciences; the Office of Biological and Environmental Research; and the Assistant Secretary for Fossil Energy, Office of Natural Gas and Petroleum Technology, through the National Petroleum Technology Office, Natural Gas and Oil Technology Partnership. Funding is also provided by the Laboratory Directed Research and Development Program at Berkeley Lab. Additional support comes from DOE's Office of Environmental Management Science Program.

GEOCHEMISTRY AND ISOTOPE CONSTRAINTS IN OIL HYDROGEOLOGY

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RESEARCH OBJECTIVES

This research project evaluates the sources and processes that provide, dissolve, and distribute noble gases (He, Ne, Ar, Kr, Xe) and noble-gas isotopes among liquid hydrocarbon, gaseous hydrocarbon, and aqueous phases. On a basin or field scale, this information is used to evaluate hydrocarbon sources and characteristics, groundwater end-members, and migration processes, mechanisms, and time scales over which these processes occur.

APPROACH

The mechanisms, processes, and time scales of fluid flow in sedimentary basins are fundamental questions in the earth sciences, with direct application to exploration and exploitation strategies for energy and mineral resources. This project investigates the noble-gas composition of hydrocarbon samples on a basin and field scale, where adequate commercial production and ancillary information are available, to provide a test of the use and applicability of noble gases to delineate end members, migration mechanism, and migration paths for hydrocarbons.

ACCOMPLISHMENTS

Production fluid from the North Sea's Snorre and Statfjord oil fields show clear geographical correlation in their noble-gas isotope and abundance characteristics. Mixing relationships coupled with the geographical compositional trends (Figures 1 and 2) suggest that (1) both reservoirs were filled with oil from a common source, (2) with migration into each reservoir, the inherited noble gases from the hydrocarbon source area are diluted with noble gases from the existing *in situ* reservoir fluids, and (3) fluid flow was from a direction contrary to existing migration scenarios. The fluid in each reservoir had a different *in situ* noble gas composition, and the differences may be related to the regional tectonics. Specifically, the Viking Graben, a zone of active extension, may be the source of the ^{3}He-enriched mantle-derived fluids found in the Snorre reservoir.

SIGNIFICANCE OF FINDINGS

The unique aspects of noble-gas geochemistry have led to a better understanding of processes related to the occurrence and distribution of hydrocarbon resources in large sedimentary basins. A better understanding of which hydrocarbon source areas contribute to the different reservoirs within larger hydrocarbon provinces constrains migration pathways, reservoir filling sequences, and existing (and often uncertain) migration models, potentially leading to new oil-producing prospects and hitherto unexplored fields.

RELATED PUBLICATIONS

Kennedy, B.M., and T. Torgersen, Multiple atmospheric noble gas components in hydrocarbon reservoirs: A study of the Northwest Shelf, Delaware Basin, SE New Mexico, Geochim Cosmochim Acta, 2001 (submitted).

Torgersen, T and B.M. Kennedy, Air-Xe enrichments in Elk Hills oil field gases: role of water in migration and storage, Earth Planet. Sci. Lett. 167, 239–253, 1999.

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ACKNOWLEDGMENTS

This project is supported by the Director, Office of Science, Office of Basic Energy Sciences, Division of Chemical Sciences, Geosciences, and Biosciences, of the U.S. Department of Energy under Contract No. DE-AC03-76-SF00098.

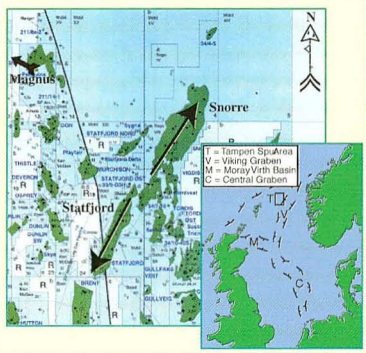

Figure 1: Map showing the location of the Snorre and Statfjord oil fields in the North Sea. The arrows indicate the proposed direction of hydrocarbon migration as inferred from trends in the elemental and isotopic composition of noble gases associated with the produced hydrocarbons (see Figure 2).

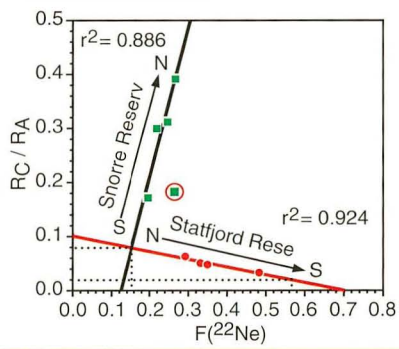

Figure 2: The helium isotopic compositions (R_c/R_A) and $^{22}Ne/^{36}Ar$ ratios [F(^{22}Ne)], normalized to their respective values in air, for hydrocarbons produced from the Snorre and Statfjord, North Sea reservoirs. The compositional trends suggest a common source (the intersection of the mixing lines, determined by a least squares fit to the data sets) with subsequent acquisition of noble gases during migration.

COMPUTATION OF SEISMIC WAVEFORMS IN COMPLEX MEDIA: CARBON DIOXIDE SEQUESTRATION IMAGING

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RESEARCH OBJECTIVES AND APPROACH

The underground sequestration of CO_2 presents a subsurface monitoring problem that requires new approaches. This specific CO_2 problem is an important example of the need for effective tools applicable to subsurface-imaging problems. Seismic tomographic imaging methods are compromised severely when the target region and/or the background medium are complex at the wavelength scale of the probing waves. The relationship between seismic response and fluid saturation in a reservoir depends on many factors. But there is a general connection between the character of porous-layer saturation and seismic response, which has to do with the frequency content of reflected waves. Our objective is to explore opportunities to use the frequency dependence of seismic reflections for underground reservoir imaging and monitoring. Our approach is to model the seismic response of dry and water-saturated porous layers in the laboratory, using ultrasonic frequencies to find differences in seismic response resulting from the character of fluid saturation.

ACCOMPLISHMENTS

The effect of stronger reflections and travel-time delays from water-saturated layers is observed at low frequencies (Figure 1). Measurements of the Q factor for porous layers revealed very low values for both dry and water-saturated cases. These values are close to seismic extremes, but their existence can be explained by very small thicknesses that cannot absorb seismic-wave energy completely. For the water-saturated layer, we found lower values of Q that showed an increase in both "frictional" and "viscous" attenuation. In all cases, Q monotonically increases with frequency. While the behavior of the reflection coefficient from the attenuative layer is rather complex, the ratio of reflection coefficients for water-saturated and dry layers reveals a strong monotonic increase in reflection amplitudes at low frequencies. The rate of this increase is more profound for the reflections from thin layers compared to the reflections from a thicker layer or a half space.

We compared the results of laboratory modeling with a "frictional-viscous" theoretical model and found that low (<5) values of attenuation parameter Q and its approximate proportionality to frequency can explain the effect. The values of Q were determined in a separate experiment, using recordings of a transmitted field for a thick, porous layer that, when saturated, had attenuation of about two times higher than under dry conditions. These findings can be used for detecting and monitoring liquid saturated areas in thin porous layers.

This reflection feature is a useful indicator of attenuative properties in thin porous layers. Attenuation for such layers strongly depends on the character of liquid saturation. The observed reflection travel-time change fits theoretical predictions quite well. Layers with higher attenuation create travel-time delays that increase as the frequency approaches zero. This property was observed on real data and can serve as an additional indication of liquid saturation in porous layers. The differences of dry and water-saturated layer reflectivities are clearly seen at high- and low-frequency domains. Physical interpretation of frictional-viscous dissipation terms remains uncertain. However, one of the applications for this theoretical model will be time-lapse imaging of gas/steam and CO_2-injection experiments in existing oil fields (with the goal of better understanding steam floods), CO_2 sequestration, gas storage, and geothermal reservoir exploitation.

ACKNOWLEDGMENTS

This project is supported by the Director, Office of Science, Office of Basic Energy Sciences, Division of Chemical Sciences, Geosciences, and Biosciences of the U.S. Department of Energy under Contract No. DE-AC03-76-SF00098.

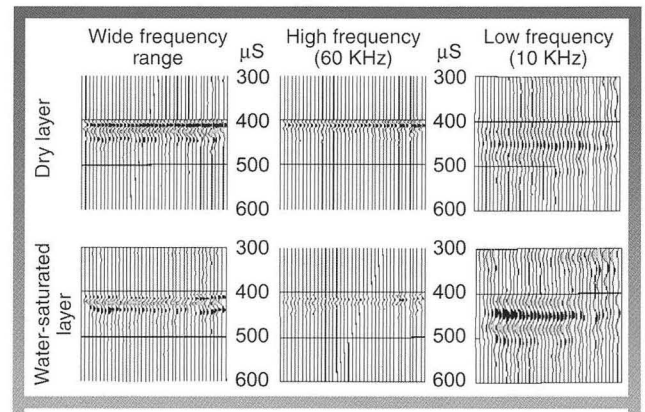

Figure 1. Data (left panels) and imaging of thin porous layers using common offset gathers by different filtering for dry and water-saturated cases.

WAVE PROPAGATION THROUGH A POROUS MEDIUM CONTAINING TWO IMMISCIBLE FLUIDS

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RESEARCH OBJECTIVES

It has been suggested recently that the application of either periodic compression and relaxation, or continuous perturbation under constant external pressure, to a fluid-containing porous medium can increase fluid flow rates. The generalization of theory to describe this wave-excitation effect in an unsaturated porous medium is of considerable relevance to many applications (e.g., enhanced oil recovery, water-resource exploitation, and chemical-pollutant removal). Despite more than 50 years of research devoted to explaining the physical mechanisms involved in the phenomenon of linear wave propagation and attenuation in an unsaturated elastic porous medium, the theory is not well established. The objective of this study is to develop a mathematical description of this phenomenon in a systematic manner.

APPROACH

The theory of continuum mechanics in principle deals with one component, which is not appropriate for multicomponent materials. Therefore, we applied the theory of continuum mixtures, which provides a very useful framework for dealing with a multicomponent system, to derive the mass- and momentum-balance equations for each phase. Because the balance equations are insufficient in number to provide a solution for all dependent variables, constitutive relationships must be constructed to supplement the balance equations. This construction is based on requirements of symmetry, objectivity, and linearity, along with the entropy inequality—well-known constraints used in continuum mechanics. To describe the coupling of fluid and solid behavior, we added linear stress-strain relations for a porous elastic solid containing compressible fluids to the balance equations.

ACCOMPLISHMENTS

Mass- and momentum-balance equations, with constitutive relationships for a multiphase system containing two compressible fluids and an elastic solid matrix, have been developed. The resulting momentum-balance equations feature new terms describing the reaction of the fluids to an acceleration of the solid matrix. The momentum-balance equations can be reduced to a set of coupled partial differential equations after substitution of the linear stress-strain relations. These coupled equations, expressed in terms of the displacements of solid and fluids, govern the propagation and attenuation of elastic waves. When specialized to the case of a porous medium containing one fluid and an elastic solid, they successfully reproduce the well-known Biot theory for a fluid-saturated porous medium.

SIGNIFICANCE OF FINDINGS

Coupled momentum balance equations for a porous medium containing two viscous, compressible, immiscible fluids have been derived. With the neglect of inertial terms, we found that the linearized increment of fluid content and the Laplacian of the solid-phase dilatation both satisfy a homogeneous diffusion equation with the same diffusivity parameter. Thus, porosity diffusion, hypothesized to be the phenomenon underlying permeability enhancement by a compressional wave traveling through a reservoir, has been demonstrated for the first time in an elastic porous medium containing two immiscible fluids. Because the fluid pressure and the solid stress tensor can be described as linear combinations of dilatations of the solid and fluid, two different linear combinations of fluid pressure and dilatational stress satisfy a Laplace equation and a homogeneous diffusion equation, respectively. Under specified initial and boundary conditions, the pore pressure distribution for a porous medium containing oil and water can be determined. Thus, the time-variation of the flow rate can be predicted as the function of the frequency of pressure pulsing.

RELATED PUBLICATION

Lo, W.-C., and G. Sposito, The physics of immiscible two-phase flows in deformable porous media, Water Resour. Res., 2001 (submitted).

ACKNOWLEDGMENTS

This work has been supported by the Assistant Secretary for Fossil Energy, Office of Natural Gas and Petroleum Technology, through the National Petroleum Technology Office, Natural Gas and Oil Technology Partnership, of the U.S. Department of Energy under Contract No. DE-AC03-76SF00098. This project was performed in conjunction with the Seismic Stimulation Project, (Peter Roberts, primary investigator) at Los Alamos National Laboratory.

MECHANICAL AND ACOUSTIC PROPERTIES OF WEAKLY CEMENTED GRANULAR ROCKS

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RESEARCH OBJECTIVES

Young, poorly consolidated geological formations (often encountered in drilling and excavation) are composed of rocks with weak intergranular cementation. Because such rocks lack strength, they can be a potential threat to the stability of boreholes and other stress-bearing structures. They are, in addition, difficult to characterize because their mechanical behavior is intermediate between rock and soil.

One of the fundamental differences between granular rock (sandstone) and soil (sand) is the strength of intergranular cohesion. Because of the lack of this cohesion, sand under differential stress exhibits significant permanent deformation that overwhelms the elastic deformation of the grains and grain contacts. In contrast, the deformation of competent sandstone (e.g., Berea sandstone) consists of both elastic deformation of grains and grain contacts and frictional slip between grains.

The objective of this study is to understand the effect of micromechanical properties of weakly cemented sandstone (such as grain size, shape, porosity (packing density), and intergranular cohesion and friction) on macroscopic behavior. Among these properties, our main focus is on the intergranular cohesion.

APPROACH

To study the effect of micromechanical properties on macroscopic behavior (such as load-displacement response and acoustic-wave propagation), we conducted laboratory tests using synthetic sandstone samples. These samples were fabricated by cementing pure silica sand, using sodium silicate binder. By changing the degree of compaction and the amount of binder, we can control both porosity and intergranular cohesive strength. For a range of porosities and degrees of intergranular cementation, we performed mechanical measurements (including uniaxial compression tests and KIc fracture toughness tests) and acoustical measurements for wave velocities.

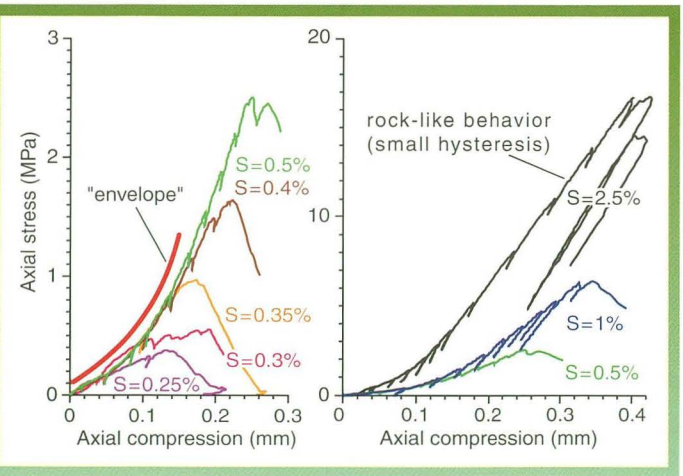

Figure 1. Transition from "soil-like" behavior to "rock-like" load-displacement behavior of weakly cemented granular rock samples. S(%) is the volumetric ratio of sodium silicate cement occupying the pore space.

ACCOMPLISHMENTS

During uniaxial compression tests, weakly cemented rock samples showed large permanent deformation with frictional intergranular slip. Such stress-strain behavior is more analogous to that of soils than competent rocks. The mechanical behavior of samples became increasingly rock-like as the intergranular cohesive strength was increased (Figure 1). For a range of uniaxial compression strengths (Uc) below 7 MPa, Uc increased linearly with the cement content within the sample. The amount of sodium silicate cement required to achieve these strengths was less than 1% of the pore space, which allowed us to change the intergranular cohesive strength of samples independently of porosity. For a given amount of cement, a reduction in porosity resulted in an increase in Uc, which indicates an increasing contribution from intergranular friction and locking to the strength of the rock.

Acoustical measurements were performed on both dry and vacuum-saturated samples (using high-purity alcohol). For weak samples with Uc less than 0.5 MPa, the velocity of the compressional wave was as low as 1,000 m/s. For a given porosity of samples, both compressional and shear velocities increased nonlinearly with increasing intergranular cementation. Interestingly, however, Poisson's ratios determined from the wave velocities were virtually unaffected.

SIGNIFICANCE OF FINDINGS

Mechanical tests revealed a transitional behavior of weakly cemented granular rocks with increasing intergranular cohesion. However, the observed failure mode of the rock during the uniaxial compression tests was always brittle, exhibiting extensile fracturing instead of ductile failure (which would be expected for soils). Acoustical measurements showed a Poisson's ratio that was not affected by intergranular cohesion. This indicates that it may be possible to determine the porosity of weak rock from Poisson's ratio.

RELATED PUBLICATION

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ACKNOWLEDGMENTS

This work has been supported by the Director, Office of Science, Office of Basic Energy Sciences, Division of Chemical Sciences, Geosciences, and Biosciences of the U.S. Department of Energy under Contract No. DE-AC03-76SF00098.

DECOMPOSITION OF SCATTERING AND INTRINSIC ATTENUATION IN ROCK WITH HETEROGENEOUS MULTIPHASE FLUIDS

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RESEARCH OBJECTIVES

This project investigates scattering and intrinsic attenuation of seismic waves in rock with heterogeneous distributions of fluids and gas. This research represents a departure from past studies on seismic attenuation in that the focus here is not a detailed study of a specific attenuation mechanism, but rather an investigation of theoretical and laboratory methods for obtaining separate estimates of scattering and intrinsic attenuation in rock with heterogeneous pore-fluid distributions.

This project combines laboratory, numerical, and theoretical studies in an investigation of scattering and intrinsic attenuation in rock with heterogeneous fluid distributions. The objectives of this project are threefold: (1) to adapt and further refine methods for decomposing scattering and intrinsic attenuation in rock with heterogeneous multiphase fluids, (2) to apply these methods to laboratory seismic measurements in porous rock with heterogeneous fluid distributions and compare these results with direct laboratory measurements, and (3) to examine a new method for focusing seismic waves in heterogeneous media, using time-reversal mirrors. These objectives are addressed in three tasks to be performed over a period of three years.

APPROACH

During the second year of the project, we have focused our efforts on full-waveform imaging methods for fracture detection using converted waves. Our approach for imaging fractures using converted elastic waves is an adaptation of the excitation-time imaging condition used in reverse-time migration to acquisition geometries, in which a direct wave from a compressional wave source is recorded (e.g., crosswell and vertical seismic profiling—VSP). In this method, we exploit the results of modeling work we have conducted, which shows large P-S converted waves that are generated at a fracture by an incident P-wave.

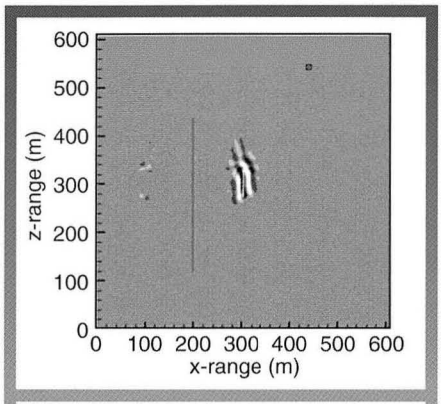

Figure 1. Composite image of the fracture formed by taking the product of the back-propagated curl (V^S) and div (V^O) wavefields and summing over all time steps

We first assume an average velocity model of the subsurface or incorporate a more precise velocity model (if this information is available from well logs or other sources). The direct P-wave is extracted from the multicomponent particle-velocity data, forming two datasets—one containing only the direct P-wave and the other containing scattered P-P and P-S waves generated by the direct P-wave. The particle velocities from the two datasets are applied as sources in two finite-difference models. At each time step in the finite-difference back-propagations, an image resulting from the product of the particle-velocity divergence of the transmitted P-wave ($\nabla \times V^O$) and the particle-velocity curl of the scattered wavefield ($\nabla \times V^S$) is formed at each cell in the finite-difference model. This image is added to the image from the previous back-propagation time step to form a composite image of the features that generated the P-S converted waves. Figure 1 displays the back-propagated divergence and curl wavefields and the composite image for a single-fracture model in a VSP configuration.

SIGNIFICANCE OF FINDINGS

A simple, full-waveform elastic approach has been developed for imaging discrete fractures. This method is applicable to source-receiver configurations in which the direct wave from the source is recorded (e.g., crosswell and VSP geometries). Present work is focused on testing this approach for more complex stratigraphy (with multiple fractures) and providing a mathematical basis for this approach.

ACKNOWLEDGMENTS

This project is supported by the Director, Office of Science, Office of Basic Energy Sciences, Division of Chemical Sciences, Geosciences, and Biosciences, of the U.S. Department of Energy under Contract No. DE-AC03-76-SF00098.

DENSITY FUNCTIONAL THEORY CALCULATIONS ON THE STRUCTURES OF 2:1 CLAY MATERIALS

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RESEARCH OBJECTIVES

The objectives of this project are (1) to assess the validity of our density functionality theory (DFT) calculations by determining the equilibrium structure of the clay mineral pyrophyllite and (2) to determine the structure of the clay mineral Na-montmorillonite with varying layer charge created by $Al^{3+} \rightarrow Mg^{2+}$ substitution at octahedral sites.

APPROACH

Our approach uses DFT as implemented in the program CASTEP in conjunction with ultrasoft pseudopotentials and plane-wave basis functions. The structures of pyrophyllite and montmorillonite with differing layer charge were determined by energy optimization. The triclinic half-unit cell of pyrophyllite $[Si_4Al_2O_{10}(OH)_2]$ was derived from available x-ray diffraction data. A half-unit cell of montmorillonite $[Si_4(Al_{1.0}\ Mg_{1.0})O_{10}(OH)_2]$ with x = 2.0 e (x = layer charge per unit cell) was obtained by substituting one of the octahedral Al^{3+} with Mg^{2+} (Figure 1a). By doubling the structure shown in Figure 1a, montmorillonite with layer charge x = 1 was created (Figure 1c). An interlayer Na^+ was then added for these two cases (Figures 1b and 1d). Additional simulations were performed by doubling the unit cell with and without Na^+ (x = 0.5, structure not shown). A uniform positively charged background was used for the cases without Na^+. All CASTEP calculations have been performed on the T3E and IBM SP supercomputers at the National Energy Research Scientific Computing Center (NERSC).

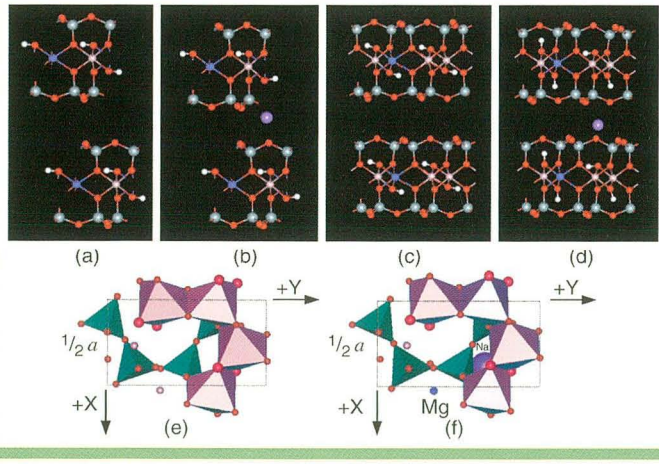

Figure 1. (a) to (d) Optimized structure of montmorillonite as determined by *ab initio* energy minimization, based on the local density approximation using gradient-corrected density functional theory. (Si are shown in gray and O are shown in red. The substituted octahedral-sheet cation is Mg^{2+} [blue] and the interlayer cation is Na^+ [purple]. Octahedral-sheet Al^{3+} cations are shown in pale red.) Note the positions of the proton [white] and the angle made by OH relative to horizontal. (e) Top view of optimized pyrophyllite structure. (f) Top view of optimized Na-montmorillonite with layer charge = –0.5e.

ACCOMPLISHMENTS

The structure of pyrophyllite determined theoretically was compared with x-ray data and showed excellent agreement in terms of characteristic structural parameters, including tetrahedral rotation angle (10.1°), surface corrugation angle (6.7°), and all interatomic distances. The calculated structures of montmorillonite were compared to pyrophyllite, which is structurally isomorphic to montmorillonite but without charge substitution. For example, the angles of surface corrugation (5°) and tetrahedral rotation (3.4°) were less for montmorillonite than for pyrophyllite (Figures 1e, 1f). There was a significant structural effect on the OH groups in the octahedral sheet. Those nearest Na^+ (upper layer in Figure 1b, bottom layer in Figure 1d) moved toward the octahedral sheet and away from the interlayer cation, while the rest (i.e., all other protons in Figures 1b and 1d) either moved similarly (Figure 1b) or even moved toward the interlayer region (Figure 1d).

SIGNIFICANCE OF FINDINGS

Detailed DFT structural optimization for pyrophyllite and montmorillonite has been achieved for the first time. Experimentally unavailable but important features such as OH orientation were determined for pyrophyllite (26°) and montmorillonite. These quantum mechanical calculations of electronic structure in clay minerals are state-of-the-art and give excellent results for both equilibrium structures and total energies.

RELATED PUBLICATIONS

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Park, S.-H., and G. Sposito, Methane hydrate structure and stability in montmorillonite interlayers, 2. Molecular dynamics simulations, J. Phys. Chem. B., 2001 (in press).

Sutton, R., and G. Sposito, Molecular simulations of interlayer structure and dynamics in 12.4 Å Cs-Smectite hydrates, J. Colloid Interface Sci. 237, 174–184, 2001

Greathouse, J. A., K. Refson, and G. Sposito, Molecular dynamics simulation of water mobility in magnesium-smectite hydrates, J. Am. Chem. Soc. 122, 11459–11464, 2000. URL: http://esd.lbl.gov/GEO/aqueous_geochem/index.html.

ACKNOWLEDGMENTS

This project is supported by the Director, Office of Science, Office of Basic Energy Sciences, Division of Chemical Sciences, Geosciences, and Biosciences, of the U.S. Department of Energy under Contract No. DE-AC03-76-SF00098. The authors also wish to thank the staff of NERSC at Berkeley Lab.

NUMERICAL SIMULATION STUDIES OF MULTIPHASE FLOW DYNAMICS DURING CO_2 DISPOSAL INTO SALINE FORMATIONS

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RESEARCH OBJECTIVES

Disposal of CO_2 into brine formations will give rise to a variety of coupled physical and chemical processes. These processes include pressurization of reservoir fluids, immiscible displacement of an aqueous phase by the CO_2 phase, partial dissolution of CO_2 into the aqueous phase, chemical interactions between aqueous CO_2 and primary aquifer minerals, and changes in effective stress. Such processes may alter aquifer permeability and porosity, and may give rise to seismicity as well. Nonisothermal effects may arise from phase partitioning, chemical reactions, and (de)compression effects.

The objective of this work is to develop and demonstrate accurate and efficient capabilities for numerical simulation of CO_2 injection into brine formations.

APPROACH

Considerable experience with subsurface flow systems that involve water, CO_2, and dissolved solids exists in geothermal reservoir engineering. The geothermal work generally addresses higher temperatures and lower CO_2 partial pressures than would be encountered in aquifer disposal of CO_2. For example, the EWASG fluid properties package of our TOUGH2 general-purpose simulator was designed to represent H_2O/ CO_2/NaCl mixtures for temperatures greater than 100°C and for relatively small CO_2 partial pressures, on the order of a few bars. Treatment of CO_2 disposal into brine formations requires modifications of the thermophysical-properties description, so that systems with temperatures down to approximately 30°C and CO_2 pressures of several hundred bars may be described.

ACCOMPLISHMENTS

A new fluid-properties module called "ECO_2" was developed. It represents density, viscosity, and enthalpy of CO_2 within experimental accuracy by the correlations of Altunin (1975), using computer programs kindly provided to us by Victor Malkovsky of IGEM, Russia. Treatment of CO_2 dissolution in water was enhanced by including fugacity effects. The thermophysical-properties package was tested extensively against experimental data and against correlations found in the literature. ECO_2 is presently limited to supercritical conditions, i.e., temperatures and pressures in excess of the critical point of CO_2 (Tcrit = 31.04°C, Pcrit = 73.82 bar).

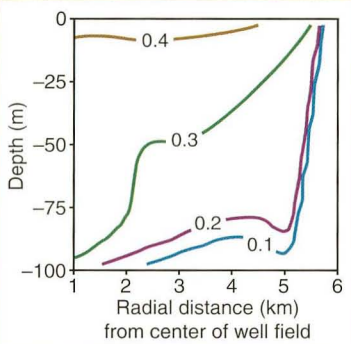

Figure 1. Simulated gas saturations after injection of 10 million tonnes of CO_2 per year for 30 years.

The TOUGH2/ECO_2 simulator has been applied to analysis of injection pressures at a CO_2 disposal well, CO_2 discharge along a fault zone, and evaluation of the storage capacity of brine formations. The amounts of CO_2 that would need to be disposed of at large fossil-fueled power plants are very large. Our simulations predict that injection of the CO_2 generated over the lifetime of a 1,000 MWe coal-fired plant (10 million tonnes per year for 30 years) would produce a plume with an approximate 100 km^2 areal extent in a typical disposal aquifer (Figure 1). Significant aquifer pressurization (1 bar or larger) would occur over an area of several thousand km^2.

RELATED PUBLICATIONS

Pruess, K., and J. García, Multiphase flow dynamics during CO_2 injection into saline aquifers, Environmental Geology, 2001 (in press).

Pruess, K., T. Xu, J. Apps, and J. García, Numerical modeling of aquifer disposal of CO_2, Paper SPE-66537, presented at SPE/EPA/DOE Exploration and Production Environmental Conference, San Antonio, Texas, February 2001.

ACKNOWLEDGMENTS

This project is supported by the Director, Office of Science, Office of Basic Energy Sciences, Division of Chemical Sciences, Geosciences, and Biosciences, of the U.S. Department of Energy under Contract No. DE-AC03-76-SF00098. We are grateful to Victor Malkovsky of IGEM, Moscow (Russia) for kindly providing us with his computer programs of the correlations for CO_2 properties by V.V. Altunin.

MODELING OF HYDROMECHANICAL CHANGES ASSOCIATED WITH BRINE AQUIFER DISPOSAL OF CO_2

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RESEARCH OBJECTIVES

The objective of this research is to study the impact of rock mechanical changes on the performance of a CO_2 injection operation into brine aquifers.

APPROACH

Two existing computer codes, TOUGH2 and FLAC3D, have been joined to form a numerical simulator (TOUGH-FLAC) that analyzes coupled THM processes in complex geological media under two-phase flow conditions. To model the geological disposal of CO_2, the two codes were joined with two hydromechanical coupling functions that account for multiphase fluid-pressure-induced stress and porosity changes and corresponding changes in hydraulic properties. Then, using laboratory data on stress-induced porosity and permeability changes, along with the TOUGH-FLAC code, we conducted a 2D study of hydromechanical processes during a deep-underground injection of supercritical CO_2 in a hypothetical brine aquifer/caprock system. As part of this study, we investigated the possibility of rock mechanical failure in the form of hydraulic fracturing or shear-slip reactivation of existing faults.

ACCOMPLISHMENTS

In this modeling, CO_2 was injected at a constant rate over a 10-year period at a depth of 1,300–1,500 m. The injection zone is overlain by a 100-meter-thick caprock, located at 1,200–1,300 m, which in one of the studied cases is intersected by a vertical fault. The hydraulic, mechanical, and hydromechanical responses caused by the injection were studied. This study included the spread of the CO_2 plume, effective stress changes, ground-surface uplift, stress-induced permeability changes, and a mechanical-failure analysis. The analysis showed that most hydromechanical changes were induced in the lower part of the caprock, near its contact with the injection zone, while the sealing mechanism of the upper part apparently remained intact, despite an injection pressure close to the lithostatic stress value (Figure 1).

SIGNIFICANCE OF FINDINGS

The rate (or amount) of CO_2 that can be injected into a brine aquifer is proportional to the injection pressure. The higher the pressure, the more CO_2 can be injected during a fixed time period. However, if the injection pressure approaches the lithostatic stress, strongly coupled hydromechanical come into play, and rock failure may occur. The simulation shows that if rock failure occurs, it would at first be limited to the lower part of the caprock, while the upper part could remain intact. At this stage, with an immediate lowering of the injection rate, further propagation of the rock failure could be prevented.

RELATED PUBLICATION

Rutqvist, J., and C.-F. Tsang, A study of caprock hydromechanical changes associated with CO_2 injection into a brine aquifer, Environmental Geology (in press); Berkeley Lab Report LNBL-48145, 2001.

ACKNOWLEDGMENTS

This work was supported by the Director, Office of Science, Office of Basic Energy Sciences, Division of Chemical Sciences, Geosciences, and Biosciences, of the U.S. Department of Energy under Contract No. DE-AC03-76SF00098.

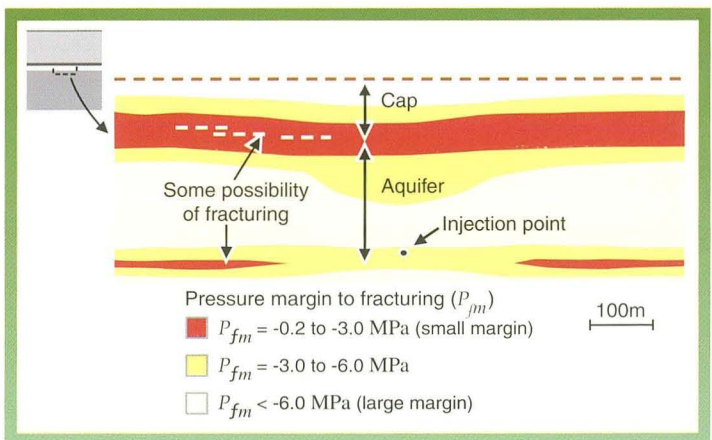

Figure 1. Potential for fracturing in the aquifer/caprock system after 10 years of CO_2 injection, when the injection pressure has increased up to the lithostatic stress value. The contour plot shows the potential for fracturing expressed in a pressure margin (pressure margin is the current fluid pressure minus the critical fracturing pressure). The white dashed lines indicate the orientation of potential hydraulic fractures in the lower part of the caprock.

FRACTURE SURFACE-ZONE FLOW AND THE SORPTIVITY-PERMEABILITY RELATION

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RESEARCH OBJECTIVES

Fast flow along unsaturated fractures can occur within "fracture surface-zones" when fracture coatings, skins, or microcracked damage zones have higher permeabilities than the underlying bulk rock matrix. When the local flux of water is high enough to sustain satiated water contents within fracture surface-zones, water is expected to flow preferentially within the fracture surface-zone. When the energy of pore waters in the fracture surface-zone rises to its near-zero matric potential range, film flow becomes possible on the fracture surface. Thus, surface-zone flow, local aperture saturation, and film flow can all contribute to flow along unsaturated fractures. The quantification of surface-zone permeabilities is difficult because this region is typically quite thin and therefore not amenable to cutting for testing independently of the bulk rock. We have identified a theoretical correlation between water imbibition rates and permeabilities that appeared promising for deducing fracture surface-zone permeabilities. This study focuses on the permeability-sorptivity relation, its experimental testing, and identification of significant limitations.

APPROACHES

By combining recent analyses by Kao and Hunt—of wetting-front time dependence during water imbibition into porous media—with the classic infiltration analyses of Green and Ampt (and of Philip), it can be shown that permeability is proportional to the 4th power of the sorptivity. The same proportionality can be established from the classic scaling analysis of Miller and Miller. This relation appeared promising for determining the permeability of thin fracture surface-zones, based upon transient imbibition experiments. To test the usefulness of this relation, imbibition experiments were performed on tuffs and rhyolites to determine sorptivities of their fracture surface-zones and bulk matrices. Fracture surface-zone and matrix permeabilities were calculated from measured sorptivities. Permeabilities of the bulk rock were then measured for comparison with values predicted based on sorptivities. Additional sorptivities were measured on highly wettable ceramics to extend the permeability range over which the sorptivity-permeability relation is tested.

ACCOMPLISHMENTS

Transient imbibition tests on some rock samples showed significantly higher sorptivities within visible fracture surface-zones than in the bulk rock. Based on the sorptivity-permeability relation, it was predicted that permeabilities of some fracture surface-zones were about 200 times greater than their associated matric rocks. However, direct measurements of rock matrix permeabilities consistently yielded much higher values than those predicted from imbibition rates. Such discrepancies did not exist in the data set analyzed by Kao and Hunt. Testing on ceramics also yielded results in compliance with the sorptivity-permeability relation. Contact- angle measurements on the rock samples showed that their air-dry surfaces were not strongly water wetting (contact angles ranged from 28° to 57°), indicating that imperfect wettability invalidates the sorptivity-permeability relation.

SIGNIFICANCE OF FINDINGS

The possibility of fast flow along unsaturated fractures within fracture surface-zones was identified. A relationship between permeability and the 4th power of sorptivity was also identified. Experimental testing showed that this relationship cannot be used reliably for media with imperfect wettability.

RELATED PUBLICATIONS

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ACKNOWLEDGMENTS

Funding was provided by the Director, Office of Science, Office of Basic Energy Sciences, Division of Chemical Sciences, Geosciences, and Biosciences, of the U.S. Department of Energy under Contract No. DE-AC03-76SF00098.

REACTIVE CHEMICAL TRANSPORT IN STRUCTURED POROUS MEDIA: X-RAY MICROPROBE AND MICRO-XANES STUDIES

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RESEARCH OBJECTIVES

Large differences in chemical composition can be sustained in boundary regions such as those at sediment-water interfaces, interior regions of soil aggregates, and surfaces of fractured rocks. Predicting transport between various environmental compartments is currently often unsuccessful, partly because of a lack of sufficient spatial and temporal resolution in measurements. Batch studies can yield insights into kinetics and equilibrium in well-mixed systems, but the subsurface is very poorly mixed. Without *in situ*, spatially and temporally resolved chemical information, transport between compartments can only be described with system-specific, nonmechanistic, mass-transfer models. We are testing the impact of transport limitations on redox-precipitation reactions in sediments.

APPROACH

Past efforts in this project focused on selenium transport and reduction in two types of microenvironments: (1) that found at surface water-sediment boundaries and (2) that found within soil aggregates. Since FY 1998, the project emphasis has shifted to reactive transport of another environmentally important contaminant, chromium. The oxidized Cr(VI) species are mostly soluble, environmentally mobile, and toxic. Most forms of reduced Cr(III) are insoluble precipitates of low toxicity. Our studies on reactive transport of Cr have included flow-through and diffusion-limited experiments in soils, including spatially resolved, real-time tracking of initial contamination processes. Distributions of total Cr, Cr(III), and Cr(VI) are determined with x-ray microprobe and micro-XANES (x-ray absorption near edge structure) analyses conducted at the Advanced Photor Source (Argonne National Laboratory) and the Nationa Synchrotron Light Source (NSLS, at Brookhaven Nationa Laboratory).

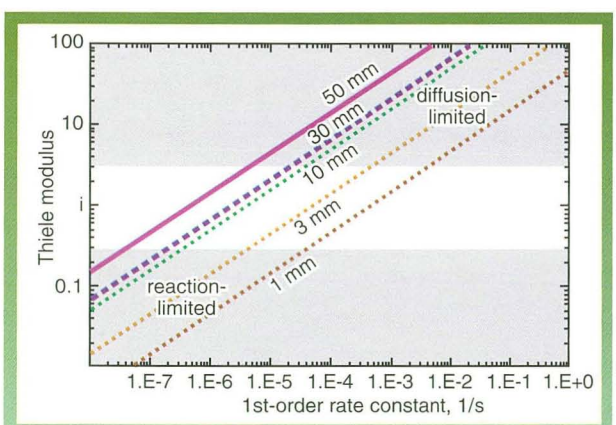

Figure 1. Dependence of the Thiele modulus on 1st-order reaction-rate constant and diffusion distance (radius of soil aggregate or sediment block). Even relatively small sediment blocks have diffusion-controlled reactions for a wide range of rate constants.

ACCOMPLISHMENTS

Our comparisons of Cr(VI) reduction rates (whether directly or indirectly microbially mediated) with diffusion-controlled transport rates show that in water-saturated, microbially active sediments, transport limitations exert two main influences. The first influence occurs through developing steeply decreasing redox potentials with distance from oxygenated boundaries resulting from oxygen diffusion-limited microbial respiration. This results in the second influence, increasing Cr(VI) reduction rates with distance. Under such conditions, Cr diffusion fronts terminate sharply. As a consequence, highly Cr-contaminated zones can coexist with pristine sediments, with transition zones as narrow as 1 mm. We have generalized analyses of reaction rates and diffusion distances using the Thiele modulus to show that many subsurface reactions of environmental interest are transport limited.

SIGNIFICANCE OF FINDINGS

These results illustrate the importance of diffusion-limited Cr reduction in sediments and the need for chemical characterization with sufficient spatial resolution to identify redox zonation. Bulk measurements on samples yield spatially averaged chemical information. When such averaged measurements are obtained over steep chemical gradients, they do not allow correct interpretations. The Thiele analysis of rates can be applied to many other chemical species to deduce the relative importance of reaction kinetics and transport.

RELATED PUBLICATION

Tokunaga, T.K., J. Wan, M.K. Firestone, T.C. Hazen, E. Schwartz S.R. Sutton, and M. Newville, Chromium diffusion and reduction in soil aggregates, Environ. Sci. Technol., 2001 (in press).

ACKNOWLEDGMENTS

This project is supported by the Director, Office of Science Office of Basic Energy Sciences, Division of Chemical Sciences Geosciences, and Biosciences, of the U.S. Department of Energy under Contract No. DE-AC03-76-SF00098. Research was in par carried out at NSLS, Brookhaven National Laboratory, which is supported by the Division of Material Sciences and Division o Chemical Sciences. We thank Tony Lanzirotti and the staff o NSLS.

JOINT INVERSION FOR MAPPING SUBSURFACE HYDROLOGICAL PARAMETERS

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RESEARCH OBJECTIVES

One of the main objectives of studying geophysical inversion is to use the results from inversion to describe various subsurface processes involving fluid flow. Hydrological properties such as fluid electrical conductivity and rock porosity cannot be directly obtained with conventional inversion techniques. The electromagnetic (EM) field propagating through the subsurface medium is a function of the bulk conductivity, which in turn may be empirically related to porosity, pore fluid conductivity, saturation, and occasionally the temperature. Within a particular medium, seismic travel time along a ray path depends on its propagation velocity, which may again be related to several factors (such as porosity, density, elastic constants, temperature, and pressure). The complex interrelationship among these variables renders direct mapping of these parameters very difficult. However, joint analysis of different geophysical data, along with information about the relationships between geophysical and hydrological parameters, may allow us to achieve direct parameter mapping.

APPROACH

To assess the feasibility of deriving hydrological properties directly, we have developed a joint-inversion technique using EM and seismic travel-time data. The objective is to derive the fluid conductivity and rock porosity of a medium between two boreholes. Archie's law and the Wyllie time-average relations are used to relate geophysical parameters to two of the hydrological variables: rock porosity and fluid conductivity. The inversion is based on least-squares criteria that minimize the misfit between the observed data (synthetic data in this study) and that of the inverted hydrological model. A smoothness constraint is used to reduce nonuniqueness. To begin with, the inversion is tested on a two-dimensional model. For the EM method, the model is axially symmetric near the transmitter borehole, and numerical simulation is carried out with the algorithm developed by Alumbaugh and Morrison (1995). The bulk electrical conductivity used for the EM simulation is estimated using Archie's law. A straight ray path is assumed for the seismic method, and travel-time data are calculated based on the simplified Wyllie equation.

ACCOMPLISHMENTS

Based on the preliminary results of this research, we have demonstrated (see Figure 1) that hydrological parameters can be obtained directly with joint inversion of two geophysical survey methods. The optimum result of the joint inversion has been obtained by alternating the selection of inversion parameters, with only one parameter allowed to change (while the other parameter is held fixed) at each iteration.

SIGNIFICANCE OF FINDINGS

Joint analysis of geophysical data for subsurface imaging is not new. However, the study presented here is the first to directly obtain hydrological parameters using different geophysical data. Successful application of the technique will greatly improve our understanding of various subsurface processes involving fluid flow.

RELATED PUBLICATION

Alumbaugh, D.L., and H.F. Morrison, Theoretical and practical considerations for crosswell electromagnetic tomography assuming a cylindrical geometry, Geophysics 60, 846–870, 1995.

ACKNOWLEDGMENTS

This project is supported by the Director, Office of Science, Office of Basic Energy Sciences, Division of Chemical Sciences, Geosciences, and Biosciences, of the U.S. Department of Energy under Contract No. DE-AC03-76-SF00098. Contract No. DE-AC03-76-SF00098.

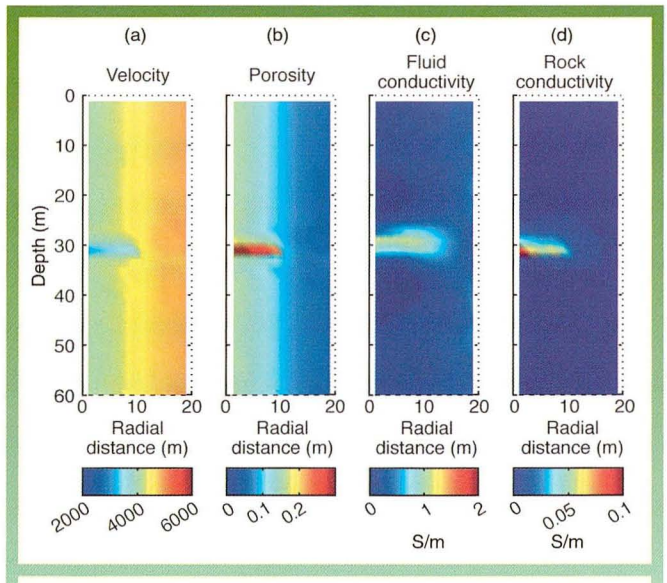

Figure 1. Joint inversion results using both EM and seismic data. The conductivity is fixed to obtain a better porosity model in a first iteration; then porosity is fixed for a better conductivity model in the next iteration.

PARTITIONING OF CLAY COLLOIDS TO GAS-WATER INTERFACES

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RESEARCH OBJECTIVES

Clays, humic acids, and microorganisms have been found preferentially sorbed at air-water interfaces in unsaturated soils. For solutions containing surface-active molecules, the measurement of changes in surface tension (with changes in solute concentration) permits calculation of their surface excess through the Gibbs adsorption equation. However, for suspensions of particles, surface-tension changes are often not measurable. To quantify colloid partitioning at air-water interfaces under surfactant-poor conditions typical of subsurface environments, an alternative means is needed. Wan and Tokunaga (1998) developed a simple dynamic method to characterize colloid-surface excesses at air-water interfaces, without requiring assumptions concerning the thickness of interfacial regions and without the use of surfactants. The objective of this study is to use this newly developed method to measure the partition coefficients (K) of different clay minerals and latex microspheres at the air-water interface, under environmentally relevant solution-chemistry conditions.

APPROACH

The bubble-column method (Wan and Tokunaga, 1998) was used to measure the K of different clays (kaolinite, montmorillonite, and illite) and polystyrene latex microspheres at the gas-water interface. In the bubble column, air is bubbled through a vertical column containing the dilute colloidal suspension, with an open free surface at the top. The rising bubbles sorb and carry the surface-active species upward, then release them back to the solution at the free surface, where the bubbles burst. The steady-state concentration profile along the column reflects the balance between upward transport by partitioning onto rising bubbles and downward transport by eddy dispersion. By measuring the steady-state concentration profile, the partitioning between bulk and surface regions can be determined.

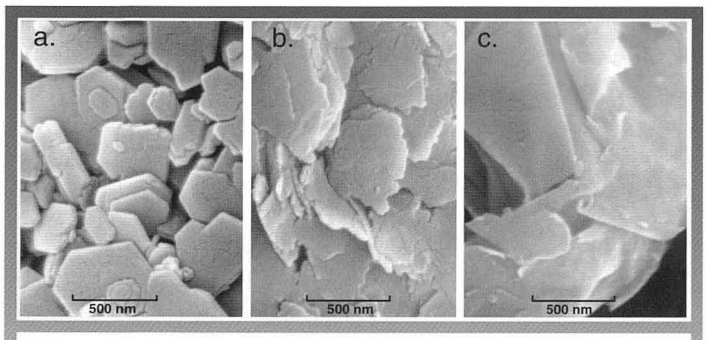

Figure 1. Scanning electron micrographs of clays used in this study: (a) kaolinite, (b) illite, and (c) Na-montmorillonite

ACCOMPLISHMENTS

Kaolinite exhibited extremely high affinity to the air-water interface at pH values below 7. Na-montmorillonite and bentonite clay were found excluded from the air-water interface at any given pH and ionic strength. The results show the importance of electrostatic interactions between the air-water interface and colloids, including pH-dependent edge charges on mineral colloids and influences of particle shape (Figure 1). Low partitioning of latex particles at the air-water interface relative to kaolinite appears to result from particle charge distribution and particle geometry.

SIGNIFICANCE OF FINDINGS

The implications of these types of measurements are especially relevant in the vadose zone, because this portion of the environment can have high values of air-water interfacial area per unit bulk volume. Because of the common existence of thin water films in the vadose zone, the distribution of surface-active colloids between bulk water and the air-water interface can be significant. Calculated ratios of colloid distribution at the air-water interface to bulk water ranged from approximately 1:1 to 1:20 for a wide range of soil saturations and colloid types. High partitioning of colloids between the air-water interface and the bulk solution has important implications on colloid transport and transformation in vadose environments.

RELATED PUBLICATIONS

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ACKNOWLEDGMENTS

This project is supported by the Director, Office of Science, Office of Basic Energy Sciences, Division of Chemical Sciences, Geosciences, and Biosciences, of the U.S. Department of Energy under Contract No. DE-AC03-76-SF00098.

Fe^{3+} SORPTION ON QUARTZ SURFACES: GRAZING INCIDENCE X-RAY ANALYSIS

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RESEARCH OBJECTIVES

Iron oxyhydroxides are powerful agents for metal scavenging in the environment. Recently, we have determined that the surface reactivity of quartz aquifer grains is dominated by coatings consisting of nanometer-thick iron oxyhydroxides. We seek to understand the processes by which these coatings are formed, determine their reactivity compared to bulk iron minerals, and describe the structure and crystal chemistry of the coatings as completely as possible on the nanometer-to-micron scale.

APPROACH

Both laboratory model studies and field sampling have been performed. In the laboratory, we are using both perfect quartz crystals with m-, r-, and c-plane surfaces, and high-surface-area aerosil silica for sorption and coating-development experiments. In the field, we have emplaced samples of the perfect quartz substrates into wells at the U.S. Geological Survey Cape Cod aquifer site, as well as in Naturita, Colorado, to study natural coating formation.

Samples are being studied by x-ray spectroscopy (XAS) at the Stanford Synchrotron Radiation Laboratory, by high-resolution transmission electron microscopy (HRTEM) at the National Center for Electron Microscopy at Berkeley Lab, and by atomic force microscopy (AFM) at the U.S. Geological Survey in Menlo Park. Grazing incidence XAS measurements (GIXAS) allow us to determine the molecular structure of sorbed iron atoms or multinuclear precipitates, as well as their relationship to the surface Si atoms. Total reflection x-ray fluorescence (TRXRF) allows unprecedented sensitivity in chemical analysis. The HRTEM and AFM studies produce nanometer-resolution images that aid in relating molecular structure to nanometer-and-larger surface structures and defects.

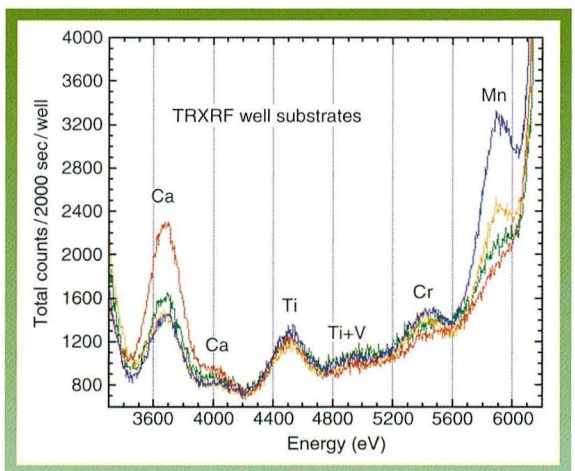

Figure 1. Energy spectrum of the upper 3 nanometers of quartz well samples as determined via TRXRF. The diagram shows the geometry of a grazing-incident experiment.

ACCOMPLISHMENTS

During the past year, GIXAS and TRXRF spectra have been obtained on well samples deposited for 8 and 14 months. One set of results from the 14-month samples is shown in Figure 1. As few as 10^{10} atoms can be detected, equivalent to about 10^{-14} moles of material. The analyses show that the surface contains Fe, Ca, and a range of other transition metal ions. Mn, Cr, and Fe surface concentrations are correlated with each other, but anti-correlated with Ca concentration. This is interesting because the concentration of Ca is very low in the Cape Cod aquifer waters, with calcite unstable under the conditions in the well. The Ca may result from colloid transport, or perhaps from microorganisms utilizing surface Fe^{3+} and rendered it soluble, while releasing Ca and acids at the quartz surface.

SIGNIFICANCE OF FINDINGS

Extended x-ray absorption fine structure (EXAFS) analysis can be done on even the small amounts of Fe found on quartz samples within one year of emplacement, so that the nature of the coating can be analyzed in terms of mineral structure as well as composition. This allows us to analyze the mode of formation, whether via biological, colloidal transport-deposited, or nucleation and growth mechanisms.

RELATED PUBLICATIONS

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ACKNOWLEDGMENTS

This project is supported by the Director, Office of Science, Office of Basic Energy Sciences, Division of Chemical Sciences, Geosciences, and Biosciences, of the U.S. Department of Energy under Contract No. DE-AC03-76-SF00098. Rebecca Reitmeyer and James A. Davis were supported by the U.S. Geological Survey.

THE GEOMETRY OF Zn COMPLEXATION ON FERRIHYDRITE

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RESEARCH OBJECTIVES

Aqueous Zn is readily sorbed by ferrihydrite and other iron oxyhydroxides at moderate pH values. However, experimental sorption isotherms vary from linearity some four orders of magnitude in aqueous Zn concentration below the saturation level with zinc hydroxide. This suggests that a precipitation process or a change in complexation mechanism is occurring. We wish to understand the processes that create this nonlinear behavior in the sorption isotherm and describe the molecular geometry of aqueous Zn uptake.

APPROACH

Samples were created at the U.S. Geological Survey to follow the composition range (i.e., sorption density and aqueous Zn concentration) of the isotherm showing nonlinear behavior. The samples were prepared in both co-precipitation and sorption modes (i.e., formed respectively with and without Zn present). While still fresh and wet, samples were examined by wet chemical and x-ray absorption methods (x-ray absorption near-edge structure [XANES] and extended x-ray absorption fine structure [EXAFS]) at the Stanford Synchrotron Radiation Laboratory. EXAFS analysis was done, both on the samples and on a set of well-characterized model compounds, to extract sample interatomic distances and coordination numbers. XANES spectra were simulated using the ab initio Feff 8.0 code to complement the EXAFS analysis.

ACCOMPLISHMENTS

The combined analysis shows a remarkable set of changes in molecular geometry as a function of Zn solution concentration (see Figure 1). In an aqueous solution with pH of 6 to 7, the zinc ion is coordinated by six water molecules in an octahedral complex (green). However, this coordination changes to tetrahedral (green) after sorption on ferrihydrite (represented by red FeO_6 octahedra) even at the lowest observable sorption densities. Depending on the type of sample preparation (sorption or co-precipitation) the number of second-neighbor Fe ions about a given sorbed Zn differs. For co-precipitation samples where Zn ions have abundant aqueous Fe^{3+} available during formation, the number of Fe^{3+} second neighbors is larger. With further increase in aqueous Zn, the complexation changes because new Zn tetrahedral units polymerize onto existing sorbed ones. Finally, at the highest aqueous Zn concentrations, a new type of precipitate forms, dominated by octahedrally coordinated Zn and with a layer structure.

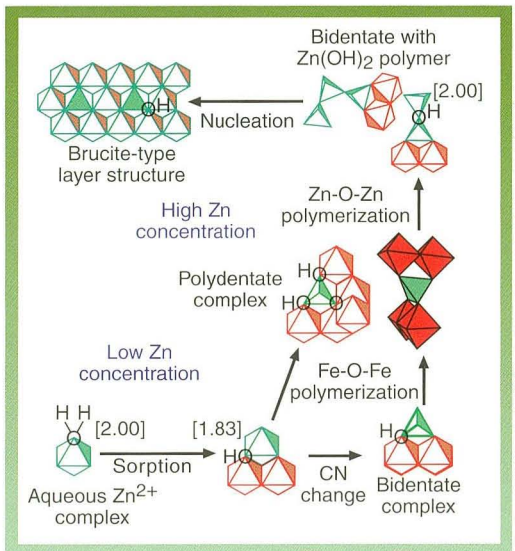

Figure 1: Changes in the geometry of Zn complexes on ferrihydrite as a function of aqueous Zn concentration. The bond valence on the relevant oxygen is shown.

SIGNIFICANCE OF FINDINGS

Our results show the complexity of even this simple sorption system, and hence the difficulty of predicting sorption geometry, sorption mechanism, and the chemical fate of certain pollutant agents without molecular information. We also find that a simple so-called "bond valence" argument explains the octahedral-to-tetrahedral change in Zn coordination upon sorption. The oxygen ion has perfectly balanced bond valence (2.00) at the H_2-O-Zn aqueous linkage and also at the tetrahedral Zn-OH-Fe linkage. Hence, once sorption occurs and a proton is lost, the change in coordination returns the ligand oxygen to perfect bond valence.

RELATED PUBLICATIONS

Waychunas, G.A., C.C. Fuller, J.A. Davis, Surface complexation and precipitate geometry for aqueous Zn(II) sorption on ferrihydrite: I. EXAFS analysis, Geochimica et Cosmochimica Acta, 2001 (in press).

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ACKNOWLEDGMENTS

This project is supported by the Director, Office of Science, Office of Basic Energy Sciences, Division of Chemical Sciences, Geosciences, and Biosciences, of the U.S. Department of Energy under Contract No. DE-AC03-76-SF00098; the U.S. Geological Survey Water Resources Research Program (Christopher C. Fuller and James A. Davis); and Laboratory Directed Research and Development funding from Berkeley Lab.

STRUCTURAL ANALYSIS OF SULFATE IN SCHWERTMANNITE

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RESEARCH OBJECTIVES

Schwertmannite is an iron oxyhydroxide with presumed intrinsic sulfate that forms in large quantities in acid-mine-drainage environments at low pH values. It is a powerful sink for toxic metals and oxyanions, and its structure appears to be similar to that of a hollandite, but with sulfate bonded into the tunnel sites of this structure. However, our recent work indicates that the proposed structure for schwertmannite must be incorrect, and that the nature of the sulfate group in the structure may be intermediate between the classical "inner sphere" and "outer sphere" complexes. We have investigated this by examining a series of synthetic schwertmannites formed with varying sulfate contents, and at different pH and water-saturation conditions.

APPROACH

L- and K-edge x-ray absorption near-edge structure (XANES) spectroscopy can be used to distinguish inner sphere, outer sphere, and intermediate hydrogen-bonded sulfate groups. This information can be combined with other structural studies to fully characterize changes in sulfate binding as a function of environmental conditions. Sulfate is generally thought to sorb as either an inner sphere (IS) (directly bonded to a surface metal ion) or outer sphere (OS) (separated from the surface by an intervening water molecule) geometry, depending on mineral surface chemistry, charge, and topology. However, recent work we have done using K-edge XANES spectroscopy at SSRL has indicated that schwertmannite may contain a third type of sulfate, a hydrogen-bonded complex intermediate between inner and outer sphere geometries. This complex has an IR spectrum indicative of an inner sphere complex (because there is considerable splitting of IR bands consistent with low sulfate symmetry), but a XANES spectrum indicative of an outer sphere complex (because no Fe-O-S features are seen). The picture is complicated by the effect of drying on samples, which can drive the local pH up and thus possibly change the nature of a sorbed or bound complex. With this in mind, we are aiming at accomplishing two goals with this study: first, determine the nature of sulfate and its complexation in schwertmannite (to be combined with other data to resolve the full structure); and second, determine the evolution of sulfate complexation at lower pH in environmental (and catalytic) materials.

ACCOMPLISHMENTS

Our XANES spectra on the S-K edge shows conclusively that in schwertmannite, sulfate is not bonded in the tunnels in the normal way. It is probably a hydrogen-bonded complex in larger tunnel-structure defect regions or is largely hydrogen bonded on the outside of crystallites. Fe-K-edge extended x-ray absorption fine structure (EXAFS) spectroscopy indicates that schwertmannite has fewer Fe-O-Fe corner linkages than its nominally structural cousin akaganeite. This points towards a highly disordered structure, probably with larger tunnel sites.

SIGNIFICANCE OF FINDINGS

The possibility of sulfate and other anion complexation changing from inner sphere to hydrogen-bonded complexes with varying pH or other mineral surface characteristics (such as water saturation) has important consequences for anion sequestration. In particular, vadose zone complexation may differ substantially from that in (laboratory) saturated systems. The mode of sulfate incorporation in schwertmannite may also give insight into other types of chemical entrapment by natural nanocrystallites.

ACKNOWLEDGMENTS

This project is supported by the Director, Office of Science, Office of Basic Energy Sciences, Division of Chemical Sciences, Geosciences, and Biosciences, of the U.S. Department of Energy under Contract No. DE-AC03-76-SF00098, and by Laboratory Directed Research and Development funding from Berkeley Lab.

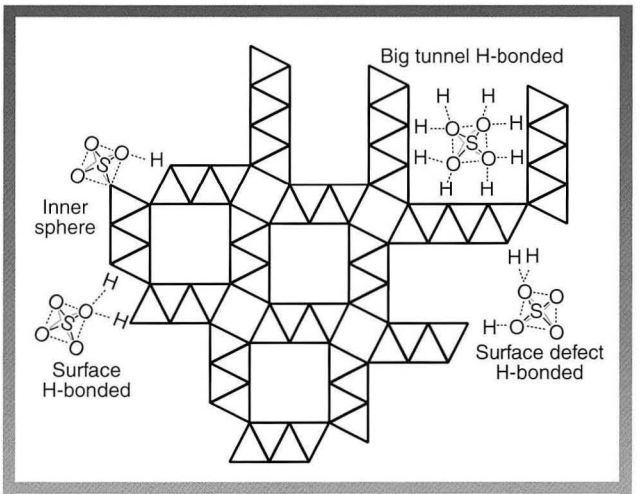

Figure 1. A model for the defect structure of schwertmannite showing positions of various types of sulfate. The framework is made up of FeO_6 octahedra linked into a tunnel structure along the axis normal to the figure.

NUMERICAL SIMULATION TO STUDY MINERAL TRAPPING FOR CO_2 DISPOSAL IN DEEP AQUIFERS

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RESEARCH OBJECTIVES

Carbon dioxide (CO_2) disposal into deep aquifers has been suggested as a potential means whereby atmospheric emissions of greenhouse gases may be reduced. As a prelude to a fully coupled treatment of physical and chemical effects of CO_2 injection, we sought to analyze the impact of CO_2 immobilization through carbonate precipitation.

APPROACHES

We performed batch reaction modeling to simulate the geochemical evolution of three different aquifer mineralogies in the presence of CO_2 at high pressure. Our modeling considered (1) redox processes that could be important in deep-subsurface environments, (2) the presence of organic matter, (3) the kinetics of chemical interactions between the host rock minerals and the aqueous phase, and (4) CO_2 solubility dependence on pressure, temperature, and salinity of the system. The geochemical evolution under both natural background and CO_2 injection conditions was evaluated. Changes in porosity were monitored during the simulations.

ACCOMPLISHMENTS

Modeling results indicate that CO_2 sequestration by matrix minerals varies considerably with rock type. Under favorable conditions, the amount of CO_2 that may be sequestered by precipitation of secondary carbonates is comparable with (and can be larger than) the effect of CO_2 dissolution in pore waters. The precipitation of ankerite and siderite is sensitive to the rate of reduction of ferric mineral precursors such as glauconite, which in turn is dependent on the reactivity of associated organic material. The accumulation of carbonates in the rock matrix and induced rock mineral alteration caused by the presence of dissolved CO_2 lead to a considerable decrease in porosity. Figure 1 shows simulated mineral abundances and CO_2 sequestration for Gulf Coast sediments.

SIGNIFICANCE OF FINDINGS

These numerical models provide a detailed understanding of a particular geochemical system's dynamic evolution. A critical evaluation of these modeling results can provide useful insight into sequestration mechanisms and control of geochemical conditions and parameters.

RELATED PUBLICATIONS

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ACKNOWLEDGMENTS

This work was supported by the Office of Sciences, Office of Basic Energy Sciences, Division of Chemical Sciences, Geosciences, and Biosciences, of the U.S. Department of Energy, under Contract No. DE-AC03-76SF00098.

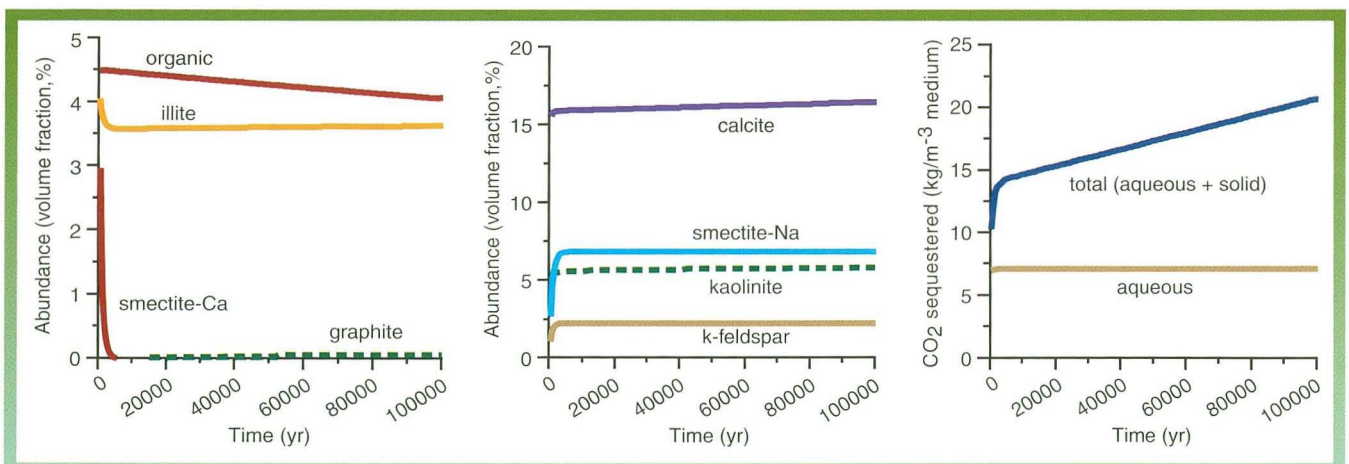

Figure 1. Mineral abundances and CO_2 sequestration obtained with CO_2 injected at 260 bar for Gulf Coast sediments

DEVELOPMENT OF A HIGH-PERFORMANCE MASSIVELY PARALLEL TOUGH2 CODE

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RESEARCH OBJECTIVES

Large-scale simulation (i.e., at the multimillion gridblock level) of multiphase fluid and heat flow in heterogeneous reservoirs remains a challenge. It can be a formidable task for a single-processor computer. However, the development of parallel-computing techniques makes it possible to perform such large-scale reservoir simulations. The main objective of this work is to parallelize the TOUGH2 code, a general-purpose numerical simulation program for modeling multidimensional, multiphase, multicomponent fluid and heat flows in porous and fractured media. Our work is intended to enhance computational performance of TOUGH2 on multiprocessor computers by 1–2 orders of magnitude, both in problem size and in CPU time requirements.

APPROACH

The two most time-consuming parts of a TOUGH2 simulation are (1) assembling the Jacobian matrix and (2) solving the linear equations. With that in mind, the most important aim of a parallel version code is to parallelize these two parts. This goal is achieved by using simulation domain partitioning and parallel linear solving of linearized equations. Three partitioning algorithms from the METIS package (version 4.0) are implemented for grid domain partitioning. The linear solver part of the TOUGH2 code is restructured, and the Aztec parallel solver is selected and incorporated into the parallel code.

In addition to parallel computing in the Jacobian matrix assembly and linear equation solver, efficient use of computer memory is also very important. This is because a several-gigabyte memory is generally required for a typical large-scale, three-dimensional simulation. Then the need arises to distribute the memory requirement to all processors. We have optimized the data input procedure and made use of computer memory shared by all processors. The parallel code is currently implemented for TOUGH2 EOS3 and EOS9 modules.

ACCOMPLISHMENTS

The TOUGH2 code has been parallelized for both computing time and memory sharing, including optimization for solving extremely large reservoir-simulation problems. The parallel code has been successfully used to develop three-dimensional models of fluid and heat flow in the unsaturated zone of Yucca Mountain, using up to two million gridblocks. One of the 3D models uses 1,075,522 gridblocks and 4,047,209 connections to represent the unsaturated zone of the highly heterogeneous fractured tuffs at Yucca Mountain. This problem involves solving of 3,226,566 linear equations at each iteration step. Simulation results indicate that the developed parallel code is very efficient and capable of modeling large-scale problems with multimillion gridblocks. Figure 1 shows the speedup of the parallel code for this application problem.

SIGNIFICANCE OF FINDINGS

The major benefits of the developed parallel code are that it (1) allows accurate representation of reservoirs with sufficient spatial resolution, using multimillion gridblocks, (2) allows adequate description of reservoir heterogeneities, and (3) enhances our modeling capability for solving large-scale, real-world simulations.

RELATED PUBLICATIONS

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ACKNOWLEDGMENTS

This work was supported by the Laboratory Directed Research and Development (LDRD) program of Berkeley Lab, in turn supported by the Director, Office of Science, of the U.S. Department of Energy under Contract No. DE-AC03-76SF00098.

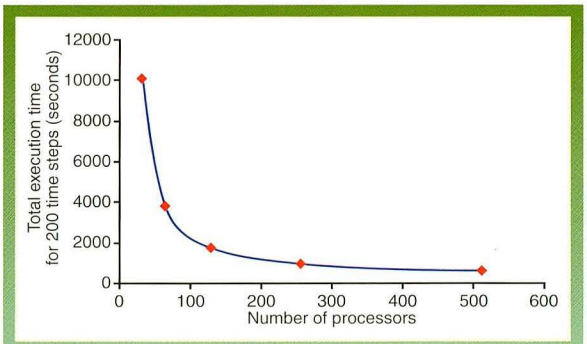

Figure 1. Reduction of execution time with the increase of processor number for a one-million-gridblock problem on Cray T3E-900

RESEARCH PROGRAM

NUCLEAR WASTE

Gudmundur S. Bodvarsson

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The role of the Nuclear Waste Program is to assist the U.S. Department of Energy, the United States, and other countries in solving the problem of safe disposal of nuclear waste through high-quality scientific analyses and technology development. The primary work of the program involves investigating the feasibility and potential of the Yucca Mountain site in Nevada for permanent storage of high-level nuclear waste. The Nuclear Waste Program also does collaborative work on nuclear-waste disposal issues with such countries as Japan, Switzerland, Sweden, China, and Romania. The program has established the Center for International Radioactive Waste Studies, the main purpose of which is to foster relationships with other countries to promote the exchange of ideas and research results.

The Yucca Mountain site is located about 120 km northwest of Las Vegas in a semi-arid region. The potential repository would be located about 350 m below ground surface within a thick unsaturated zone (UZ). Subsurface rocks at Yucca Mountain consist primarily of fractured volcanic tuffs that vary in degree of welding. To date, a total of 60 deep surface boreholes have been drilled in the area. In 1996, an 8 km long underground tunnel, the Exploratory Studies Facility (ESF), was completed at Yucca Mountain to facilitate more extensive subsurface testing.

Berkeley Lab's work at Yucca Mountain consists of solving many problems related to multiphase, nonisothermal flow and transport through the UZ. Some of the key questions that Berkeley Lab scientists are addressing include:

- How much water percolates through the UZ to the repository at Yucca Mountain?
- What fraction of the water flows in fractures and how much flows through the rock matrix blocks?
- How much of this water will seep into the waste-canister emplacement drifts?
- How will radionuclides migrate from the repository to the water table?
- How will coupled TH (thermal-hydrologic), THC (thermal-hydrologic-chemical) and THM (thermal-hydrologic-mechanical) processes affect flow and transport?

To address these questions, the Nuclear Waste Program is organized into Ambient Testing, Thermal Testing, and Modeling groups, with support from geophysicial studies.

AMBIENT TESTING GROUP

The Ambient Testing group investigates how water flows through the mountain and how much of this water will seep into the emplacement drifts. The group performs various tests within the ESF, including fracture-matrix interaction tests, drift-to-drift tests, the Paint Brush Unit test (PTn test), and niche (short drift) testing. Fracture-matrix interaction tests are relatively small-scale (i.e., a few meters) tests that focus on the components of water flow in fractures and matrix blocks and on the interaction between the two continua. The drift-to-drift tests address the same issues, but on a much larger spatial scale (10–20 m). The test in the Paint Brush unit, which is an unwelded tuff unit, addresses issues of episodic flow, effects of faults and large-scale features, and lateral continuity of flow and transport. This unit, directly above the potential repository, is key to dispersed fracture flow from the above fractured units and buffers the transient behavior of episodic flow. The niche studies address perhaps the most crucial problem of Yucca Mountain, i.e., determining the fraction of water that will flow into the emplacement drifts. The niche studies are carried out by introducing water into boreholes above the drift opening and measuring what fraction actually seeps into the opening.
Results to date suggest that there is a seepage threshold below which no water will seep into the drifts.

THERMAL TESTING GROUP

The Thermal Testing group works in collaboration with other national laboratories to evaluate the effects of heat on thermodynamic conditions, fluid flow and transport, and permanent property changes at and near the emplacement drifts. The Yucca Mountain Project has completed the first *in situ* heater test, called the Single Heater Test. The project is now involved with a large-scale heater test in a 50 m long drift. This second test, called the Drift Scale Test (DST), is intended to resemble the actual conditions that would exist when the high-level radionuclide waste is placed in the emplacement drifts. Berkeley Lab's roles in the heater tests are to characterize the heater-test rock block (area) prior to testing; monitor potential changes in fracture and matrix saturations through air injections, tracer testing, and ground-penetrating radar measurements; and to perform predictive thermal-hydrologic and thermal-hydrologic-chemical calculations.

The initial characterizations of the heater test areas are performed with air-injection tests that yield the 3D permeability structure of the fracture network. Continued air-injection testing during heating yielded changes that can be attributed to changes in fracture saturations or mechanical effects. Crosshole radar tomography has also yielded very promising results regarding change in global saturations of the system caused by heating. Laboratory scientists are also involved with measurements of the isotopic compositions of gases and condensate water collected in instrumented boreholes. Detailed 3D thermal-hydrologic and thermal-hydrologic-chemical calculations were used to predict the behavior of the tests. These are being refined as the test progresses.

MODELING GROUP

Berkeley Lab has the primary responsibility for the development of the UZ Flow and Transport Model. This is a comprehensive, 3D, dual-permeability numerical model that represents the entire UZ at and near Yucca Mountain. The model is intended to integrate, in a single computational framework, all of the relevant geological, hydrological, geochemical, and other observations that have been made at the surface, in boreholes, and in tunnels at Yucca Mountain. The model is calibrated against pneumatic moisture tension, matrix potential, temperature, geochemical, perched water, and other data from the UZ. The model is then used to predict all of these variables in new boreholes and new drifts to be drilled. The degree of agreement between model predictions and subsequent field observations indicates the reliability of the model, and provides guidance as to what additional data need to be collected and incorporated.

A very important submodel of the UZ model is the seepage model, which is on a tens-of-meters scale, versus the UZ model's hundreds-of-thousands-of-meters scale. The seepage model, similarly to the UZ model, predicts the results of the niche tests, which are subsequently modified to match the actual observations. Another submodel of the UZ model is the coupled process THC model, calibrated using the heater test data and used to estimate the chemistry of water and gas entering the drifts. All these models—the UZ model, the seepage model and the THC model—are key process models for Total System Performance Assessment (TSPA); performance of the potential repository is only as reliable as these key models.

FUNDING

The Nuclear Waste Program's Yucca Mountain Project research is supported by the Director, Office of Civilian Radioactive Waste Management, U.S. Department of Energy, through Memorandum Purchase Order EA9013MC5X between Bechtel SAIC Company, LLC, and Berkeley Lab. The support is provided to Berkeley Lab through U.S. Department of Energy Contract No. DE-AC03-76SF00098.

FRACTURES AND UZ PROCESSES AT YUCCA MOUNTAIN

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RESEARCH OBJECTIVES

The objective of this research is to evaluate the importance of fractures at different scales on a variety of processes in the unsaturated zone at Yucca Mountain. These processes are ambient liquid flow, radionuclide transport, and coupled thermal-hydrological processes. Additionally, we evaluate the importance of including all fractures or a subset of mapped fractures in the analysis of these processes.

APPROACH

Fractures are integral structural features at Yucca Mountain, providing highly permeable pathways for air and liquid to flow through unsaturated rocks. They are also potential pathways for radionuclide migration. Though millions of fractures exist in the unsaturated zone, the portion of these fractures relevant to assessing the performance of a potential repository depends upon the process being evaluated.

Ambient Flow Processes—Water flows mainly through fractures in the low-porosity welded tuffs occurring in the unsaturated zone at Yucca Mountain. Yet only a fraction of the widely dispersed and connected fractures is believed to actively conduct water under ambient conditions. Also, within an active fracture, only a limited area of the rock matrix is in contact with percolating water (as a result of flow fingering). Thus, much of the fracture system does not participate in liquid flow, and the transfer of water between fractures and the rock matrix is limited.

Radionuclide Transport Processes—Transport patterns are expected to mimic flow patterns under ambient conditions. Consequently, only fractures contributing to flow are important. However, the existence of small fractures and microfractures connected to larger fractures that transmit water may be important for transport, because they penetrate matrix blocks and can enhance matrix diffusion, thereby improving repository performance.

Coupled Thermal-Hydrological Processes—If a repository is constructed at Yucca Mountain, the heat generated from radioactive decay may cause boiling and vaporization of pore water in the rock surrounding the waste packages. Much of the vapor generated will migrate into fractures and be driven away from the repository drifts, creating a dryout zone. When the vapor encounters cooler rock away from the drifts, it will condense, and saturation will increase locally in all fractures. Part of the condensate may then imbibe into the matrix, while some of the condensate will remain in the fractures, become mobile, and drain around the drift opening.

ACCOMPLISHMENTS

Tens of thousands of fractures have been mapped and described as part of the site characterization of Yucca Mountain. The majority of the mapped fracture data come from fractures with trace lengths greater than 1 m; however, small fractures (< 1 m in length) are far more numerous. Some small-scale fracture-mapping studies have been conducted in the ECRB Cross Drift, and additional studies have been proposed.

SIGNIFICANCE OF FINDINGS

Numerical analyses should consider all fracture data in light of the processes to be modeled. For mountain-scale ambient-flow-modeling applications, only fractures that actively contribute to large-scale flow are believed to be significant. Since the specific fractures transmitting water are unknown, we recommend using mapped data for coarse fractures (≥ 1 m in length) to estimate fracture-network characteristics and suggest adopting a fracture-matrix interaction variable to match observed field data. For mountain-scale transport modeling, small fractures and microfractures connected to larger active fractures may be important for diffusion and should be evaluated. Coupled thermal-hydrological models should reflect information about fractures at all scales within the condensation zone, and the full fracture-matrix interface area should be used.

RELATED PUBLICATION

Hinds, J.J., and G.S. Bodvarsson, Role of fractures in processes affecting potential repository performance, Proceedings of the Ninth International High-Level Radioactive Waste Management Conference, Las Vegas, Nevada, April 29–May 3, 2001.

ACKNOWLEDGMENTS

This work was supported by the Director, Office of Civilian Radioactive Waste Management, U.S. Department of Energy, through Memorandum Purchase Order EA9013MC5X between Bechtel SAIC Company, LLC, and Berkeley Lab. The support is provided to Berkeley Lab through U.S. Department of Energy Contract No. DE-AC03-76SF00098.

MOISTURE MONITORING ALONG A NONVENTILATED SECTION OF TUNNEL AT YUCCA MOUNTAIN

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RESEARCH OBJECTIVES

The monitoring study conducted in the Enhanced Characterization of the Repository Block (ECRB) East-West Cross Drift is designed to detect drips in sealed drift sections (Figure 1). The ECRB bulkhead sections are located in the area of the drift most likely to show seepage under ambient conditions. This monitoring effort is an integrated part of the field seepage testing and monitoring program at Yucca Mountain. The seepage studies, together with hydrological measurements in boreholes and benches, provide field measurements and data to be used for calibration and validation of unsaturated zone models related to seepage.

APPROACH

To observe potential seepage, ventilation effects on the terminal section of the ECRB were minimized with the construction of two bulkheads. These bulkheads were installed in the ECRB in June 1999. A third bulkhead was installed in July 2000 to ameliorate (but not eliminate) the influence of some nearby heat sources on the tunnel conditions. Along the tunnel bore (before and after the bulkhead) humidity, temperature, and barometric pressure are being measured at various stations to provide information on moisture dynamics along the ECRB. Additionally, psychrometer measurements of water potential are being made along the length of boreholes installed before and after the bulkhead.

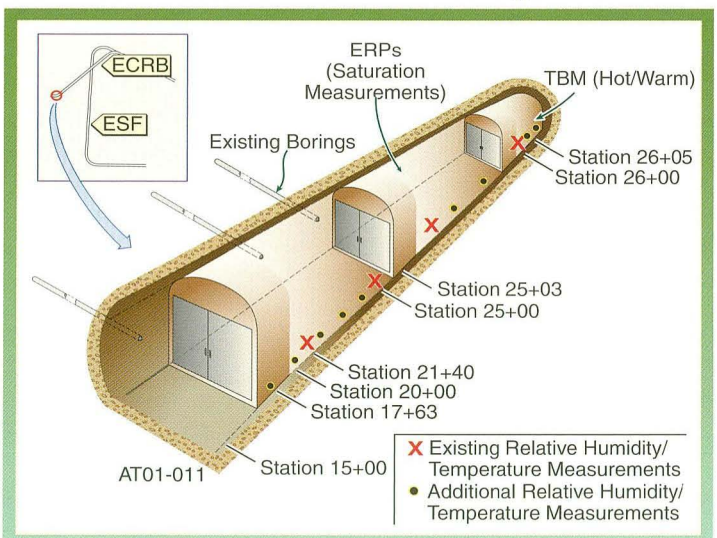

Figure 1. Terminal 944 m of the ECRB showing the location of monitoring stations and three bulkheads

ACCOMPLISHMENTS

Six moisture-monitoring stations have been located before and after the bulkhead. Data from these stations, along with periodic observations from the nonventilated zone of the ECRB, have allowed for a better understanding of moisture dynamics in the ECRB. When the bulkhead doors were opened briefly in January 2001, the cross drift was observed to be dry from the first bulkhead (17+63 to 19+00 m). While there was evidence of water from 24+75 to 24+95 m (between the first and second bulkheads), most of it was concentrated between the second and third bulkheads. Temperature and relative humidity data from the three nonventilated zone (for the first four months in 2001) show that the temperature ranged between 24 and 33°C, and the relative humidity ranged from ~80% to close to saturation.

SIGNIFICANCE OF FINDINGS

Condensation observed in the nonventilated section in the ECRB could be from seepage or temperature fluctuations associated with air moving through the fault (or with the hot, moist air leaking through the third bulkhead). Our preliminary data suggest that the observed condensation could have been caused from warmer, moist air moving away from a heat source into cooler zones. Without eliminating the heat source, the cause of the observed condensation cannot be identified definitively.

ACKNOWLEDGMENTS

This work was supported by the Director, Office of Civilian Radioactive Waste Management, U.S. Department of Energy, through Memorandum Purchase Order EA9013MC5X between Bechtel SAIC Company, LLC, and Berkeley Lab. The support is provided to Berkeley Lab through U.S. Department of Energy Contract No. DE-AC03-76SF00098.

SYSTEMATIC HYDROLOGIC CHARACTERIZATION OF THE TOPOPAH SPRING LOWER LITHOPHYSAL UNIT

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RESEARCH OBJECTIVES

Over 80% of the potential repository for the permanent disposal of high-level radioactive nuclear waste will be situated in the lower lithophysal unit of the Topopah Spring welded tuff, Yucca Mountain, Nevada. This unit is traversed by a 5 m diameter drift (the East-West Cross Drift) in the Yucca Mountain underground testing facility (the Exploratory Studies Facility). The welded tuff is intersected by many small fractures (less than 1 meter in length) and interspersed with lithophysal cavities ranging in size from 15 to 100 cm. Size and spacing of both fractures and lithophysal cavities vary appreciably along the 5 m drift walls over an 800 m stretch. This indicates that hydrological characteristics at one particular location may not be representative of the entire lower lithophysal unit. Therefore, systematic testing at regular intervals along the drift, regardless of the presence of specific features (such as large fractures, extra abundance of fractures, or cavities), is being conducted to understand the hydrological characteristics and associated heterogeneity of this potential repository unit.

APPROACH

Air-injection and liquid-release tests are being carried out in 20 m long boreholes that are drilled into the crown of the drift, parallel to and inclined at low angle (~15°) from the drift axis. These boreholes are systematically installed at 30 m intervals along the length of the drift. Air-injection tests give a measure of fracture permeability, while liquid-release tests determine the ability of the open drift to act as a capillary barrier (diverting water around itself), as well as the potential of water to seep into the drift. This is important because water seepage into the drifts increases the potential for corrosion of waste canisters and subsequent release of radionuclides.

The systematic test equipment is designed to fit on flatbed rail cars, allowing it to be efficiently transported from one test station to another along the drift. A schematic of the equipment system is shown in Figure 1. Field-scale measurements involving liquid flow in unsaturated rocks require continuous testing, lasting for weeks to months, while the underground facility is open only eight hours for four days every week. Therefore, the control of test equipment has been fully automated, allowing remote manipulation via computer network when there is no human presence at the field site.

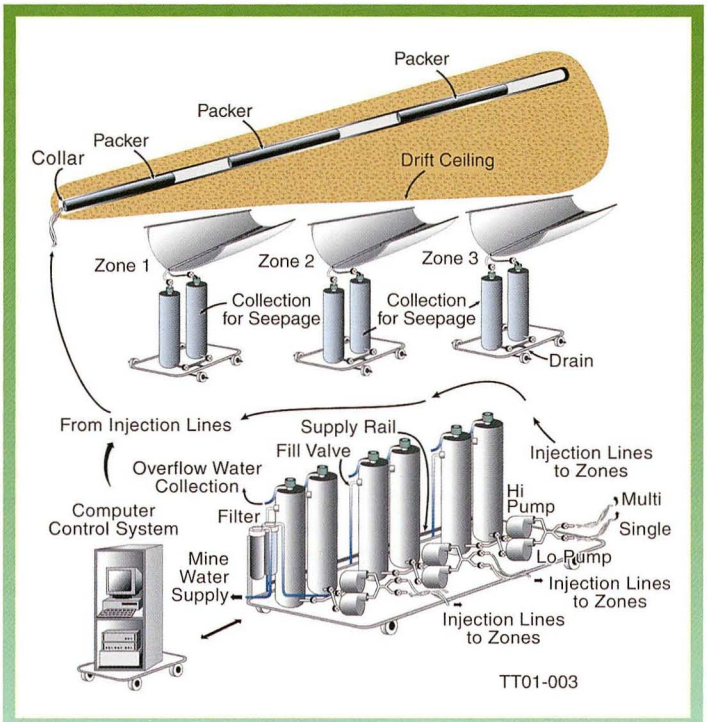

Figure 1. A schematic of the equipment system: packer assembly, water supply, air- injection component, seepage-collection component, and data acquisition and control

ACCOMPLISHMENTS AND SIGNIFICANCE OF FINDINGS

We are presently at the third systematic test station. Data to date are consistent with the conceptual model that lithophysal cavities act as capillary barriers, causing lateral diversion of percolation flux. We have also found that lithophysal cavities (when filled with water) can act as obstructions to fast paths. The tests indicate that, until the first arrival of recorded seepage, water introduced into the formation was being imbibed and stored in the matrix pores. Once seepage was initiated, flow was likely to go through the least resistive fast paths (connected fractures) with weak capillary suction.

ACKNOWLEDGMENTS

This work was supported by the Director, Office of Civilian Radioactive Waste Management, U.S. Department of Energy, through Memorandum Purchase Order EA9013MC5X between Bechtel SAIC Company, LLC, and Berkeley Lab. The support is provided to Berkeley Lab through U.S. Department of Energy Contract No. DE-AC03-76SF00098.

AUTOMATED SEEPAGE TESTING AT NICHE 5, EXPLORATORY STUDIES FACILITY, YUCCA MOUNTAIN

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RESEARCH OBJECTIVES

The objective of this research is to carry out field studies at Yucca Mountain, Nevada, to characterize the hydrogeologic processes and conditions leading to water seepage into a potential underground waste repository constructed in unsaturated fractured rock. Seepage into an underground cavity or drift depends upon the effectiveness of a capillary barrier present at the ceiling of the opening. A capillary barrier is created when the relatively strong capillary forces in the overlying rock matrix and fractures hold the water in the formation like a sponge, preventing it from dripping into the drift. Seepage into the potential repository may cause premature corrosion and failure of metal canisters, allowing the waste contained therein to migrate.

APPROACH

We are testing the physical concept of a capillary barrier and its ability to prevent or reduce seepage by introducing water at different rates into boreholes installed above specially constructed drifts (called niches) and collecting the seepage (if any) into the niche. Four niches have been constructed and tested for this purpose in the Topopah Spring Tuff middle nonlithophysal zone (Tptpmn), a densely welded, highly fractured rock containing few natural cavities. These tests were performed using manually operated test equipment.

A fifth niche site (Niche 5) was constructed in the lower lithophysae zone (Tptpll), containing abundant lithophysae cavities ranging from a few centimeters to over a meter in diameter. Automated test equipment is being used at Niche 5, allowing the remote control, operation, and monitoring of seepage experiments over the Internet (Figure 1). (Deployment of this automated test equipment reduces field test costs, produces consistent experimental results, and allows real-time monitoring and control of the experiments.)

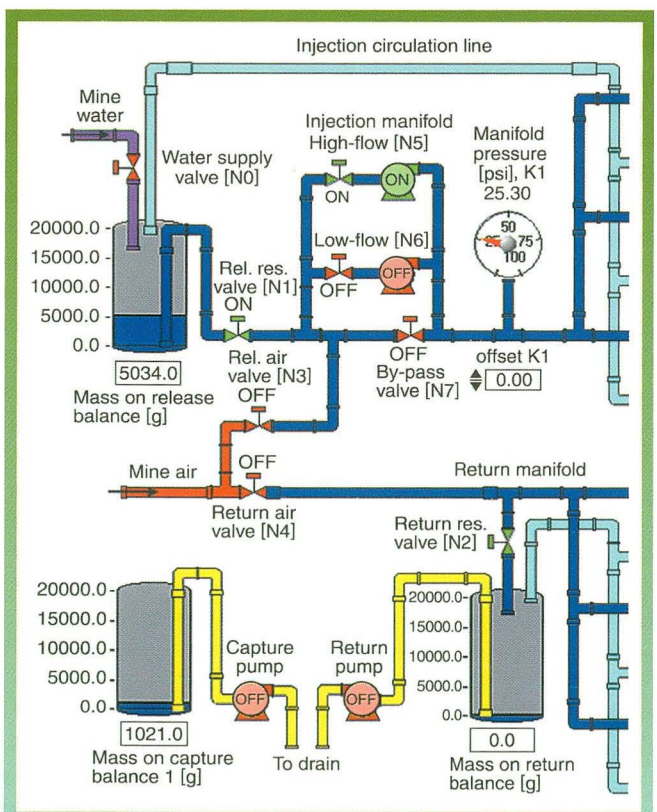

Figure 1. Virtual instrument panel used to control, operate, and monitor seepage experiments over the Internet

ACCOMPLISHMENTS

To date, over 50 tests have been conducted in the Tptpmn and initial tests are underway in the Tptpll at Niche 5 to characterize seepage. During the initial test conducted at Niche 5, approximately 300 L of water were released only 1.5 m above the drift, but the wetting front did not arrive at the niche ceiling, nor did water seep after 38 days of continuous water injection. In contrast, the wetting front typically arrived at the niche ceiling and seeped (after releasing only a couple of liters of water) within a few hours of starting the release at the niches constructed in the Tptpmn.

SIGNIFICANCE OF FINDINGS

Field tests conducted in the Tptpmn indicate that a capillary barrier is present at the ceiling of an underground opening that prevents seepage into the drift; results from Niche 5 are too preliminary to draw this same conclusion for the Tptpll. Initial tests performed in the Tptpll, however, indicate that some lithophysae cavities may act as dead-end pores that can store large volumes of water and potentially arrest or slow the progress of a transient pulse of natural water before it reaches and seeps into a drift.

RELATED PUBLICATION

Wang, J.S.Y., R.C. Trautz, P.J. Cook, S. Finsterle, A.L. James, and J. Birkholzer, Field tests and model analyses of seepage into drift, Journal of Contaminant Hydrology, 38, 323–347, 1999.

ACKNOWLEDGMENTS

This work was supported by the Director, Office of Civilian Radioactive Waste Management, U.S. Department of Energy, through Memorandum Purchase Order EA9013MC5X between Bechtel SAIC Company, LLC, and Berkeley Lab. The support is provided to Berkeley Lab through U.S. Department of Energy Contract No. DE-AC03-76SF00098.

SEEPAGE INTO DRIFTS LOCATED IN A LITHOPHYSAL ZONE

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RESEARCH OBJECTIVES

Seepage of liquid water into an underground opening such as a waste emplacement drift is a key factor affecting the performance of the potential national nuclear waste repository at Yucca Mountain, Nevada. Predicting drift seepage relies on capturing the relevant flow processes in an unsaturated fracture-network model as well as accurately representing the conditions encountered at the drift surface. The objective of this research is to design a strategy for the development, calibration, and testing of drift-seepage models. This strategy is applied to the analysis of liquid-release tests conducted at Yucca Mountain, specifically in the lower lithophysal zone of the Topopah Spring tuff.

APPROACH

Air-injection and liquid-release tests were conducted from packed-off intervals of a slanted borehole drilled into the crown of a drift located in the lower lithophysal zone. Water injection occurred over several weeks, during which the water that seeped into the drift was collected and its seepage rate measured. We then developed a three-dimensional model with a cylindrical drift opening. The fractured formation was modeled as a stochastic continuum, based on the permeabilities inferred from the air-injection tests, and lithophysal cavities were added randomly. Figure 1a shows the saturation distribution during a simulated liquid-release test, revealing flow diversion around the drift as a result of the capillary-barrier effect. The model was automatically calibrated against seepage-rate data to estimate an effective capillary strength, which is the parameter most strongly affecting seepage and for which direct measurements are not available. Calibration by inverse modeling is a critical step in the procedure because it provides effective, model-related, seepage-specific flow parameters at the scale of interest. To test the ability of the model to make seepage predictions, we performed Monte Carlo simulations and compared them to data from additional liquid-release tests not used during calibration (Figure 1b).

ACCOMPLISHMENTS

Detailed analyses of the seepage data and model results show that average seepage can be both reproduced and predicted by the calibrated model. However, the estimated parameters are specific to the conceptual model and its numerical implementation, as well as to the conditions encountered during testing. Lithophysal cavities tend to increase seepage because they lead to flow focusing and a jagged drift ceiling. Both effects increase the probability of capillary-barrier failure at a lower percolation flux. Finally, evaporation (currently not explicitly modeled) has been identified as a key mechanism affecting seepage data and thus the estimated parameters.

SIGNIFICANCE OF FINDINGS

The combination of field testing and inverse modeling enables the estimation of seepage-relevant parameters that can be used in subsequent model predictions and sensitivity analyses of seepage into waste emplacement drifts. If test conditions are accurately monitored and the key features affecting seepage are included in the numerical model, the approach developed in this research can provide the means to make seepage predictions even in the absence of microscale characterization data. This finding is of practical interest, specifically for studies related to the performance of a potential nuclear waste repository at Yucca Mountain.

RELATED PUBLICATION

Finsterle, S., Using the continuum approach to model unsaturated flow in fractured rock, Water Resour. Res., 36(8), 2055–2066, 2000.

ACKNOWLEDGMENTS

This work was supported by the Director, Office of Civilian Radioactive Waste Management, U.S. Department of Energy, through Memorandum Purchase Order EA9013MC5X between Bechtel SAIC Company, LLC, and Berkeley Lab. The support is provided to Berkeley Lab through U.S. Department of Energy Contract No. DE-AC03-76SF00098.

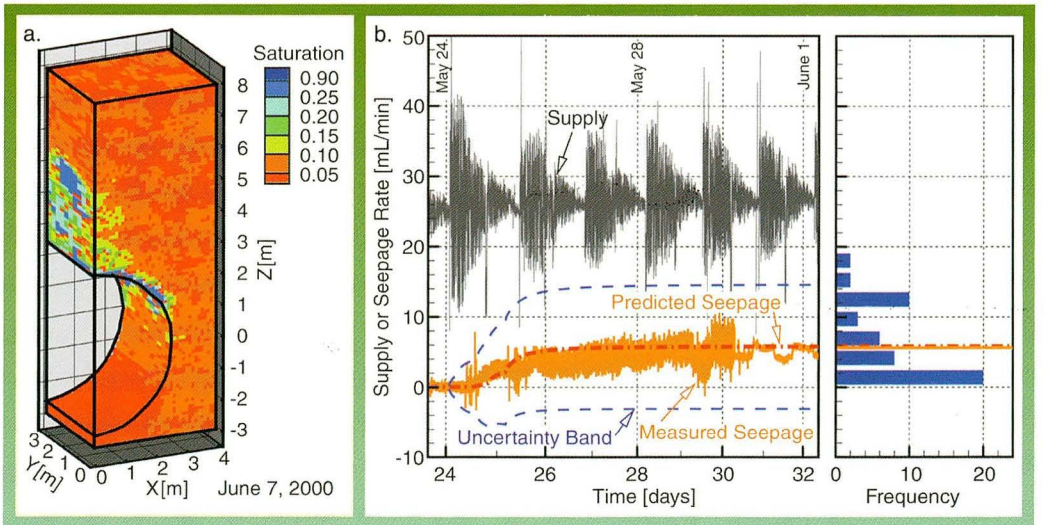

Figure 1a. Saturation distribution during simulation of liquid-release test performed to calibrate 3D, heterogeneous drift seepage model (injection at indicated supply rate occurs approximately 2.75 m above niche crown); 1b. Comparison between measured and predicted seepage rates (uncertainty band calculated from linear analysis, histogram from Monte Carlo simulations).

IMPACT OF ROCK BOLTS ON SEEPAGE

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RESEARCH OBJECTIVES

Characterization of seepage into drifts in unsaturated fractured tuff is a key factor for assessing the long-term viability of the proposed high-level nuclear waste repository at Yucca Mountain. Rock bolts are among the methods proposed for ground control in the emplacement drifts. Rock bolts may, however, also provide a conduit whereby percolating water that would otherwise bypass the drift will seep into the drift (see Figure 1). The objective of this study is to assess the impact that the use of rock bolts may have on seepage.

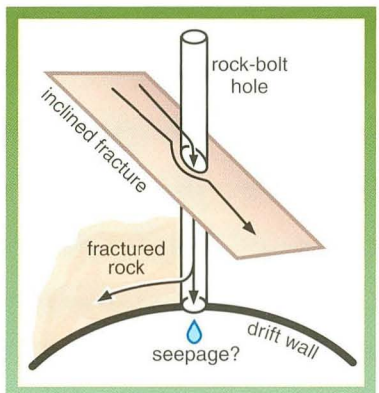

Figure 1. Schematic of rock-bolt interaction with percolation through unsaturated fractured tuff

APPROACH

The impact of rock bolts on seepage is studied using a numerical model that is finely discretized around the rock bolt. Several sources of uncertainty and variability exist with respect to the flow system around the drift and rock bolt. There is uncertainty about the capillary strength of the fractures around the drift, as well as about how the permeability and capillary strength of the grout (used to cement the steel rock bolts into the bolt holes) will change over time. Variability is expected in the percolation rates incident upon the drifts, depending on location. The uncertainty and variability of these parameters are approached by evaluating the rock-bolt impact over a range of values for several model parameters. It is also important to consider where the last fracture capable of carrying flow away from the rock bolt intersects the rock bolt. Three models are used in which the last fracture is 0, 10, and 50 cm (respectively) above the drift.

ACCOMPLISHMENTS

When the rock bolt and grout are much less permeable than the surrounding fractures, as they are expected to be for several hundred years after installation, they should not enhance seepage because water will preferentially flow in the more permeable fracture system. At much later times, when the grout has degraded, the effectively open rock-bolt hole will form a capillary barrier, with the water again preferentially flowing in the fracture system (i.e., the greater capillary strength of the fracture system will keep water from entering the rock bolt hole). For the cases in which the permeability and capillary strength of the rock bolt and grout system are on the same order as that of the fracture system, the model indicates that the rock bolts do not enhance seepage, which is reasonable considering the small volume occupied by the rock bolts.

SIGNIFICANCE OF FINDINGS

A simpler model previously developed to study this problem indicated that for the planned rock bolt spacing of 1.5 m, seepage would be enhanced by as much as 40%. The results of this more detailed study will allow the amount of seepage predicted to enter the drifts to be reduced for the Total System Performance Assessment (TSPA) for Yucca Mountain. These results also reduce uncertainty about the amount of seepage and thus will reduce uncertainty about TSPA results.

RELATED PUBLICATION

Ahlers, C.F., Y.S. Wu, Q. Hu, G. Li, H.H. Liu, J. Liu, L. Pan, Unsaturated zone flow processes and analysis, MDL-NBS-HS-000012 REV00, Bechtel SAIC Company, Las Vegas, Nevada, Berkeley Lab, 2001 (submitted).

ACKNOWLEDGMENTS

This work was supported by the Director, Office of Civilian Radioactive Waste Management, U.S. Department of Energy, through Memorandum Purchase Order EA9013MC5X between Bechtel SAIC Company, LLC, and Berkeley Lab. The support is provided to Berkeley Lab through U.S. Department of Energy Contract No. DE-AC03-76SF00098.

SEEPAGE ENHANCEMENT RESULTING FROM ROCKFALL

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RESEARCH OBJECTIVES

Seepage into drifts in unsaturated tuff is an important issue for the long-term performance of the potential nuclear waste repository at Yucca Mountain, Nevada. Waste emplacement drifts are subject to drift-ceiling rockfall induced by excavation or long-term degradation caused by seismic or thermal effects. The objective of this research is to calculate seepage rates—for various rockfall scenarios and different values of percolation flux—through the Topopah Spring middle nonlithophysal (Tptpmn) and the Topopah Spring lower lithophysal (Tptpll) units at Yucca Mountain.

APPROACH

Seepage enhancement caused by rockfall is addressed by (1) defining a heterogeneous permeability model on the drift scale that is consistent with field data, (2) selecting calibrated parameters associated with the Tptpmn and the Tptpll units in which the potential repository will be situated, and (3) applying rockfall scenarios from detailed degraded drift profiles calculated in a separate rock mechanical analysis.

Detailed 3D degraded drift profiles calculated using a discrete-region key-block analysis were used to define three scenarios of rockfall from the drift ceiling: worst degradation (largest rockfall volume) profile, profile at the 75th percentile, and no degradation. The 75th percentile case corresponds to a rockfall valume per unit length greater than the rockfall volume per unit length in 75% of the overall emplacement drift length for that rock unit. Seepage was calculated in each of the three scenarios for a series of percolation fluxes and for three realizations of the heterogeneous permeability field.

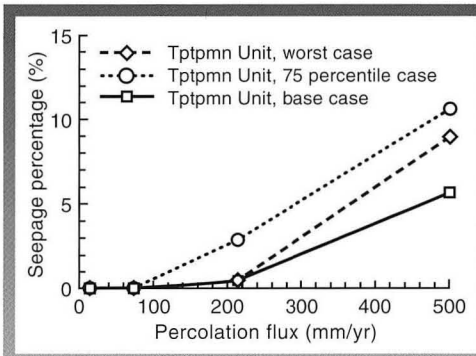

Figure 1. Seepage percentage as a function of percolation flux Q_P for three scenarios in the Tptpmn unit, Realization 1

ACCOMPLISHMENTS

Figure 1 shows that seepage enhancement for the scenarios in the Tptpmn unit decreases with decreasing percolation flux. The results indicate that seepage enhancement resulting from the worst case and the 75th percentile case rockfall ranges from 0 to 5% for percolation flux up to 500 mm/yr. For the scenarios in the Tptpll unit, values of percolation flux up to 2,500 mm/yr were used because of the low seepage. The seepage enhancement caused by rockfall in the Tptpll is 2% or less.

SIGNIFICANCE OF FINDINGS

For both the Tptpmn and Tptpll units, seepage enhancement caused by rockfall was predicted to be larger for larger percolation flux. The magnitude of the enhancement appears to be limited to the scenarios and parameters used. The enhancement does not appear to depend on whether the worst (i.e., largest rockfall) or 75th percentile case is used.

ACKNOWLEDGMENTS

This work was supported by the Director, Office of Civilian Radioactive Waste Management, U.S. Department of Energy, through Memorandum Purchase Order EA9013MC5X between Bechtel SAIC Company, LLC, and Berkeley Lab. The support is provided to Berkeley Lab through U.S. Department of Energy Contract No. DE-AC03-76SF00098.

UPSCALING OF CONSTITUTIVE RELATIONS IN UNSATURATED, HETEROGENOUS POROUS MEDIA

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RESEARCH OBJECTIVES

When numerical models are used for modeling field-scale flow and transport processes in the subsurface, the problem of "upscaling" arises. Typical scales, corresponding to spatial resolutions of subsurface heterogeneity in numerical models, are generally much larger than the measurement scale of the parameters and physical processes involved. The upscaling problem is, then, one of assigning parameters to large (gridblock) scales based on parameter values measured on small scales. The focus of this study is to determine upscaled constitutive relations (relationships among relative permeability, capillary pressure, and saturation) from small-scale measurements, for porous media with large air-entry values representative of the unsaturated zone tuff matrix at Yucca Mountain, Nevada (the potential site of a national high-level nuclear waste repository).

APPROACH

For porous media with large air-entry values, capillary forces play a key role in determining spatial water distribution at large scales. Consequently, an approximately uniform capillary pressure exists even for a relatively large gridblock scale under steady-state flow conditions. Based on this reasoning, we developed formulations that relate upscaled constitutive relationships to ones measured at core scale. Numerical studies with stochastically generated heterogeneous porous media were then used to evaluate these upscaling formulations.

ACCOMPLISHMENTS

General formulations for upscaling constitutive relations were developed for heterogeneous porous media with large air-entry values. We then applied the upscaled constitutive-relationship formulations to the tuff matrix in the unsaturated zone of Yucca Mountain. Numerical simulation results are in good agreement with the relations calculated from the upscaling formulations, supporting the validity of these formulations.

SIGNIFICANCE OF FINDINGS

Upscaling is always needed for field-scale modeling studies. Although considerable progress has been made in upscaling flow parameters describing saturated flow, our knowledge about upscaling unsaturated flow parameters is very incomplete. This work represents the first effort to rigorously determine large-scale constitutive relations from small-scale measurements for porous media with high air-entry values.

RELATED PUBLICATION

Liu, H.H., and G.S. Bodvarsson, Upscaling of constitutive relations in unsaturated heterogeneous porous media with large air entry values, Water Resour. Res., 2001 (submitted).

ACKNOWLEDGMENTS

This work was supported by the Director, Office of Civilian Radioactive Waste Management, U.S. Department of Energy, through Memorandum Purchase Order EA9013MC5X between Bechtel SAIC Company, LLC, and Berkeley Lab. The support is provided to Berkeley Lab through U.S. Department of Energy Contract No. DE-AC03-76SF00098.

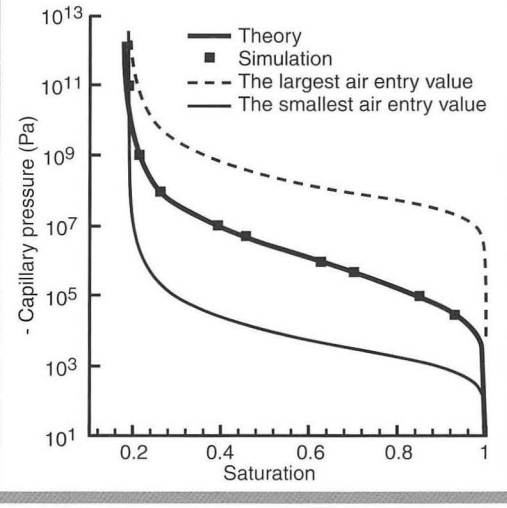

Figure 1. Comparison between upscaled water retention curves and simulated data points. Local water-retention curves with the largest and smallest air-entry values are also shown to demonstrate the spatial variability within the porous medium used in numerical experiments.

CONSTITUTIVE RELATIONS FOR UNSATURATED FLOW IN A FRACTURE NETWORK

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RESEARCH OBJECTIVES

The continuum approach is frequently used for modeling unsaturated flow in both porous and fractured media. Such a continuum model requires specifying constitutive relationships (relative permeability and capillary-pressure functions) originally developed for porous media. While proven successful for describing flow in porous media, the applicability of these concepts to fracture networks remains to be demonstrated. The objective of this study is to examine the usefulness and limitations of the widely used van Genuchten and Brooks-Corey models, and to develop improved models for the specific characteristics of fracture networks.

APPROACH

Because it is generally difficult to directly measure constitutive relationships for a fracture network in the field, we have determined these relationships from numerical simulations of steady-state unsaturated flow in two-dimensional fracture networks (Figure 1). In these simulations, a fracture network is considered to be an effective porous medium. The rock matrix is treated as impermeable for the purpose of focusing on the fracture continuum. Fracture networks consist of vertical and horizontal fractures with different hydraulic properties.

ACCOMPLISHMENTS

Our investigations found that the van Genuchten model could reasonably well match the simulated water-retention curves except for high saturations, but both van Genuchten and Brooks-Corey models generally underestimate relative permeability values except at low saturations. On the basis of this finding, we propose a new relative permeability-saturation relationship for the fracture continuum by modifying the Brooks-Corey approach. The combination of this new relationship and the van Genuchten capillary pressure-saturation relationship can represent the simulated curves and may provide an improved set of constitutive relationships for the fracture continuum. However, this study is based largely on numerical results, and further investigation based on relevant field observations are needed.

SIGNIFICANCE OF FINDINGS

The constitutive relationships developed for porous media to describe unsaturated flow in subgrid-scale fracture networks may not be valid for a fracture continuum, because the geometry of a fracture network is considerably different from pore geometry in a porous medium. Moreover, unsaturated flow behavior in a fracture network, which is mainly determined by gravity, is not necessarily the same as that in a porous medium. This study represents an effort to deal with this important issue.

RELATED PUBLICATION

Liu, H.H., and G.S. Bodvarsson, Constitutive relations for unsaturated flow in a fracture network, Journal of Hydrology (in press).

ACKNOWLEDGMENTS

This work was supported by the Director, Office of Civilian Radioactive Waste Management, U.S. Department of Energy, through Memorandum Purchase Order EA9013MC5X between Bechtel SAIC Company, LLC, and Berkeley Lab. The support is provided to Berkeley Lab through U.S. Department of Energy Contract No. DE-AC03-76SF00098.

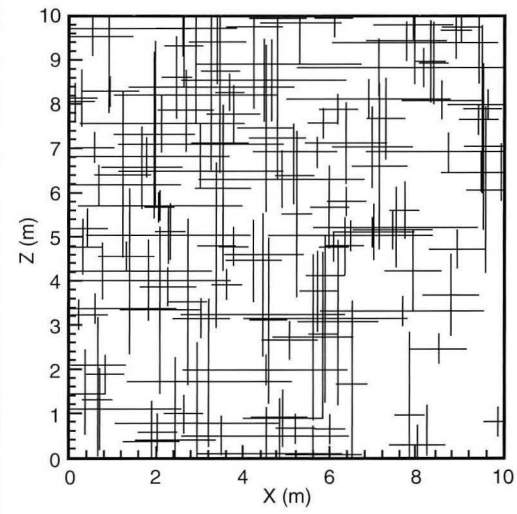

Figure 1. Computationally generated fracture networks with the scanline density of 2.2 (fracture/m)

CAPILLARY-BARRIER EFFECTS IN UNSATURATED FRACTURED ROCKS OF YUCCA MOUNTAIN

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RESEARCH OBJECTIVES

Naturally occurring capillary barriers have been of considerable interest for many subsurface flow and contiminant transport problems. The objective of this study is to investigate the effects of capillary barriers on water-flow processes in the unsaturated zone (UZ) of Yucca Mountain. We identify factors controlling the formation of capillary barriers and estimate their effects on the extent of possible large-scale lateral flow within the unsaturated, fractured rocks. This study indicates that the UZ of Yucca Mountain is capable of producing strong capillary-barrier effects, which may laterally divert significant amounts of flow.

APPROACH

This modeling study uses five different 2D vertical cross-sectional models to explore capillary-barrier formation and lateral diversion under current ambient flow conditions. The conceptual hydrogeological framework is based on the one used to develop the current UZ flow model of Yucca Mountain (Wu et al., 2000). In this framework, the UZ is represented by a stack of three-dimensional layers, each with its own set of fracture and matrix properties. In addition, these layers are intersected by several major faults.

Numerical simulations in this study are performed with the TOUGH2 code. Hydrogeological layers and faults along the cross-sectional models are captured by refined numerical grids. A dual-permeability approach is used to handle fracture-matrix interactions. The bottom model boundary is located at either the water table or at the interface between the Paintbrush (PTn) and Topopah Spring (TSw) units of Yucca Mountain, while the top model boundary coincides with the bedrock surface of the mountain. Surface net infiltration of water is applied to the top boundary to approximate present-day mean infiltration rates.

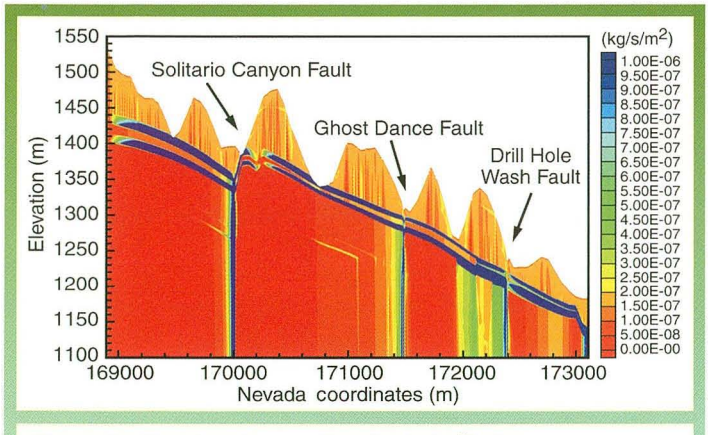

Figure 1. Simulated mass flux (kg/s/m^2) along an east-west cross section, showing lateral flow along naturally occurring capillary boundaries and vertical flow along faults

ACCOMPLISHMENTS

Examination of simulated percolation fluxes at the PTn–TSw interface using the five cross-sectional models reveals that significant lateral flow occurs within the PTn unit, with a large amount of water being diverted to down-slope faults. Faults serve as major downward flow pathways crossing the PTn under the current conceptual model. Figure 1 shows two simulated layers within the PTn with high fluxes. These layers control lateral flow within the PTn unit as a result of the contrast in rock properties between these layers and adjacent layers. The figure also shows that major faults provide the main flow pathways for vertical percolation flux.

SIGNIFICANCE OF FINDINGS

This study indicates that with the current conceptualization, significant capillary-barrier effects may exist within the PTn unit and, as a result, large-scale lateral flow could occur. Faults serve as major downward pathways for laterally diverted water. Capillary barriers within the PTn unit are mainly the result of contrasts in matrix hydraulic parameters, while fracture properties have a less significant impact on water flow. Compared with detailed, spatially varying distributions, the magnitude of the average net-infiltration rate has a larger impact on flow patterns through the PTn unit. The model results also show that capillary-barrier effects are strongly correlated with surface infiltration rates, with lower infiltration leading to larger lateral flow.

RELATED PUBLICATION

Wu, Y.S., J. Liu, T. Xu, C. Haukwa, W. Zhang, H.H. Liu, and C.F. Ahlers, UZ flow models and submodels, Report MDL-NBS-HS-000006, CRWMS M&O, 2000.

ACKNOWLEDGMENTS

This work was supported by the Director, Office of Civilian Radioactive Waste Management, U.S. Department of Energy, through Memorandum Purchase Order EA9013MC5X between Bechtel SAIC Company, LLC, and Berkeley Lab. The support is provided to Berkeley Lab through U.S. Department of Energy Contract No. DE-AC03-76SF00098.

AN IMPROVEMENT TO DCPT: THE PARTICLE-TRANSFER PROBABILITY AS A FUNCTION OF PARTICLE'S AGE

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RESEARCH OBJECTIVES

Multiscale features of transport processes in fractured porous media make numerical modeling a difficult task, in both conceptualization and computation. In response to this difficulty, investigators have found the dual-continuum particle-tracker (DCPT) numerical model an attractive method for numerically modeling large-scale problems typically encountered in the field, such as those in the unsaturated zone (UZ) of Yucca Mountain, Nevada (the site for a potential national repository of high-level nuclear waste). This method's particular advantage is its ability to capture the major features of flow and transport in fractured porous rock (i.e., a fast fracture subsystem combined with a slow matrix subsystem) with reasonably few computational resources. However, as with other conventional dual-continuum approach-based numerical methods, DCPT (v1.0) is often criticized for failing to capture the transient features of the diffusion depth into the matrix. It tends to overestimate the transport of tracers through the fractures, especially for the cases with large fracture spacing, and thus predict artificial early breakthroughs. The objective of this study is to develop a theory for calculating the particle-transfer probability that captures the transient features of diffusion depth into the matrix within the framework of the dual-continuum random-walk particle method.

APPROACH

Our approach is to relate the particle-transfer probability to the particle's age by introducing the concept of particle activity range. Particle activity range is used to describe the transient features of the diffusion depth into the matrix. A quantitative relationship between the activity range of a particle and the particle's age is derived from an analytical solution for a system of parallel-plate fractures (separated by porous rock) responding to a pulse injection in the fractures. The method was incorporated into an enhanced version of DCPT (DCPT v2.0), used to model particle transport in heterogeneous, fractured porous media, and then verified against proven analytical solutions.

ACCOMPLISHMENTS

This new method was verified against analytical solutions for a variety of fracture spacings (Figure 1). Both the old modeling system (DCPT v1.0) and new (DCPT v2.0) predict breakthrough curves that agree well with the analytical solutions for the case with a fracture spacing of 1 m. However, for the case of the larger fracture spacing of 10 m, the old method seriously overestimates the breakthrough at early times (see Figure 1). On the other hand, Figure 1 shows that DCPT v2.0 predicts breakthrough curves that are almost identical to the analytical solutions for both cases (Figure 1). Thus, the new method shows the ability to effectively capture transient features of the diffusion depth into the matrix, using only one matrix block to represent the matrix. It does not assume a passive matrix medium (as required by a residence-time particle tracking approach) and can be applied to cases where global water flow exists in both continua.

This method was then applied to calculate the breakthrough curves of radionuclides from a potential nuclear-waste repository (i.e., Yucca Mountain, Nevada) to the water table. Our findings demonstrate the effectiveness of this new technique for simulating 3D, mountain-scale transport in a heterogeneous, fractured porous medium under variably saturated conditions. The results show that transient effects (of the diffusion depth into matrix) on the breakthrough of radionuclides are significant.

SIGNIFICANCE OF FINDINGS

The results of this study show DCPT v2.0 capturing transient features of the diffusion depth into the matrix (using only one matrix block to represent the matrix) without assuming a passive matrix medium. DCPT v2.0 thus proves to be a uniquely powerful simulation tool, both in terms of accuracy and efficiency, for modeling transport in fractured porous media.

The results would also suggest the importance of transient features in any further studies. Application of DCPT v.2.0 to the Yucca Mountain case indicates that transient-feature effects (of the diffusion depth into matrix) on solute breakthrough are significant in many cases, especially when fracture spacing is large and the effective diffusion coefficient is small. These effects may need to be accounted for in future modeling of real-world transport problems.

RELATED PUBLICATION

Pan, L., and G.S. Bodvarsson, Modeling transport in fractured porous media with the random-walk particle method: The transient activity range and the particle-transfer probability, Water Resour. Res., 2001 (submitted).

ACKNOWLEDGMENTS

This work was supported by the Director, Office of Civilian Radioactive Waste Management, U.S. Department of Energy, through Memorandum Purchase Order EA9013MC5X between Bechtel SAIC Company, LLC, and Berkeley Lab. The support is provided to Berkeley Lab through U.S. Department of Energy Contract No. DE-AC03-76SF00098.

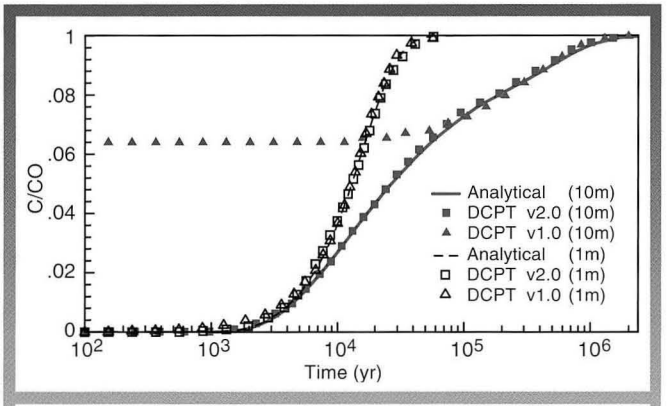

Figure 1. Predicted breakthrough curves by DCPT v1.0, DCPT v2.0, and analytical solutions for the case with smaller fracture spacing (1 m) and larger fracture spacing (10 m), respectively

THERMAL-LOADING STUDIES USING THE UNSATURATED ZONE MODEL

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RESEARCH OBJECTIVES

At Yucca Mountain, Nevada, the potential site of a high-level radioactive waste repository, several factors affect the thermal-hydrologic (TH) response of the unsaturated zone (UZ) to thermal load at the potential repository. These factors include small- and large-scale heterogeneity, the thermal load within the repository drifts, and the presence of lithophysal cavities. The objective of this study is to use numerical modeling to simulate and quantify these factors.

APPROACH

Numerical modeling is used to investigate the effects of heat on UZ flow, temperature, and liquid saturation on two spatial scales, for a range of potential repository operating modes. Two TH models are derived from two dual-permeability numerical grids. The first model is produced from a refined north-south mountain-scale 2D grid. The second model is produced from a refined half-drift (1 m grid near drift) 2D grid with several realizations of spatially variable fracture permeability for the Topopah Spring welded unit (TSw), the geological unit in which the potential repository would be located.

In the TSw lithophysal units, thermal capacity and thermal conductivity of the lithophysal units were scaled within these models, using the lithophysal porosity. The first model provides an overview of layer-wise constant-fracture-permeability behavior at the mountain scale. The second model includes both small-scale (<1 m correlation length) heterogeneity in the fracture permeability and discrete high-permeability fractures. Monte Carlo methods were used to generate several realizations of spatially variable fracture permeability (up to four orders of magnitude) in the TSw, based on the measured distribution of fracture permeability within the exploration drifts. Above-boiling and below-boiling repository operating modes were investigated by varying the initial thermal load and the amount of heat removed by ventilation. The simulations of coupled heat and mass flow were conducted using TOUGH2 (EOS3 module) over a simulated period of 100,000 years.

ACCOMPLISHMENTS

The models accounted for the uncertainty in repository heat load, the effectiveness of the ventilation process, spatial heterogeneity in flow properties, and the effect of lithophysal cavities. For both the above-boiling and below-boiling cases, the drift and the zone below (drift shadow) are dry (Figure 1a), but liquid saturation increases above drifts and within the drift pillars. Therefore, while liquid flux up to 5 m above the drifts and within the pillars may be enhanced by condensation, the liquid flux below drifts is zero (Figure 1b) or significantly reduced (by a combination of thermal and capillary barrier effects) for over 1,000 years. Spatial heterogeneity in fracture permeability and even the presence of highly permeable features does not substantially alter the predicted liquid percolation flux.

SIGNIFICANCE OF FINDINGS

The TH models provide insight into how decay heat from emplaced waste will affect the magnitude and spatial distribution of temperature, liquid saturation, and percolation flux reaching the potential waste emplacement drifts, which in turn affects the potential for seepage into the drifts. Reduced liquid percolation below the drift means that there is little potential for transport of radionuclides away from the drifts for thousands of years. However, the above-boiling operating mode may result in higher-than-desired temperatures in the waste emplacement drifts as well as parts of other units above and below TSw.

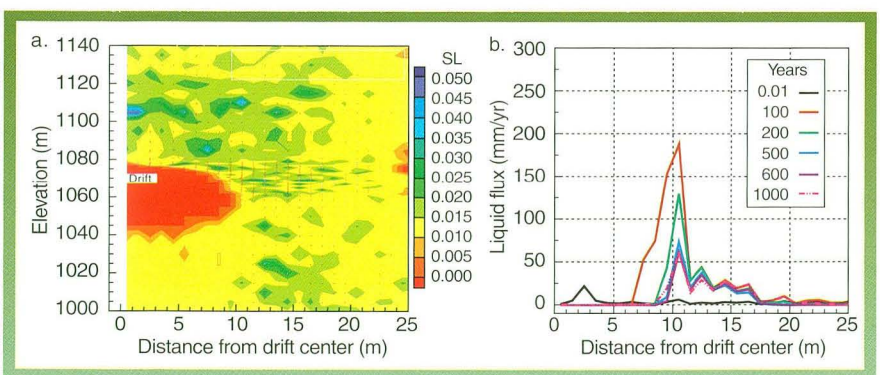

Figure 1a. Fracture liquid saturation and flux at 1,000 years. Spatially variable fracture permeability, Var. #1: 1.45 kW/m, 50 years 70% ventilation. High permeability fracture $k_f \times 100$ into drift.

Figure 1b. Fracture liquid flux at drift centerline. Variable fracture permeability, Var. #1: 1.45 kW/m, 50 years 70% ventilation. High permeability fracture $k_f \times 100$ into drift.

RELATED PUBLICATION

C.B. Haukwa, S. Mukhopadhay, Y.W. Tsang, and G.S. Bodvarsson, Liquid seepage at the repository horizon under thermal loading, Water Resour. Res., 2001 (submitted).

ACKNOWLEDGMENTS

This work was supported by the Director, Office of Civilian Radioactive Waste Management, U.S. Department of Energy, through Memorandum Purchase Order EA9013MC5X between Bechtel SAIC Company, LLC, and Berkeley Lab. The support is provided to Berkeley Lab through the U.S. Department of Energy Contract No. DE-AC03-76SF00098.

UNDERSTANDING THE IRREGULAR DATA FROM THE LARGE BLOCK TEST

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RESEARCH OBJECTIVES

The Large Block Test (LBT) is one of three thermal tests at Yucca Mountain, Nevada. The test block, with a size of 3 × 3 × 4.5 m, is highly fractured, , with at least four-orders-of-magnitude variation in permeability. Recent temperature data from the LBT contained some features that differed from what would normally be expected of thermal-hydrologic coupled processes in a fracture continuum. In this project, we attempt to develop a better understanding of these irregular temperature data.

APPROACH

The test block in the LBT was excavated from the surrounding Topopah Spring fractured nonlithophysal tuff in the Fran Ridge area of Yucca Mountain. The bottom of the block remained attached to the underlying rock, while the top and four side faces were kept open to the atmosphere. Mapping of all the fractures from the four sides and the top surface of the block revealed the existence of some large fractures in the block. The presence of such large fractures indicated that the flow of water and heat-induced vapor could be very different in different zones of the block, with vapor and water flowing more easily through the highly permeable fractures than elsewhere. It is our hypothesis that the irregular temperature data arose out of thermal-hydrological (TH) processes taking place in the heterogeneous fracture system. We show, through simulations that incorporated discrete fractures into a 3D dual-permeability numerical model (based on the TOUGH2 simulator), that a heterogeneous fracture system can indeed give rise to the observed irregular temperature data.

ACCOMPLISHMENTS

While certain LBT temperature data at first glance appeared anomalous, our studies found that these anomalies can be attributed to thermal-hydrologic processes in a heterogeneous fractured block. As an illustration of the impact of heterogeneities on TH processes, a comparison between measured and simulated temperatures in a vertical borehole (TT1) is shown in Figure 1. The irregular temperature data in Figure 1 can be correlated to a rain event that occurred at about 4,470 hours of heating in the LBT. As seen in the figure, simulations performed with a 3D dual-permeability numerical model, specifically accounting for rain water flowing down fractures in the vicinity of the temperature borehole, show good agreement with this measured data. As rain water trickled down the fractures in the heated rock, complex TH processes occurred in its heterogeneous environment. Temperatures at Sensor TT1-28 (at the top of the block), originally at 60°C, went up to 100°C before declining to 60°C when the rain stopped. However, Sensor TT1-14, which was at 140°C, fell sharply to 100°C before returning to 140°C. As rain water came in contact with the heated rock (maximum temperature at Sensor TT1-14, closest to the heaters), it vaporized. When the vapor passed upward through cooler zones away from the heaters, temperatures at those locations increased to 100°C. Thus, though certain temperature signatures from the LBT appear irregular, they can be explained in terms of thermal-hydrologic processes within fracture heterogeneities, for which the model provides a good understanding.

ACKNOWLEDGMENTS

This work was supported by the Director, Office of Civilian Radioactive Waste Management, U.S. Department of Energy, through Memorandum Purchase Order EA9013MC5X between Bechtel SAIC Company, LLC, and Berkeley Lab. The support is provided to Berkeley Lab through U.S. Department of Energy Contract No. DE-AC03-76SF00098.

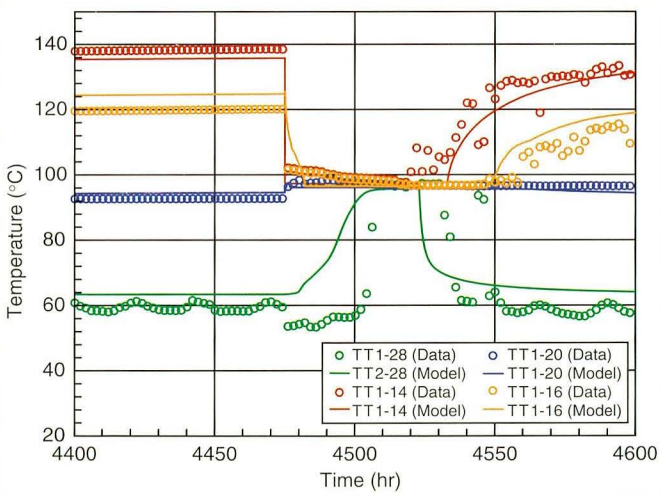

Figure 1. Comparison of measured and simulated temperatures at selected sensors of borehole TT1 in the LBT.

MODELING OF THERMAL-HYDROLOGIC-CHEMICAL LABORATORY EXPERIMENTS

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RESEARCH OBJECTIVES

The objective of this research is to use coupled thermal-hydrologic-chemical (THC) models to simulate previously conducted laboratory experiments investigating (1) tuff dissolution and (2) mineral precipitation in a boiling, unsaturated fracture. Mineral dissolution and precipitation could affect the total system performance of the potential nuclear waste repository at Yucca Mountain, Nevada, where heat-generating nuclear waste will induce vaporization of water present in the rock matrix and fractures. Vaporized water will migrate via fractures to cooler regions where condensation and mineral dissolution would occur. Mineralized water flowing back towards the heated zone would boil, depositing the dissolved minerals, reducing porosity and permeability above the repository, and potentially altering the flow paths of percolating water.

APPROACH

Numerical simulations of tuff dissolution and mineral precipitation in a fracture were performed using a modified version of the TOUGHREACT code developed at Berkeley Lab by T. Xu and K. Pruess. These simulations consider the transport of heat, water, gas, and dissolved constituents; reactions between gas, mineral, and aqueous phases; and the coupling of porosity and permeability to mineral dissolution and precipitation. Model dimensions and initial fluid chemistry, rock mineralogy, permeability, and porosity were defined to reproduce the experimental conditions. A 1D plug-flow model was used to simulate mineral dissolution in water. A 2D model was developed to simulate the flow of mineralized water through a planar fracture within a nonisothermal block of ash flow tuff, where boiling conditions led to mineral precipitation. In this model, fluid flow was confined to the fracture. Fracture permeability changes were calculated using the cubic law.

ACCOMPLISHMENTS

Simulations were conducted for both the tuff dissolution and fracture mineral deposition experiments. Predicted concentrations of the major dissolved constituents for the tuff dissolution were within a factor of 2 of the measured average steady-state compositions (Figure 1). The fracture mineral deposition simulations are ongoing, with initial model results indicating the precipitation of a narrow band of silica at the base of the boiling front. While the overall reduction of fracture porosity is small (~2–3% over 5 days), fracture permeability is reduced by over an order of magnitude because of the highly focused silica precipitation. Both of these results are in agreement with experimental observations.

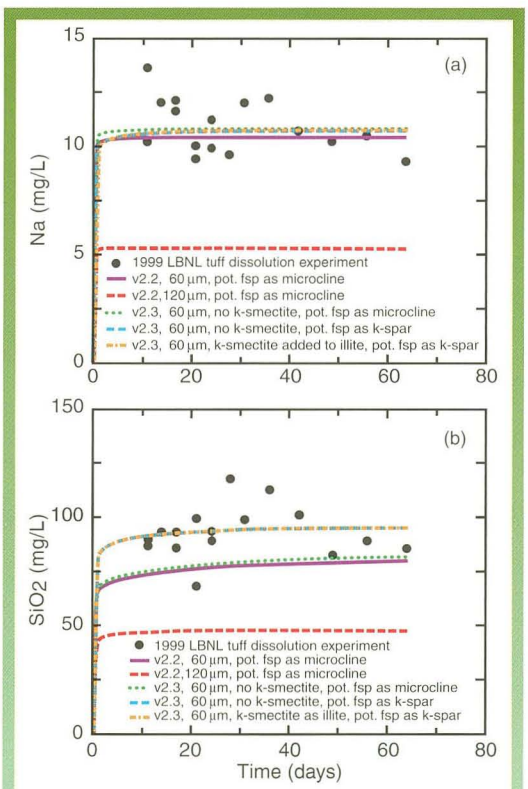

Figure 1. Comparison of measured and simulated results for the tuff dissolution plug-flow experiment. Legend descriptions refer to versions 2.2 and 2.3 of TOUGHREACT, use of 60 and 120 mm grain-size models, and variations in model mineralogy. Plots show variations with time for Na (a) and SiO_2 (b).

SIGNIFICANCE OF FINDINGS

This study demonstrates that carefully constructed THC models can successfully replicate laboratory experiments, thus validating the use of similar models in the prediction of changes in permeability, porosity, and resulting fluid flow for the potential nuclear waste repository at Yucca Mountain.

RELATED PUBLICATIONS

Kneafsey, T.J., J.A. Apps, and E.L. Sonnenthal, Tuff dissolution and precipitation in a boiling, unsaturated fracture, Proceedings of the 9th International High-Level Radioactive Waste Management Conference, Las Vegas, Nevada, April 29–May 3, 2001.

Sonnenthal, E.L., and N. Spycher, Drift-scale coupled processes (DST and THC seepage) models, Report MDL-NBS-HS-000001 REV01, Bechtel SAIC Company, Las Vegas, Nevada, Berkeley Lab, 2001 .

ACKNOWLEDGMENTS

This work was supported by the Director, Office of Civilian Radioactive Waste Management, U.S. Department of Energy, through Memorandum Purchase Order EA9013MC5X between Bechtel SAIC Company, LLC, and Berkeley Lab. The support is provided to Berkeley Lab through U.S. Department of Energy Contract No. DE-AC03-76SF00098. We thank Stefan Finsterle for his assistance in model design.

MOUNTAIN-SCALE COUPLED THERMAL-HYDROLOGIC-CHEMICAL PROCESSES AROUND THE POTENTIAL NUCLEAR WASTE REPOSITORY AT YUCCA MOUNTAIN

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RESEARCH OBJECTIVES

The objective of this study is to evaluate the thermal-hydrological-chemical (THC) effects on flow and geochemistry in the unsaturated zone (UZ) at Yucca Mountain, Nevada, at a mountain scale. The major THC processes important in the UZ are (1) mineral precipitation/dissolution affecting flow and transport to and from the potential repository, and (2) changes in the compositions of gas and liquid that may seep into drifts.

APPROACH

The conceptual model developed for THC processes provides the basis for modeling mineral-water-gas reactions, because they influence the chemistry of water and gas and associated changes in mineralogy and hydrologic properties. Data incorporated in the model include hydrologic and thermal properties, geologic layering from the UZ 3D flow and transport model, geochemical data (fracture and matrix mineralogy, water and gas geochemistry), and thermodynamic and kinetic data. Simulations included coupling among heat, water, and vapor flow; aqueous and gaseous species transport; kinetic and equilibrium mineral-water reactions; and feedback of mineral precipitation/dissolution on porosity, permeability, and capillary pressure for a dual-permeability (fracture-matrix) system. Simulations were performed using TOUGHREACT V2.3.

The effects of coupled THC processes on the evolution of flow fields and water and gas chemistry in the UZ were evaluated for an above-boiling thermal operating mode. A cross section was chosen from the UZ 3D flow and transport model that follows a north-south trend through the potential repository. Minerals include calcite, silica phases, feldspars, zeolites, clays, gypsum, fluorite, and iron oxides with the relevant aqueous species. The gas phase consists of air, water vapor, and CO_2. The composition of the initial and infiltrating water was derived from the matrix pore water extracted from the Topopah Spring welded tuff near the ongoing Drift Scale Test.

ACCOMPLISHMENTS

The simulations revealed that 5,000 years after waste emplacement, most of the region above and directly below the potential repository undergoes a small reduction in fracture porosity of less than 1% (Figure 1). Above the northern edge, a region of slight porosity increase persists, owing to enhanced vapor convection and condensation. The areas that show the most effect as a result of heating are the zeolitic units below the potential repository, where calcic zeolites dissolve to form alkali feldspars, leading to increased aqueous calcium concentrations and increased porosity. The predicted range in pH from 7 to 9 is linked to changes in gas-phase CO_2 concentrations induced by heating of pore waters.

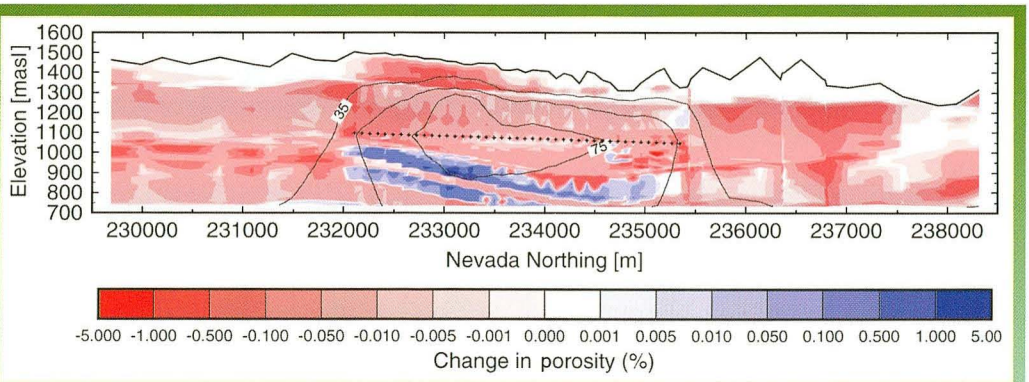

Figure 1. Porosity changes and temperature contours after 5,000 years. Crosses represent potential repository drift locations.

SIGNIFICANCE OF FINDINGS

The results of these simulations, based on a limited range of input parameters, suggest that mineral precipitation/dissolution will not significantly affect the percolation flux above the potential repository compared to the effects on flow induced solely by increased temperature. Edge effects owing to gas convection produce mineral precipitation below the drifts at the potential repository edge and in wider ranges in water and gas compositions than has been observed in drift-scale THC simulations. The results of this modeling will be used to bound uncertainties in potential repository performance.

RELATED PUBLICATION

Sonnenthal, E.L., and N. Spycher, Drift-scale coupled processes (DST and THC seepage) models, Report MDL-NBS-HS-000001 REV01, Bechtel SAIC Company, Las Vegas, Nevada, Berkeley Lab, 2001.

ACKNOWLEDGMENTS

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TEMPERATURE EFFECTS ON SEEPAGE FLUID COMPOSITIONS AT YUCCA MOUNTAIN

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RESEARCH OBJECTIVES

This project investigated the effect of two repository operating-temperature modes on coupled thermal, hydrological, and chemical processes around potential nuclear waste-emplacement tunnels (drifts) at Yucca Mountain, Nevada. The main objective of this study was to evaluate the composition of fluids (water and gas) that could enter the drifts, because these data directly relate to the performance of waste canisters and other in-drift engineered systems over the life of the potential repository.

APPROACH

Multicomponent reactive transport simulations were performed using TOUGHREACT, initially written by T. Xu and K. Pruess at Berkeley Lab and modified here to handle high-temperature and boiling environments. Two repository operating- temperature modes were investigated: (1) a high-temperature mode, which considered a short preclosure ventilation period (50 years) and gave rise to above-boiling temperatures in rocks around the drift for hundreds of years, and (2) a low-temperature mode with a smaller heat load and longer preclosure ventilation (300 years), yielding temperatures at the surface of the waste package below 85°C (a design threshold) and thus below boiling conditions. Simulations under ambient conditions (no heat load) were also conducted to serve as a baseline for comparing results of thermal-loading simulations.

ACCOMPLISHMENTS

For each considered temperature mode, time profiles of various calculated thermal, hydrologic, and chemical parameters were generated for several locations around a simulated drift (Figure 1). In the high-temperature case, fractures around the drift dry out as soon as preclosure ventilation ends and remain dry until approximately 1,500 years. During this time period, carbon dioxide concentrations (pore gas) fall below ambient values because of boiling and displacement by steam. In contrast, in the low-temperature case, fractures never dry out, and carbon dioxide concentrations remain above ambient values, because this gas is exsolved from matrix pore waters (by heating) and transported into fractures. For most major cations and anions, predicted concentrations immediately after dryout in the high-temperature case are significantly higher (one or more orders of magnitude) than in the low-temperature case, because of larger prior evaporative concentration. However, this effect dissipates relatively quickly as percolating waters rewet the drift wall after dryout.

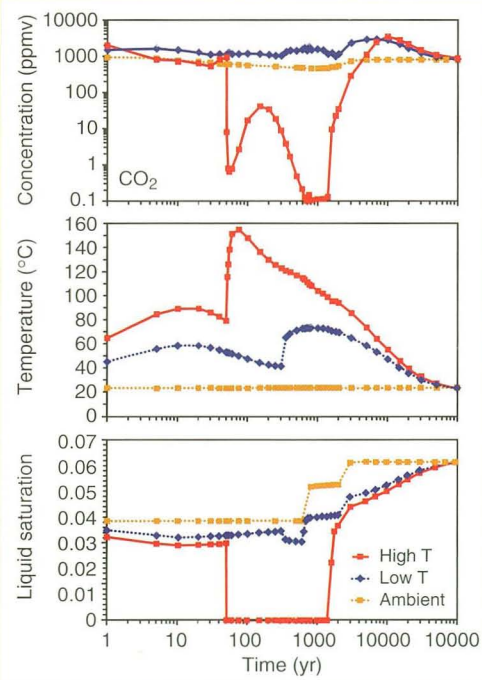

Figure 1. Predicted time profiles of thermal, hydrologic, and chemical parameters at the drift crown in fractures. The model infiltration rate was increased at 600 years and 2,000 years to account for possible future climate changes.

SIGNIFICANCE OF FINDINGS

During the first simulated 5,000 years or so, seepage water compositions around drifts are more affected by high than low temperatures, primarily as a result of evaporative concentration. However, at temperatures below boiling, the continuous presence of water in fractures around the drift increases the potential for seepage to occur. In the long term (5,000 years or more), water and gas compositions return to ambient values along with temperatures and become largely dominated by the composition of infiltrating water, regardless of the operating temperature mode of the repository. Therefore, the variability of infiltrating water compositions is also important in determining the variability of fluid compositions that could enter drifts.

RELATED PUBLICATION

Spycher, N., and E. Sonnenthal, Section 6.3.1 in Supplemental Science and Performance Analyses, Scientific Bases and Analyses, TDR-MGR-MD-000007, Vol. 1, REV 00D (Draft), Bechtel SAIC Company, Las Vegas, Nevada, Berkeley Lab, 2001.

ACKNOWLEDGMENTS

This work was supported by the Director, Office of Civilian Radioactive Waste Management, U.S. Department of Energy, through Memorandum Purchase Order EA9013MC5X between Bechtel SAIC Company, LLC, and Berkeley Lab. The support is provided to Berkeley Lab through U.S. Department of Energy Contract No. DE-AC03-76SF00098.

COUPLING OF TOUGH2 AND FLAC3D FOR COUPLED THERMAL-HYDROLOGIC-MECHANICAL ANALYSIS UNDER MULTIPHASE FLOW CONDITIONS

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RESEARCH OBJECTIVES

The objective of this research is to develop a numerical simulator for coupled thermal-hydrologic-mechanical (THM) analysis in complex geological media under multiphase flow conditions, with possible coupling to reactive transport modeling.

APPROACH

Two existing computer codes, TOUGH2 and FLAC3D, have been joined to develop a numerical simulator (TOUGH-FLAC) for analysis of coupled THM processes in complex geological media under two-phase flow conditions. Both codes are well established and widely used in their respective fields. The TOUGH2 code is designed for geohydrological analysis of multiphase, multicomponent fluid flow and heat transport, while the FLAC-3D code is designed for rock and soil mechanics involving thermo-mechanical and hydromechanical interactions. The two codes are executed on two separate meshes and joined with two coupling modules (Figure 1). One set of coupling modules can be exchanged with another set, depending on the type of rock and the problem being considered.

ACCOMPLISHMENTS

Two sets of coupling modules have been developed over the past year. One set has been developed for highly fractured rocks and has been applied to the Yucca Mountain site in Nevada. A second set has been developed for porous rocks and applied to geological sequestration of CO_2. Each set requires two coupling modules (Figure 1). The first module is used to transfer temperature and multiphase fluid pressures from the thermal-hydraulic analysis in TOUGH2 to the stress-strain analysis in FLAC3D. This also involves interpolation of TOUGH2 pressures, saturation, and temperatures from TOUGH2 nodes (mid-element) to FLAC3D nodes (element corners). The second coupling module takes the stress field calculated by FLAC3D and corrects the hydraulic properties for the TOUGH2 simulation. In the case of fractured rock, the aperture is a nonlinear function of the stress across each fracture set. The aperture changes are then used to correct fracture porosity, permeability, and the capillary pressure function. Through various iterative schemes, either explicitly or implicitly coupled solutions are obtained.

SIGNIFICANCE OF FINDINGS

We have successfully constructed a coupled THM numerical simulator for two-phase flow conditions, and its use has been demonstrated. The results from these simulations will be important for performance assessments of geological disposal of CO_2 and spent nuclear fuel, and are also valuable in other applications such as geothermal energy extraction and oil and gas reservoir engineering.

RELATED PUBLICATION

Rutqvist, J., Y.-S. Wu, C.-F. Tsang, and G. Bodvarsson, Coupling of TOUGH2 and FLAC3D codes for analysis of multiphase fluid flow, heat transfer, and rock deformation, International Journal of Rock Mechanics, 2001 (submitted).

ACKNOWLEDGMENTS

This work was jointly supported by the Director, Office of Science, Office of Basic Energy Sciences, Chemical Sciences and Geosciences Division of the U.S. Department of Energy, and the by the Office of Civilian Radioactive Waste Management, U.S. Department of Energy, through Memorandum Purchase Order EA9013MC5X between Bechtel SAIC Company, LLC, and Berkeley Lab. The support is provided to Berkeley Lab through U.S. Department of Energy Contract No. DE-AC03-76SF00098.

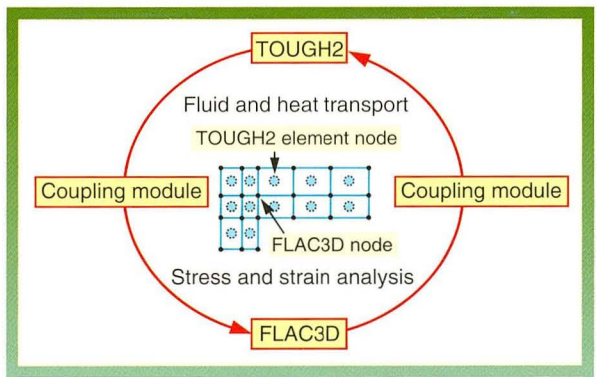

Figure 1. Schematic of the TOUGH-FLAC numerical simulator

MODELING OF COUPLED THERMAL-HYDROLOGIC-MECHANICAL PROCESSES AT YUCCA MOUNTAIN

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RESEARCH OBJECTIVES

The objective of this study is to investigate the impact of stress-induced permeability changes (a coupled hydrologic-mechanical effect) on the performance of a potential nuclear waste repository at Yucca Mountain, Nevada.

APPROACH

The two computer codes TOUGH2 and FLAC3D have been joined to form a numerical simulator (named TOUGH-FLAC) for analysis of coupled THM processes in complex geological media under two-phase flow conditions. For the Yucca Mountain project, the two codes are joined with hydromechanical coupling functions that account for stress-induced changes in fracture apertures and corresponding changes in fracture hydraulic properties. In our modeling, these hydromechanical coupling functions are calibrated against several field experiments conducted in the Exploratory Study Facility (ESF) at Yucca Mountain. Using the calibrated functions and the TOUGH-FLAC code, we then predict THM conditions around a future potential repository at Yucca Mountain.

ACCOMPLISHMENTS

With waste emplacement and thermal input, the coupled model predicts thermal stresses that will reduce permeability around the entire perimeter of the drift. In the long term, thermal effects will cause permeability changes far from the drift (up to 100 m), with most changes occurring in the vertical permeability. Permeability reduction is a function of initial local permeability values, which are larger for initially low values. However, despite permeability decreases to a factor of 0.2 in low-permeability regions, the effect of the hydromechanical coupling on the percolation flux around the drift is not significant (Figure 1). The reason is that the water-retention curve and the relative permeability, which can change much more than stress-induced permeability, dictates unsaturated flow. Further, a stress-induced decrease in permeability may be compensated for by an increase in relative permeability.

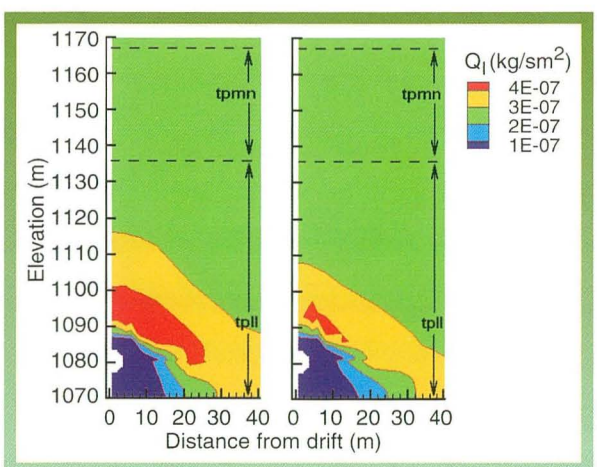

Figure 1. Distribution of percolation flux for a pure TH simulation (left) and a fully coupled THM simulation (right). In the THM calculation (right), the hydraulic properties of the rock mass are a function of stress.

SIGNIFICANCE OF FINDINGS

That the stress-induced changes in hydraulic properties have little or no impact on the flow field indicates that hydromechanical coupling for this particular case scenario is not a significant factor in the total system performance assessment of a potential repository. Work on other scenarios and sensitivity studies would be useful for further understanding of this issue.

RELATED PUBLICATIONS

Bodvarsson, G.S., J. Wang, A. Unger, J. Liu, Y-S. Wu, J. Hinds, C. Haukwa, E. Sonnenthal, C.-F. Tsang, and J. Rutqvist, Unsaturated zone flow, in Chapter 3 of Supplemental Science and Performance Analyses, Volume 1, Scientific Bases and Analyses, TDR-MGR-MD-000007, REV 00, CRWMS M&O, Las Vegas, Nevada, 2001 (in press).

Finsterle, S., G.S. Bodvarsson, C.F. Ahlers, G. Li, C-F. Tsang, Y. Tsang, E.L. Sonnenthal, and J. Rutqvist, Seepage, in Chapter 4 of Supplemental Science and Performance Analyses, Consisting of Volume 1, Scientific Bases and Analyses, TDR-MGR-MD-000007, REV 00, CRWMS M&O, Las Vegas, Nevada, 2001 (in press).

ACKNOWLEDGMENTS

This work was supported by the Director, Office of Civilian Radioactive Waste Management, U.S. Department of Energy, through Memorandum Purchase Order EA9013MC5X between Bechtel SAIC Company, LLC, and Berkeley Lab. The support is provided to Berkeley Lab through U.S. Department of Energy Contract No. DE-AC03-76SF00098.

YELLOWSTONE AS AN ANALOG FOR THERMAL-HYDROLOGIC-CHEMICAL PROCESSES AT YUCCA MOUNTAIN

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RESEARCH OBJECTIVES

Enhanced water-rock interaction resulting from the emplacement of heat-generating nuclear waste in the potential geologic repository at Yucca Mountain, Nevada, may result in changes to fluid flow (resulting from mineral dissolution and precipitation in condensation and boiling zones, respectively). Studies of water-rock interaction in active and fossil geothermal systems (natural analogs) provide evidence for changes in permeability and porosity resulting from thermal-hydrologic-chemical (THC) processes. The objective of this research is to document the effects of coupled THC processes at Yellowstone and then examine how differences in scale could influence the impact that these processes may have on the Yucca Mountain system.

APPROACH

Subsurface samples from Yellowstone National Park, one of the largest active geothermal systems in the world, contain some the best examples of hydrothermal self-sealing found in geothermal systems (Figure 1). We selected core samples from two U.S. Geological Survey research drill holes from the transition zone between conductive and convective portions of the geothermal system (where sealing was reported to occur). We analyzed the core, measuring the permeability, porosity, and grain density of selected samples to evaluate how lithology, texture, and degree of hydrothermal alteration influence matrix and fracture permeability.

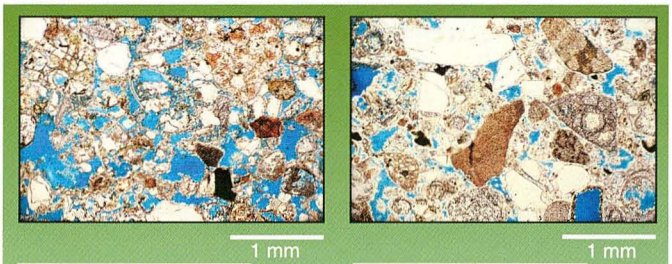

Figure 1. Silica sealing in volcaniclastic sandstone core samples from Yellowstone. Blue color in photomicrographs is dyed epoxy filling pore space in thin sections. Similar zones of silica sealing form an impermeable cap to the convective portion of the Yellowstone geothermal system.

ACCOMPLISHMENTS

We examined core samples from the Y-5 and Y-8 drill holes, describing lithology, texture, hydrothermal alteration, and veins and fractures. Observed variations in porosity and matrix permeability are primarily controlled by lithology. Volcaniclastic sandstone and nonwelded tuffs have high porosity and moderate matrix permeability, while densely welded ash-flow tuffs and rhyolite lavas have low porosity and permeability. Fractures are most abundant in the latter two lithologies and provide the dominant pathways for fluid flow there. Most of the observed fractures have been sealed by hydrothermal mineralization. A zone of secondary silica mineralization in the Y-8 core corresponds to the location of the impermeable cap for the near-isothermal, convective geothermal reservoir.

SIGNIFICANCE OF FINDINGS

Predicting changes in permeability and porosity resulting from water-rock interaction is important in evaluating the long-term performance of nuclear waste repositories and for geothermal reservoir engineering. Geothermal systems have much higher fluxes of heat and fluid flow than those predicted for the potential Yucca Mountain repository, and thus hydrothermal mineralization (and the resulting permeability and porosity reduction) at Yucca Mountain is likely to be much less extensive than that observed at Yellowstone. Scaling comparisons and THC modeling of Yellowstone could provide a more quantitative way to test THC models used for the Yucca Mountain system.

RELATED PUBLICATION

Dobson, P., J. Hulen, T.J. Kneafsey, and A. Simmons, Permeability at Yellowstone: A natural analog for Yucca Mountain processes, Proceedings of the 9th International High-Level Radioactive Waste Management Conference, Las Vegas, Nevada, April 29–May 3, 2001,

ACKNOWLEDGEMENTS

This work was supported by the Director, Office of Civilian Radioactive Waste Management, U.S. Department of Energy, through Memorandum Purchase Order EA9013MC5X between Bechtel SAIC Company, LLC, and Berkeley Lab. The support is provided to Berkeley Lab through U.S. Department of Energy Contract No. DE-AC03-76SF00098. Additional support (to Jeffery Hulen) was provided by DOE Grant DE-FG07-00ID13891 to Energy and Geoscience Institute.

U-SERIES TRANSPORT STUDIES AT PEÑA BLANCA, MEXICO, NATURAL ANALOG SITE

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RESEARCH OBJECTIVES

Natural analogs provide a line of evidence that supports the understanding of how natural and engineered processes could occur over long time frames and large spatial scales at a potential nuclear waste repository at Yucca Mountain, Nevada. Studies of U-series disequilibria within and around uranium deposits can provide valuable information on the timing of actinide mobility and hence the stability of a potential repository over geologic time scales. The Nopal I uranium deposit at Peña Blanca, Mexico, is situated in unsaturated tuff that is similar in composition to the Topopah Spring Tuff of Yucca Mountain and closely matches other evaluation criteria for suitable natural analogs. By modeling the observed radioactive isotope disequilibria at Nopal I, we can estimate the rates of sorption-desorption and dissolution-precipitation of the radionuclides over time. Such information is vital to the testing or validation of performance assessment models for geologic nuclear waste disposal.

APPROACH

A number of boreholes through and surrounding the ore deposit will be drilled to the water table (a depth of ~200 m); from these boreholes, solid core and water samples will be taken. Isotopes of ^{234}U, ^{238}U, ^{232}Th, ^{230}Th, ^{228}Th, ^{234}Th, ^{226}Ra, ^{228}Ra, ^{210}Po, and ^{210}Pb will be measured in the fluid samples. Radioactive disequilibria in sorbed phases will be obtained using leaching methods on the core samples. To correct for the possible effect of evaporative concentration on model results, Cl^- or $\delta^{18}O$ and δD compositions of water samples from the unsaturated zone will be compared with those of rainwater. The final report will include recommendations on the application of model results from the Peña Blanca analog site to testing the unsaturated zone process models that provide input to performance assessment models for Yucca Mountain.

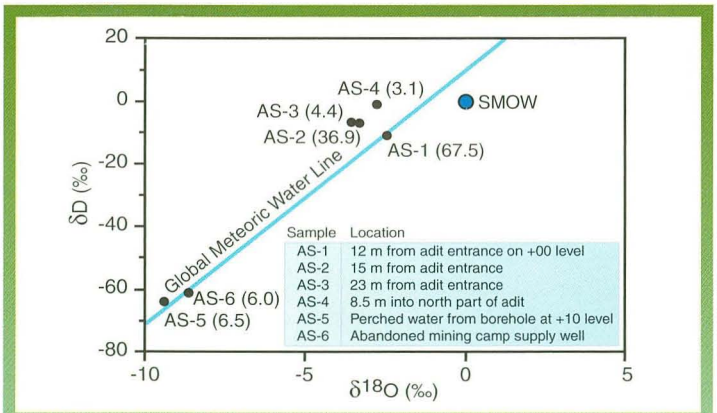

Figure 1. Uranium and stable isotope data for water samples collected (black circles) from Peña Blanca during February 2000. Also shown is the position of the global meteoric water line and SMOW (Standard Mean Ocean Water). Uranium concentrations in parts per billion (ppb) are indicated in parentheses after the sample number. Sample locations are shown on key.

ACCOMPLISHMENTS

Shown in Figure 1 are the stable isotope data and uranium concentrations for the samples collected in 2000. Samples AS-1 and AS-2 exhibit higher U concentrations because of proximity to the ore body (exposed from 0 to 2 m into the adit), indicating the rapid decrease in U concentration with distance from the ore body. Samples AS-5 and AS-6 have significantly lower δD and $\delta^{18}O$ values than the other samples. They probably represent the average composition for the precipitation at the site. The other samples were all collected from an adit in the unsaturated zone. Of these, AS-1 lies on the GMWL, but probably does not represent a rainwater sample (it is relatively enriched in D and ^{18}O for meteoric water at this latitude). The other three samples all fall significantly to the left of the GWML and may represent atmospheric water vapor that has condensed in the cooler, underground environment, followed by some evaporation in the collection bottles.

SIGNIFICANCE OF FINDINGS

U-series modeling provides a means to characterize the kinetically controlled radionuclide transport and residence time at Peña Blanca. Using an earlier data set collected by Southwest Research Institute, we estimated the ^{234}U alpha-recoil rate into fluids to be 9 dpm/L/y at Peña Blanca versus dissolution rates of 8.3 dpm/L/y for ^{238}U and ^{234}U. The kinetic model also allows determination of fluid transit time in the unsaturated zone. Uranium-238 increases linearly with increasing transit time, while $^{234}U/^{238}U$ decreases. The transit time for the seep water infiltrated into the adit 8 m below surface is estimated to be 6–29 days, and that for the perched water at 10.7 m depth in an old borehole is 0.4–0.5 years. The large values of transit time for the perched water may reflect the long residence time of water in the borehole. Although the water transit time in the unsaturated zone is quite short, detectable dissolution of U from fractured rocks does occur in this low-water flux, high-U concentration setting near the Nopal I uranium deposit.

RELATED PUBLICATION

Murrell, M.T.; P. Paviet-Hartmann, S.J. Goldstein, A.J. Nunn, R.C. Roback, P.A. Dixon, and A. Simmons, U-Series natural analog studies at Peña Blanca, Mexico: How mobile is uranium? EOS Transactions, AGU 80, F1205, 1999.

ACKNOWLEDGMENTS

Stable isotope analyses were performed by Mark Conrad, Berkeley Lab. U-series modeling was done by Shangde Luo and Teh-Lung Ku, USC. This work was supported by the Director, Office of Civilian Radioactive Waste Management, U.S. Department of Energy, through Memorandum Purchase Order EA9013MC5X between Bechtel SAIC Company, LLC, and Berkeley Lab. The support is provided to Berkeley Lab through U.S. Department of Energy Contract No. DE-AC03-76SF00098.

DEVELOPING AN EFFECTIVE-CONTINUUM SITE-SCALE MODEL FOR FLOW AND TRANSPORT IN FRACTURED ROCK

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RESEARCH OBJECTIVES

The objective of this project is to participate in a multinational program to investigate the uncertainties involved in developing conceptual and numerical models for prediction of flow and transport behavior through fractured rock.

APPROACH

In a previous study (the H-12 flow comparison), several international research organizations conducted numerical simulations with the same starting information regarding a hypothetical fractured rock mass. The results were subsequently compared. In the present work, the exercise is applied to a real site, a 4 km x 6 km x 3 km region north of the Toki River in the Tono area of Gifu, Japan.

In our conceptual model, stochastic permeability and porosity distributions are used to represent fractured rock as an effective continuum. Individual fractures are not modeled explicitly. However, large-scale features such as fault zones, lithologic layering, natural boundaries, and surface topography are incorporated deterministically. The stochastic permeability distribution results from hydrologic testing that occurs using packed-off borehole intervals of comparable length to the model gridblock dimensions (~100 m), giving us confidence that the permeability values being used in the model are reasonable. In contrast, the only data available on which to base porosity estimates are fracture density measurements. These measurements, obtained from borehole optical scanner images and core samples, are typically taken on a much smaller scale (a few centimeters) than the model gridblocks. Porosity estimates also rely on the cubic law, which is known to be unreliable. Hence, we recognize that there is a large uncertainty associated with any model result that depends on porosity, such as travel times through the model.

ACCOMPLISHMENTS

We developed the model shown in Figure 1 and used the numerical simulator TOUGH2 to simulate steady-state flow through the 4 km x 6 km x 3 km region. Regional topography determines the extent of the grid and the boundary conditions. The resulting flow fields appear consistent with local infiltration data and head profiles in boreholes. Calculated travel times from monitoring points to the model boundaries range from 1 to 25 years.

SIGNIFICANCE OF FINDINGS

A major benefit of the present project is the chance for a variety of modeling approaches to highlight which aspects of site characterization need to be improved to increase confidence in model predictions. Because the field investigation program is ongoing, model results can potentially have a significant impact on future characterization activities.

The wide range in travel times obtained by the different research groups for the present exercise (several years to millions of years) can be largely attributed to orders-of-magnitude differences in the effective porosity assumed for the fracture network. Coupled with our recognition that porosity is one of the least well-constrained parameters of our model, this finding indicates that a field program aimed at better estimating effective fracture porosity is needed. Possible areas of investigation include using naturally occurring trace elements or isotopes to estimate residence times and flow paths on a regional scale, or active tracer tests using suites of neighboring wells to estimate effective porosity on a smaller scale.

ACKNOWLEDGMENTS

This work was supported by the Japan Nuclear Fuel Cycle Corporation (JNC) and Taisei Corporation of Japan, through U.S. Department of Energy Contract No. DE-AC03-76SF00098.

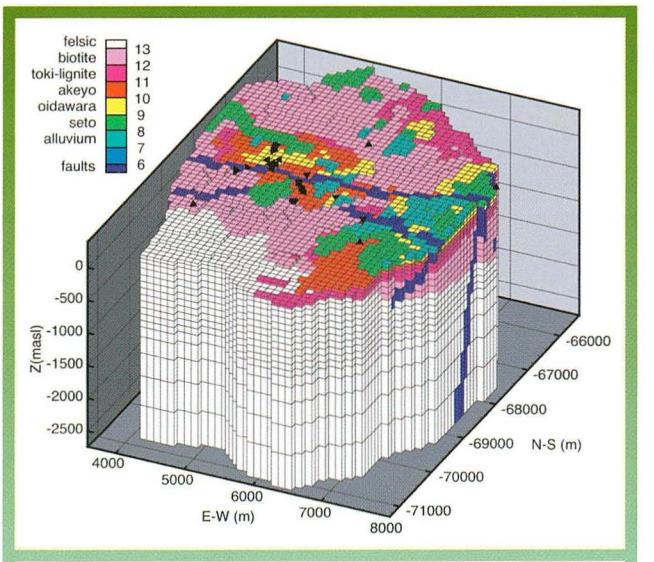

Figure 1. 3D perspective view of the model used for the TOUGH2 simulations of the 4 × 6 km region. Material types are color coded. Surface locatons of wells are black symbols.

SIMULATING INFILTRATION AT THE LARGE-SCALE PONDED INFILTRATION TEST, INEEL

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RESEARCH OBJECTIVES

This work involves using ITOUGH2 to simulate the Large-Scale Ponded Infiltration Test (LPIT) at Idaho National Engineering and Environmental Laboratory (INEEL) to calibrate parameters controlling the infiltration of water in fractured basalt, using a dual-permeability modeling approach. This supports the higher objective of building confidence in the use of the dual-permeability approach for modeling flow and transport in unsaturated fractured rock systems.

APPROACH

A 3D dual-permeability mesh representing the geological conditions at the LPIT was constructed as shown by the cross section on Figure 1a. The geology consisted of surficial sediments, two separate basalt flows (A and B basalts) underlain by a low-permeability sedimentary (BC) interbed, and a lower C basalt constituting the bottom of the model. Water was allowed to infiltrate from the pond and then pool on top of the sedimentary interbed. Water pressure was simulated at four wells screened within the fractured basalt on top of the sedimentary interbed (B04N11, C04C11, B06N11, C06C11) along two radial angles and at two radial distances. Model results were calibrated to field data using ITOUGH2.

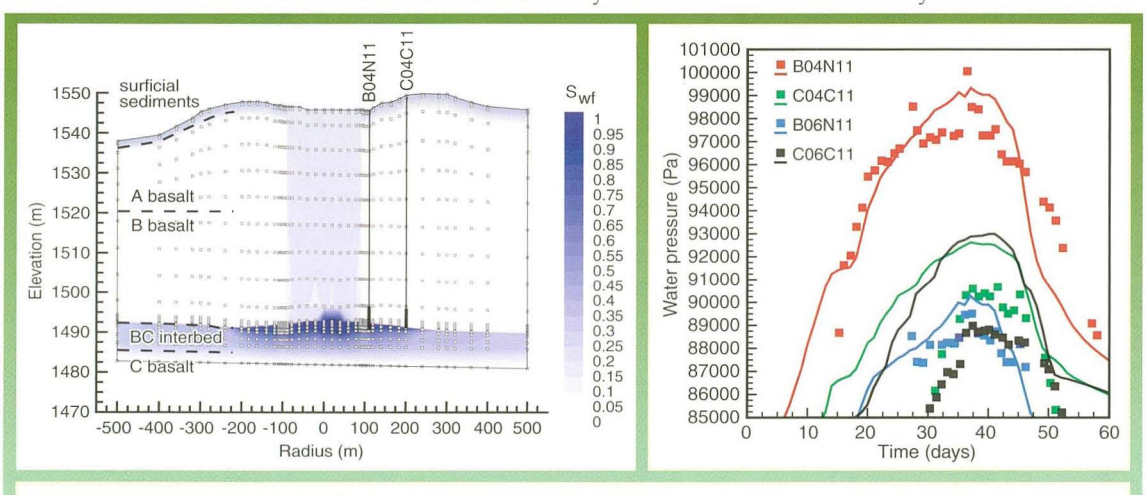

Figure 1a. Water saturation in the fracture continuum (S_{wf}) 35.5 days after the start of the infiltration test; Figure 1b. Field (symbol) and calibrated model (lines) hydrographs. Note that wells B04N11 and B06N11 are located at the same radial distance as C04C11 and C06C11, while "04" and "06" wells are on the same radial angle.

ACCOMPLISHMENTS

Five parameters were selected for calibration by ITOUGH2: (1) basalt fracture-continuum permeability, (2) basalt matrix-continuum permeability, (3) BC interbed permeability, and (4 and 5) BC interbed van Genuchten capillary-pressure parameters a and n. Inversions were performed using constant fracture-matrix continuum area scaling factors of: 0.02, 0.01, and 0.005. Results of the calibration to the hydrographs using a fracture-matrix continuum area scaling factor of 0.01 are shown in Figure 1b and are: basalt fracture continuum permeability of 3.27 x 10^{-10} m^2, basalt matrix continuum permeability of 2.51 x 10^{-15} m^2, BC interbed permeability of 5.01 x 10^{-17} m^2, BC interbed van Genuchten α of 1 x 10^{-4} Pa^{-1} and n of 0.28.

SIGNIFICANCE OF FINDINGS

The significance of this calibration effort pertains to previous modeling efforts conducted at the Box Canyon site at INEEL as well as the use of the dual-permeability modeling approach to simulate steady-state and transient infiltration at Yucca Mountain. Parameters obtained from this modeling effort agree closely with those obtained in a preliminary study conducted at the Box Canyon site. Therefore, we conclude that the use of the dual-permeability approach with a constant fracture-matrix continuum area-scaling factor is adequate for modeling transient infiltration at a variety of scales and under various wetting histories. Successful application of the dual-permeability modeling approach for simulating the LPIT lends credibility to the use of the same approach for modeling infiltration (both transient and steady state) at the Yucca Mountain site.

RELATED PUBLICATION

Unger, A.J.A., B. Faybishenko, G.S. Bodvarsson, and A.M. Simmons, A three-dimensional model for simulating ponded infiltration tests in the variably saturated fractured basalt at the Box Canyon Site, Idaho, Berkeley Lab Report LBNL-44613, 2000.

ACKNOWLEDGMENTS

This work was supported by the Director, Office of Civilian Radioactive Waste Management, U.S. Department of Energy, through Memorandum Purchase Order EA9013MC5X between Bechtel SAIC Company, LLC, and Berkeley Lab. The support is provided to Berkeley Lab through U.S. Department of Energy Contract No. DE-AC03-76SF00098.

RESEARCH PROGRAM

ENERGY RESOURCES

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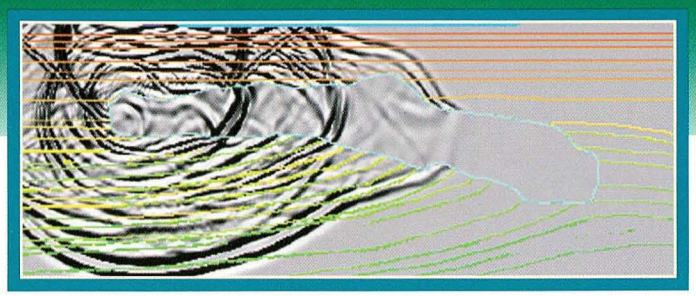

The Energy Resources Program (ER) is responsible for two major program areas: Oil and Gas Exploration and Development, and Geothermal Energy Development.

OIL AND GAS EXPLORATION AND DEVELOPMENT

Multidisciplinary research is being conducted in reservoir characterization and monitoring, optimization of reservoir performance, and environmental protection. Using basic research studies as a source of innovative concepts, ER researchers seek to transform these concepts into tangible products of use to industry within a time-frame consistent with today's rapid growth in technology. Reservoir characterization and monitoring involves development of new seismic and electromagnetic techniques focused at the inter-well scale. Field acquisition, laboratory measurements, and numerical simulation play important roles in the development activities. Optimization of reservoir performance is focused on simulation-based methods for enhancing reservoir management strategies. Emphasis is placed on the integration of geophysical data, production data, and reservoir simulation. The next major step in research will focus on methods to optimize performance through integration of monitored geophysical data, production data, and reservoir simulation.

International and national concern about the variable climatic effects of greenhouse gases produced by burning of fossil fuels is increasing, while it is also recognized that these fuels will remain a significant energy source well into the next century. In response to these concerns, ER has initiated research focused on development of technologies that will minimize the impact of fossil-fuel usage on the environment. Methane hydrates constitute a huge potential fuel source with lower carbon emissions than coal or oil. ER researchers are developing and evaluating possible methods for producing gas from such deposits. Geophysical data acquisition and inversion methods developed in the ER program are also being applied in a new project on geologic sequestration of CO_2 carried out in the Climate Variability and Carbon Management Program with the Earth Sciences Division.

Principal research activities include:

- Development of single-well and crosswell seismic technology, including instrumentation, acquisition and processing
- Applications of seismic methods for characterization of fractured reservoirs
- Laboratory measurement of the seismic properties of poorly consolidated sands
- Development of efficient 3D elastic-wave propagation codes
- Improved inversion methods for reservoir characterization, with a focus on combining production and geophysical data
- Application of x-ray CT and NMR imaging to study multiphase flow processes
- Pore-to-laboratory-scale study of physical properties and processes, with a focus on controlling phase mobility, predicting multiphase flow properties and drilling efficiency
- Development of reservoir process-control methods
- Development of new methods to mitigate environmental effects of petroleum refining and use
- Enhancement of refining processes using biological technologies
- Numerical simulation of subsurface methane hydrate systems

Since 1994, the major part of the Oil and Gas Exploration and Development program has been funded through the Natural Gas and Oil Technology Partnership Program. Begun in 1989, the partnership was expanded in 1994 and again in 1995 to include all nine Department of Energy multiprogram laboratories, and has grown over the years to become an important part of the DOE Oil and Gas Technologies program for the national laboratories. Partnership goals are to develop and transfer to the domestic oil industry the new technologies needed to produce more oil and gas from the nation's aging, mature domestic oil fields, while safeguarding the environment.

Partnership technology areas are:

- Oil and gas recovery technology
- Diagnostics and imaging technology
- Drilling, completion and stimulation
- Environmental technologies
- Downstream technologies

Projects are typically multiyear, are reviewed and reprioritized annually by industry panels, and are collaborations between national laboratories and industry.

GEOTHERMAL ENERGY DEVELOPMENT

The main objective of ER's geothermal energy development program is to reduce uncertainties associated with finding, characterizing, and evaluating geothermal resources. The ultimate purpose is to lower the cost of geothermal energy for electrical generation or direct uses (e.g., agricultural and industrial applications, aquaculture, balneology). The program encompasses theoretical, laboratory, and field studies, with an emphasis on a multidisciplinary approach to solving the problems at hand. Existing tools and methodologies are upgraded, and new techniques and instrumentation are developed for use in the areas of geology, geophysics, geochemistry, and reservoir engineering. Cooperative work with industry, universities, and government agencies draws from Berkeley Lab's 25 years of experience in the area of geothermal research and development.

In recent years, DOE's geothermal program has become more industry-driven, and the Berkeley Lab effort has been directed toward technology transfer and furthering our understanding of the nature and dynamics of geothermal resources under production, such as The Geysers geothermal field in northern California, which has begun to show the effects of overexploitation.

At present, the main research activities of the program include:

- Geothermal Reservoir Dynamics: development and enhancement of computer codes for modeling heat and mass transfer in porous and fractured rocks, with specific projects such as modeling the migration of phase-partitioning tracers in boiling geothermal systems; modeling of mineral dissolution and precipitation during natural evolution, production, and injection operations; and geophysical-signature prediction of reservoir conditions and processes
- Isotope Geochemistry: identification of past and present heat and fluid sources, development of natural tracers for monitoring fluids re-injected into geothermal reservoirs, better understanding of the transition from magmatic to geothermal production fluids, and enhancement of reservoir-simulation methods and models by providing isotopic and chemical constraints on fluid source, mixing, and flow paths
- Multicomponent 3D Seismic Imaging: development and implementation of 3D surface and borehole methods for defining permeable pathways in geothermal reservoirs
- Geochemical Baseline Studies: documentation of geothermal-fluid behavior under commercial production and injection operations (e.g., field case studies), with specific emphasis on The Geysers field
- Electromagnetic Methods for Geothermal Exploration: development of efficient numerical codes for mapping high-permeability zones, using single-hole electromagnetic data

Future research will concentrate on the development of innovative techniques for geothermal exploration and assisting in a reassessment of geothermal power potential in the U.S. The emphasis will be on expanding existing fields, prolonging their productive life, and finding new "blind" geothermal systems, i.e., those that do not have any surface manifestations, such as hot springs, fumaroles, etc., that suggest the presence of deeper hydrothermal systems.

FUNDING

Within ER, The Oil and Gas Exploration and Development program receives support from the Assistant Secretary for Fossil Energy, Office of Natural Gas and Petroleum Technology, through the National Energy Technology Laboratory, the National Petroleum Technology Office, and the Natural Gas and Oil Technology Partnership, under U.S Department of Energy Contract No. DE-AC03-76SF00098. Support is also provided from industry and other sources through the Berkeley Lab Work for Others program. Industrial collaboration is an important component of DOE Fossil Energy projects.

The Geothermal Energy Development program receives support from the Assistant Secretary for Energy Efficiency and Renewable Energy, Office of Power Technologies, Office of Wind and Geothermal Technologies, of the U.S. Department of Energy.

INTEGRATED RESERVOIR MONITORING USING SEISMIC AND CROSSWELL ELECTROMAGNETICS

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RESEARCH OBJECTIVES

The central problem in petroleum production is the development of a model or simulator that guides the drilling of wells, the management of the field, and the design of enhanced recovery processes. The objective of this research program is to integrate both seismic and electromagnetic geophysics for the mapping of reservoir properties between wells. This project will demonstrate that an integrated approach can be used to assign these properties to the flow simulation models of the interwell volume and greatly increase the effectiveness of in-fill drilling, reservoir production, and reservoir stimulation.

APPROACH

The project combines feasibility studies based on numerical models with the interpretation of field data to investigate possible methods of integrating electromagnetic (EM) and seismic data, along with well log information, to produce images of reservoir parameters (such as pressure and fluid saturations). Numerical studies have been carried out for a model of a producing North Sea oil field supplied by industrial partners. This study concentrated on well separations, which are relevant to offshore applications but have not been treated in field experiments to date. Two field data examples provided by industrial partners have been processed and interpreted to demonstrate how well log measurements, crosswell EM, and seismic data can be combined.

ACCOMPLISHMENTS

The numerical feasibility study of the Snorre Field demonstrates that crosswell EM could be measured and used to infer reservoir average water saturations in fields where well separations are on the order of 1 km. This represents an increase by a factor of 2 in well separations over what has been demonstrated to date in field measurements. This study demonstrated the necessity of integrating structural control from seismic data along with well control to provide the optimal estimates of reservoir water saturation in the interwell volume.

Crosswell, EM, and seismic field data from the Kern River and Lost Hills oil fields have been processed and interpreted. In the Kern River case, a detailed reprocessing of the seismic data to produce an equivalent CDP section between the wells was used to constrain the EM inversion for conductivity. This process increased the spatial resolution of the inferred fluid saturations as well as the correlation between logs and imaged fluid properties.

In the Lost Hills project, time-lapse seismic and EM data were able to predict both pressure and saturation changes in the inter-well volume. In addition, time-lapse changes demonstrated that small internal faults, not previously considered significant, were acting as barriers to flow. Figure 1 shows time-lapse changes in electrical conductivity, which directly maps changes in water saturation caused by an increase in oil.

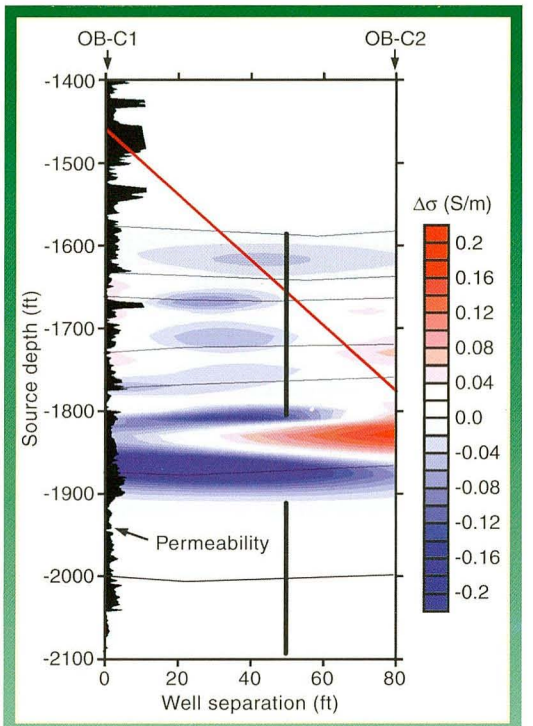

Figure 1. Time-lapse change in electrical conductivity during CO_2 injection. Large negative changes (blue) indicate an increase in oil saturation and correlate with high-permeability zones. The red line marks a small fault mapped from well logs. Changes in electrical conductivity truncate at the fault location.

SIGNIFICANCE OF FINDINGS

The addition of conductivity mapping via crosswell EM provides a robust estimate of water saturation changes that is independent from seismic data.

RELATED PUBLICATIONS

Hoversten, G.M., G.A. Newman, H.F. Morrison, and J.I. Berg, Reservoir characterization using crosswell EM inversion: A feasibility study for the Snorre Field, North Sea: Geophysics, 2001 (in press).

ACKNOWLEDGMENTS

This work was funded in part by the Assistant Secretary for Fossil Energy, Office of Natural Gas and Petroleum Technology, through the Natural Gas and Oil Technology Partnership, of the U.S. Department of Energy under Contract No. DE-AC03-76SF00098 and Sandia Contract No. DE-AC04-94AL85000.

HIGH-SPEED 3D HYBRID ELASTIC SEISMIC MODELING

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RESEARCH OBJECTIVES

The best tool for understanding and imaging complex structures and large offset data sets is an accurate, fully elastic 3D algorithm. The applications for such an algorithm are many (e.g., survey design, hypothesis testing, AVO evaluation, wave field interpretation, generation of test data sets for testing of new migration algorithms, and forward-calculation engines in 3D prestack migration algorithms and new full waveform inversion algorithms). While such algorithms have been developed, uniform grid sampling produces costly oversampling of high-velocity regions and unnecessarily small time-integration steps in low-velocity regions. Thus, the scale of the computer resources required to model the entire geologic section, from source locations to the depths of interest and with fully elastic representation, is prohibitive. In addition, the discretization of high-contrast boundaries (such as a salt-sediment interface) can produce high-energy diffraction events in the modeled data, which are often difficult to completely suppress even in processing. There is a critical need for an algorithm that can accurately model and image all of the elastic effects occurring in a complex structure, and at the same time be efficient enough to run on clusters of available workstations in a reasonable time. We seek to develop an efficient 3D elastic forward-modeling algorithm that will address these requirements.

APPROACH

Two critical concepts will provide for a significant improvement in computation efficiency and accuracy over what is currently available. The first critical concept is the decomposition of the original 3D model into parts (subdomains) where wave propagation will be computed, using the optimal spatial parameterization for each particular subdomain. The second critical concept is the use of a fourth-order time scheme (as opposed to the frequently used second-order schemes).

The new variable-grid-subdomain finite-difference (FD) algorithm is designed for parallel-cluster computing, utilizing a message-passing-interface technique. Using subdomains in FD modeling has several major advantages over current single-domain algorithms. For one thing, this approach uses fine gridding only in low-velocity regions (sea water, loosely compacted sediments) where it is required, allowing coarser gridding in the higher-velocity regions (salt, deep sediments). The innovative fourth-order differencing scheme enables improved accuracy in time differencing, and therefore increases the time-differencing step for the expense of extra computation within a single node. Since inter-CPU communication speed is a major bottleneck for parallel data-processing flow, the fourth-order scheme allows an increase in the computation-to-communication ratio, improving the effectiveness of parallel computations. The fourth-order time-differencing scheme has little effect on memory usage compared to second-order schemes. A required special formulation for absorbing boundary conditions is under development.

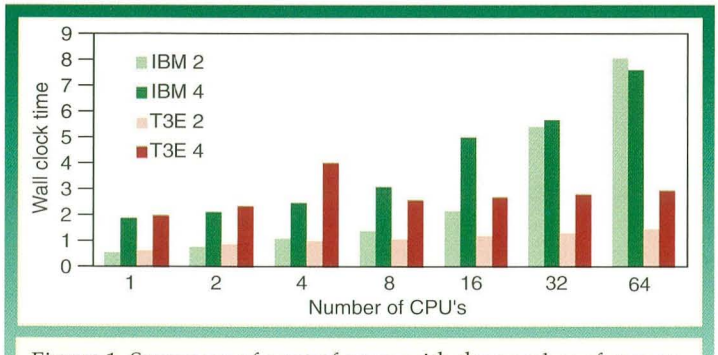

Figure 1. Summary of a set of runs, with the number of computational zones increasing linearly with the number of processors

ACCOMPLISHMENTS

Figure 1 shows a graph summarizing a set of runs performed this past year using the new variable-grid-subdomain FD algorithm scheme. The graph shows the number of computational zones increasing linearly with the number of processors. Perfect scaling results would have zero slope. Cray T3E times are encouraging. The IBM SP shows a reduction in parallel performance with increasing numbers of processors. The performance loss is less severe for the fourth-order scheme than for the second-order scheme. The IBM has slower interprocessor communications (both lower bandwidth and higher latency). (Run time reported is wall-clock time.) Cray T3E shows very efficient processor usage for both second- and fourth-order schemes. Fourth-order schemes show slower degradation of parallel performance with increasing problem size.

ACKNOWLEDGMENTS

This work has been supported by the Assistant Secretary for Fossil Energy, Office of Natural Gas and Petroleum Technology, through the National Petroleum Technology Office, Natural Gas and Oil Technology Partnership, of the U.S. Department of Energy under Contract No. DE-AC03-76SF00098.

FREQUENCY-DEPENDENT SEISMIC ATTRIBUTES OF POORLY CONSOLIDATED SANDS

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RESEARCH OBJECTIVES

The objectives of this work are to: (1) provide a theoretical basis for frequency-dependent amplitude attributes associated with multiple fluid (and gas) phases in poorly consolidated sands, for a range of consolidation conditions; (2) explore the possibility of new seismic attributes; (3) use numerical modeling to examine optimum 3D seismic-acquisition geometries and processing schemes for illuminating these attributes in poorly consolidated sand reservoirs; and (4) apply the results of these analyses to 4D seismic imaging.

APPROACH

This research combines laboratory acoustic measurements, theoretical development, and 3D visco-elastic wave simulations. The focus of the acoustic measurements and theoretical development is to obtain a frequency- dependent theory for wave propagation in poorly consolidated sands, a theory that can be used to predict the effects of fluid substitution and reservoir compaction on elastic waves. The focus of the wave-simulation effort is to embed this rock physics model into a numerical simulator to predict the changes in and effects of fluid distributions on acoustic properties in the presence of different reservoir structures. After all this work, we will analyze synthetic data for robust seismic attributes that can be used for 4D monitoring of changes in reservoir fluid/gas migration and reservoir consolidation.

ACCOMPLISHMENTS

The second year of the project has focused on three efforts: (1) analysis of the measured extensional wave velocities and attenuation (1–9 kHz) using existing rock physics models, (2) addition of torsional-wave sonic-frequency-measurement capabilities to our extensional wave apparatus, (3) completion of our lab velocity and attenuation measurements on medium-grain clean sands under a range of gas saturations and confining pressures, (4) design of a seismic- frequency (1–100 Hz) stress-strain apparatus, and (5) 3D dynamic poroelastic modeling of wave propagation in media with heterogeneous gas distributions.

Here, we describe some results for Effort 1. (Efforts 2–5 are presently ongoing.) Figure 1 displays the extensional wave velocities obtained from a 3 kHz pulse transmission test on a 0.8 m long packing of a coarse grain Monterey sand. Three different styles of gas saturation were introduced into the sample and imaged using an x-ray computerized-tomography scanner: (1) CO_2 degassing, yielding near-homogeneous gas phase; (2) injection of water into a dry horizontal sample, yielding patchy saturation consisting of horizontal stratification; and (3) injection of water into a dry vertical sample, yielding patchy saturation consisting of vertical segregation.

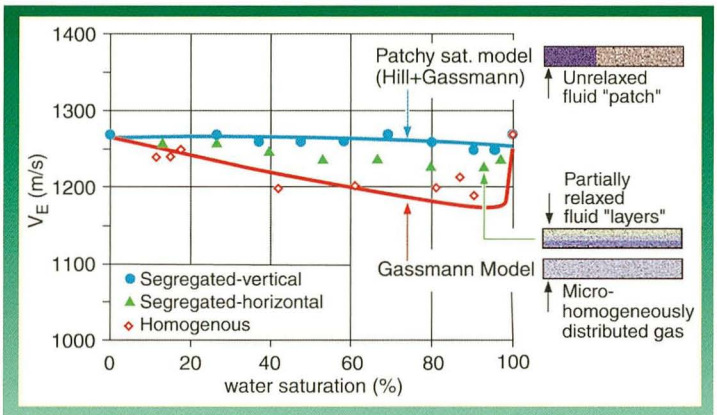

Figure 1. Comparison of measured extensional wave velocities with Gassmann theory (homogenous saturation) and Hill and Gassmann theory (patchy-vertical saturation)

Figure 1 shows that several static-effective-medium theories (Gassmann for the homogeneous case and Hill for the patchy-vertical case) show good agreement with the measured extensional wave velocities. These results demonstrate that sonic-frequency velocities for a coarse-grain sand are not unique functions of the water saturation. That is, the details of the distribution of the fluid and gas phases have an effect on the velocities. Note that measurements to date suggest that the attenuation (not shown) may provide additional information that can be used to deduce the style of saturation (i.e., homogeneous versus heterogeneous).

SIGNIFICANCE OF FINDINGS

Seismic characterization of fluids in poorly consolidated sands is a problem of growing importance, especially on the Gulf Coast. A basic understanding of sand acoustic properties under moderate stresses and in the presence of multiple fluids and gases is required to relate seismic attributes to fluid distributions. The laboratory and modeling efforts described here will provide clearer relations between heterogeneous and homogeneous partial-gas saturations in poorly consolidated sands, with sonic-frequency velocities and attenuation.

ACKNOWLEDGMENTS

This work has been supported by the Assistant Secretary for Fossil Energy, Office of Natural Gas and Petroleum Technology, through the National Petroleum Technology Office, Natural Gas and Oil Technology Partnership, of the U.S. Department of Energy under Contract No. DE-AC03-76SF00098.

IMAGING, MODELING, MEASURING, AND SCALING OF MULTIPHASE FLOW PROCESSES

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OBJECTIVE

Our objective is to develop methodologies based on advanced imaging technology for rapid and accurate measurement of petrophysical properties and prediction of engineering parameters needed for reservoir simulation.

APPROACH

To simulate multiphase flow in a reservoir, for the various facies, one needs to know petrophysical parameters such as porosity, permeability, relative permeabilities, and capillary pressures. Laboratory measurements of these parameters using core plugs are often expensive, time consuming, or unavailable because of a lack of core material. Thus, the need exists to develop rapid methods that require a minimum of core material. One promising approach uses pore-network models to compute rock properties. This project addresses (1) obtaining pore-network data to be used as input for existing network models, (2) validating the network predictions with laboratory core measurements, and (3) upscaling the core measurements to use in field simulation. The work emphasizes extracting the pore data needed for network modeling from synthetic sedimentary models constructed from grains, using grain-size distribution extracted from analysis of small reservoir rock samples not amenable to regular core-flooding techniques. This approach permits setting the spatial resolution to levels not obtainable experimentally from microtomography, but which are needed to resolve the pore throats in many rocks of economic interest. It also presents a very significant time and cost advantage compared to microtomography.

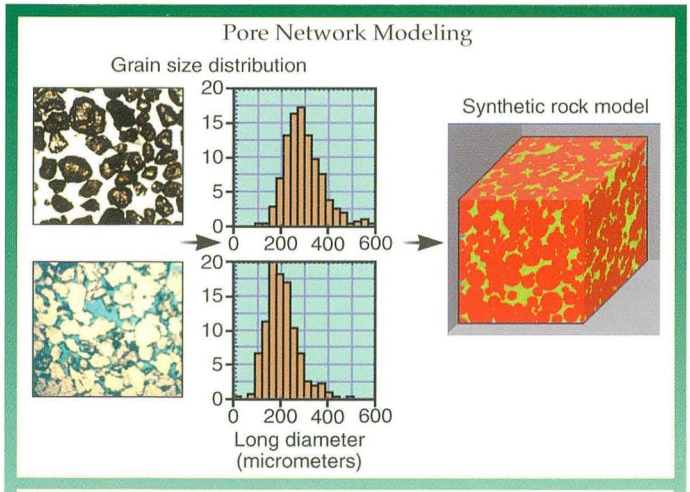

Figure 1. Synthetic sedimentary model of sandstone, based on grain data

ACCOMPLISHMENTS

A synthetic sedimentary model was used to construct 3D pore networks based on grain-size data obtained from digitized images of grains (in turn obtained from thin sections). The software package 3DMA from the State University of New York, Stonybrook, was used to extract pore-network parameters from 3D images of pore space. The extracted data were used as input in the pore-network model ANETSIM to calculate relative permeability and capillary pressure curves. The network simulations for drainage-water-oil relative permeability and capillary pressure showed good agreement with experimental data. We also completed the development of the quasi-static simulator of drainage and imbibition. To provide the ability to image the pore structure of many rocks that are of critical economic importance to oil and gas production, and to increase the basic understanding of pore-scale processes, we are involved in a cooperative project to construct a submicron-resolution rock-microtomography imaging capability at the Advanced Light Source. Also, using x-ray computer-tomagraphy imaging at the new Rock-Fluid Imaging Laboratory, we investigated foamy oil production and the effect of saturation on wave attenuation.

SIGNIFICANCE OF FINDINGS

By reducing the cost and time of petrophysical core measurements, the density of petrophysical data can be significantly increased. This higher data density, combined with proper upscaling, will yield more accurate reservoir simulations, improved oil-reservoir management, and increased oil recovery.

RELATED PUBLICATIONS

Patzek, T.W., Verification of a complete pore network simulator of drainage and imbibition, SPE 71310, SPEJ, 6, 2144–2156, June 2001.

Liu, Z., K.T. Nihei, L. Tomutsa, L.R. Myer, and J.T. Geller, Sonic - frequency attenuation in partially saturated, unconsolidated sand, presented at American Geophysical Union 2000 Fall Meeting, San Francisco, California, Dec. 15–19, 2000.

Liu, Z., J.W. Rector, K.T. Nihei, L. Tomutsa, L.R. Myer, and S. Nakagawa, Extensional wave attenuation and velocity in partially saturated sand in the sonic-frequency range, Accepted for presentation at the 38th U. S. Rock Mechanics Symposium "Rock Mechanics in the National Interest," July 7–10, Washington, D.C., 2001.

ACKNOWLEDGMENTS

This work has been supported by the Assistant Secretary for Fossil Energy, National Petroleum Technology Office of the U.S. Department of Energy under Contract No. DE-AC03-76SF00098.

SINGLE-WELL SEISMIC IMAGING

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RESEARCH OBJECTIVES

The continuing objective of this project is to identify and provide solutions to fundamental issues surrounding single-well seismic imaging to evaluate and develop the technology in a timely and cost-effective fashion. Single-well imaging is in its infancy, and there are many unanswered questions, but only limited resources to address them. Therefore, this technology must be developed in an efficient and logical manner to quickly identify the fundamental attributes that must be included in a total methodology. Such development must occur while leveraging the best-available resources to ensure the technology's successful application and acceptance.

APPROACH

The work is an integrated approach to spur the development and application of a new technology much more quickly than if it were left to individuals working separately. The project is meant to leverage resources to address issues that would not be addressed by individual companies. It is a coordinated effort between three national laboratories working closely with industry and involving university support. In addition to Berkeley Lab, the other participating laboratories are Idaho National Engineering and Environmental Laboratory (INEEL) and Sandia National Laboratories. It recognizes that in a time of shrinking funds, we have an obligation to spend wisely, while creating and maintaining fairness of opportunity to the industry (as well as bringing the appropriate capabilities of the national laboratories to complement and catalyze industry's efforts in this area).

The proposed work consists of four interdependent activities. These activities comprise facets of the technology required for the ultimate successful development of single-well seismic imaging and (to some degree) crosswell imaging:

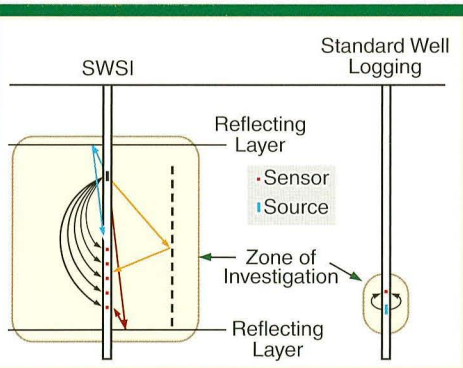
- Hardware: sources/receivers, telemetry/recording, borehole noise effects, deployment
- Modeling: synthetic seismograms, parametric studies, inversion, designs for hardware/surveys
- Field testing: quality data sets, evaluation/validation at well-characterized sites.
- Data processing and interpretation: algorithms, 3D imaging, noise reduction, visualization.

ACCOMPLISHMENTS

Several single-well surveys were run at Chevron's Lost Hills oil field in Central California. The objective of the work was to perform time-lapse imaging of a CO_2 flood in the diatomite. In August 2000 and May 2001, two separate surveys were run to gain data before injection and after injection, respectively. Additional objectives were to test tube-wave damping with a device designed and fabricated by INEEL. In each survey, different configurations of sources and receivers were run, using a high-frequency piezoelectric source (500 Hz to 200 Hz) and a low-frequency orbital source with both hydrophones and three component geophones. In the tube-wave experiments, a 10–16 dB reduction of the tube wave was obtained with the INEEL tube wave attenuator. Figure 1 shows an example of the single-well data obtained in the baseline test.

ACKNOWLEDGMENTS

This work has been supported by the Assistant Secretary for Fossil Energy, Office of Natural Gas and Petroleum Technology, through the National Petroleum Technology Office, Natural Gas and Oil Technology Partnership, of the U.S. Department of Energy under Contract No. DE-AC03-76SF00098.



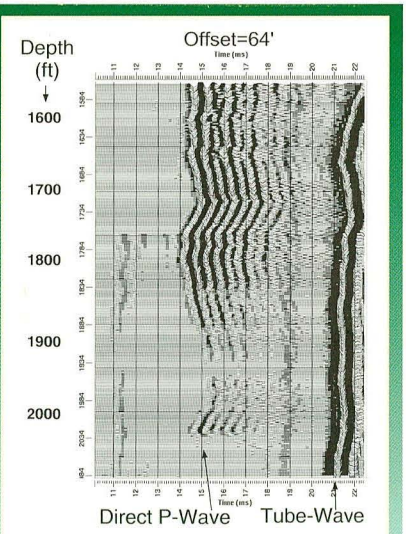


Figure 1. An example of the single-well data obtained at the Lost Hills oil field in Central California. The source was a piezoelectric bender; the receivers were 16 hydrophones with recordings at 2 ft intervals.

TUBE-WAVE SUPPRESSION FOR SINGLE-WELL IMAGING

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RESEARCH OBJECTIVES

The objective of this project is to conduct field tests of a borehole tube-wave suppressor (TWS) in conjunction with single-well seismic imaging (SWSI). We can quantify the effects of a new TWS, developed at Idaho National Engineering and Environmental Laboratory (INEEL) by using Berkeley Lab's single-well equipment.

APPROACH

We conducted two field-scale tests. The first was in shallow wells at the University of California's Richmond Field Station (RFS). The RFS has four boreholes of 100 m depth and 6 in. diameter. These wells are deep enough to deploy the SWSI system and TWS.

A follow-up test at an oil-field site was then scheduled to test the equipment in a deep well situation. We conducted this test with Berkeley Lab's SWSI field system at Chevron's Lost Hills oil field. Chevron's CO_2 flood pilot site was extensively used. This site has permanently emplaced observation wells that are available for studies without taking production wells off-line. Berkeley Lab has previously acquired crosswell and single-well surveys at this site, which has recently undergone hydrofracturing and CO_2 injection.

ACCOMPLISHMENTS

For the first test, we recorded data with hydrophones and wall-locking geophones, both with and without the TWS. These tests allow quantification of tube-wave attenuation as well as field testing of the hardware and mechanical/electrical interface. Data were recorded by Berkeley Lab using a fiber-optic borehole digitizer. The successful completion of these tests indicated a reduction of tube waves of about 10dB, relative to the compressional P-wave.

In the follow-up test, the presumed vertical fracture zone is a particularly attractive imaging target for the single-well acquisition geometry. While useful data was acquired in the initial surveys (demonstrating the baseline properties of the site), tube waves were a major problem. We expect the seismic data to be greatly enhanced by TWS. The comparison of data collected with and without the TWS is shown in Figure 1. We see a dramatic reduction of tube-wave energy.

SIGNIFICANCE OF FINDINGS

We have shown that the INEEL TWS can dramatically reduce the tube-wave energy in a single-well seismic survey. This result is very important for the future of single-well surveys as well as other borehole seismic surveys.

RELATED PUBLICATIONS

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Daley, T.M., Single-well seismic-imaging tests: November 1997 at Bayou Choctaw Site, Berkeley Lab Report LBNL-42672, 1998.

Daley, T.M., Single-well seismic imaging in a deep borehole using a piezoelectric orbital vibrator, Berkeley Lab Report LBNL-42673, 1997.

ACKNOWLEDGMENTS

This work was supported through INEEL by the Assistant Secretary for Fossil Energy, Office of Natural Gas and Petroleum Technology, the Natural Gas and Oil Technology Partnership program of the U.S. Department Energy under Contract No. DE-AC03-76SF00098. Data processing performed at the Center for Computational Seismology supported by the Director, Office of Sciences, Office of Basic Energy Sciences, Division of Chemical Sciences, Geosciences, and Biosciences, of the U. S. Department of Energy under Contract No. DE-AC03-76SF00098.

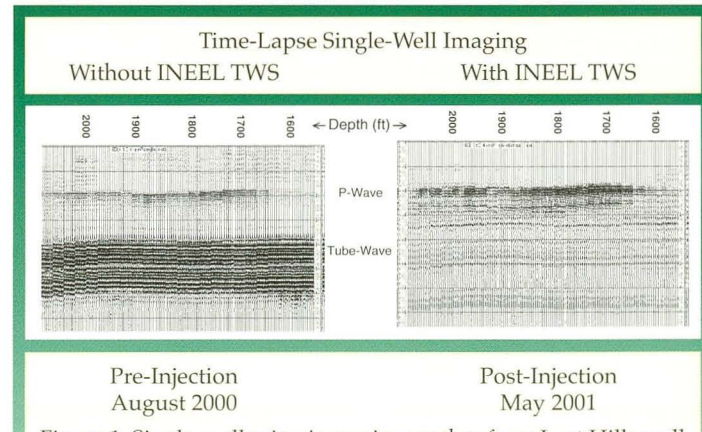

Figure 1. Single-well seismic-receiver gather from Lost Hills well OB-C1. The data were recorded using Berkeley Lab's high-frequency piezoelectric source and hydrophone sensors. A dramatic reduction in tube energy is seen when the tube-wave suppressor is used in the postinjection survey.

FRACTURE QUANTIFICATION IN GAS RESERVOIRS

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RESEARCH OBJECTIVES

Berkeley Lab is the lead institution of a comprehensive program between the Department of Energy and industry for integrated field testing and analysis. This program is aimed at improving the fundamental understanding of seismic-wave propagation in naturally fractured gas reservoirs to extend fracture characterization to fracture quantification. A cooperative research program has been organized between Berkeley Lab and Conoco, Inc., Lynn, Inc., Schlumberger, Inc., Stanford University, and Virginia Tech. This field-scale effort is focused on using field production and test facilities for both development and validation of methods for predicting fractured reservoir performance.

APPROACH

We are starting with current state-of-the-art methods and extending the surface-based information with current borehole methods (vertical seismic profiling, crosswell and single well) to quantify fracture characteristics. The approach will be an industry-coupled program, tightly linked to actual field cases, iterating between development and application. Past efforts have focused on field experiments in well-characterized field sites at both the intermediate and full field scale. We will continue with this approach, working at industry sites that are representative of other sites.

The proposed field site for this year's work was the Conoco property in New Mexico's San Juan Basin. The criteria we set for the field site are: (1) it must be in an area of ongoing commercial interest; (2) it must have a wealth of geologic and other geophysical information; and (3) we must be able to have ongoing access throughout the project. Ideally, we also would like to be involved with the producer to such an extent that if our approaches and methodology are successful, they could be integrated into future operational plans. The selected field site and industry partners meet all of these criteria.

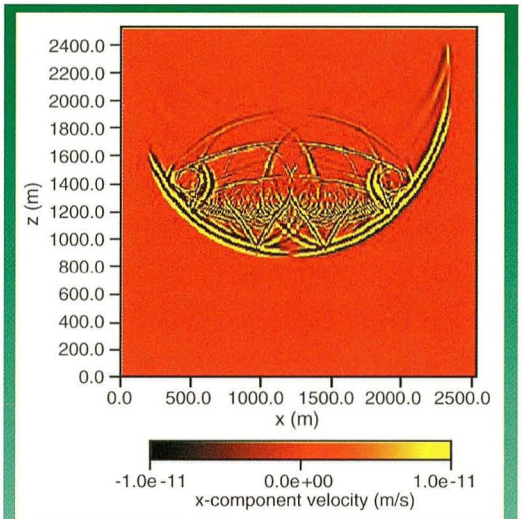

Figure 1. Model 113 Horizontal Component 400 ms. Seismic wavefield through a layered media with discrete fractures of two different sizes, large through-going "faults" ("V' shaped image) and smaller fractures within one layer (smaller diffractions). The wavefield was calculated using a finite-element discrete-fracture model rather than an equivalent media model.

We anticipate that wells will be drilled to validate the results of this work.

The overall work plan can be divided into four broad tasks:

1. Modeling
2. Field measurements
3. Processing and interpretation
4. Reservoir simulation

ACCOMPLISHMENTS

Over the past year, the effort has focused on reprocessing and interpretation of a 20-square-mile P-wave, 3D surface, seismic data set. The objective of the reprocessing by Conoco was to provide the "best" image for fracture identification by Lynn. The processing improved the past results by which Lynn targeted potentially fractured areas in the subsurface. This was in preparation for the next phase of field work, in which vertical seismic profiling (VSP) and single-well surveys will be run in two new wells drilled by Conoco in the 20-square-mile study area.

Another major thrust was the modeling of seismic waves in fractured media. Our approach is to model the effects of discrete fractures (in addition to an equivalent media approach). Figure 1 shows an example of this approach, a multilayer model with one layer having many smaller fractures and the entire model cut by several larger fractures (faults). The results of using a discrete-fracture modeling approach show that such effects as scattering, tuning, and diffraction are caused by the fractures. Future work will involve validating the different scale effects with field data.

ACKNOWLEDGMENTS

This work has been supported by the Assistant Secretary for Fossil Energy, Office of Natural Gas and Petroleum Technology, through the National Energy Technology Laboratory, of the U.S. Department of Energy under Contract No. DE-AC03-76SF200098.

SEMI-AUTOMATIC SYSTEM FOR WATERFLOOD SURVEILLANCE

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RESEARCH OBJECTIVES

A successful waterflood requires proper operation of individual wells in a pattern as well as maintained balance between water injection and production over an entire project or field. Aggressive or unbalanced injection leads to reservoir rock damage and consequent loss of wells caused by shear failure of reservoir rock and overburden.

Our ultimate goal is to design an integrated system of field-wide waterflood surveillance and supervisory control. Recently, we have introduced a new element of our system, satellite images of the field surface through Synthetic Aperture Radar Interferograms (InSAR).

APPROACH

Damage to heterogeneous soft rock caused by water injection is not well understood yet. Rock damage causes water recirculation between injectors and producers without the desirable pressure support and increased oil recovery. Water-swept, pressurized regions in the reservoir cause less surface subsidence, the evolution of which shows up on satellite images with remarkable accuracy and clarity.

ACCOMPLISHMENTS

1. Injection into a Layered Reservoir

Injection into a layered reservoir is extremely difficult. Usually, "thief-layers" or highly conductive channels of damaged rock exist. Recently, we have designed an optimal injection controller for mixed transient/steady-state flow in a layered formation. The objective of the controller is to maintain the prescribed injection rate in the presence of hydrofracture growth and injector-producer linkage. The history of injection pressure and cumulative injection, along with estimates of the hydrofracture size, are the controller inputs. After analyzing these inputs, the controller outputs an optimal injection pressure for each injector.

2. InSAR Image Analysis

Between April 1995 and December 1999, we analyzed ten differential InSAR images of the South/North Belridge and Lost Hills diatomite fields in California (Figure 1). The images show that the rate of subsidence has decreased in some parts of Lost Hills and Belridge while it increased in others. We have been able to demonstrate the remarkable behavior of both fields:

(a) There is recirculation of injected water through the "tubes" of damaged soft rock that link injectors with producers, resulting in diminished pressure support from the waterfloods.

(b) Consequently, despite more water injection, there is more subsidence in Sections 29, 34, and 33 in Belridge, and in Sections 29, 4, 5, and 32 in Lost Hills.

(c) Because much of the injected water is recirculated, the rate of subsidence is proportional to water production rate.

(d) Compaction remains an important mechanism of hydrocarbon production.

(e) In addition to accelerated compaction in the densest and most advanced waterfloods, there is a sizable oil production response to water injection.

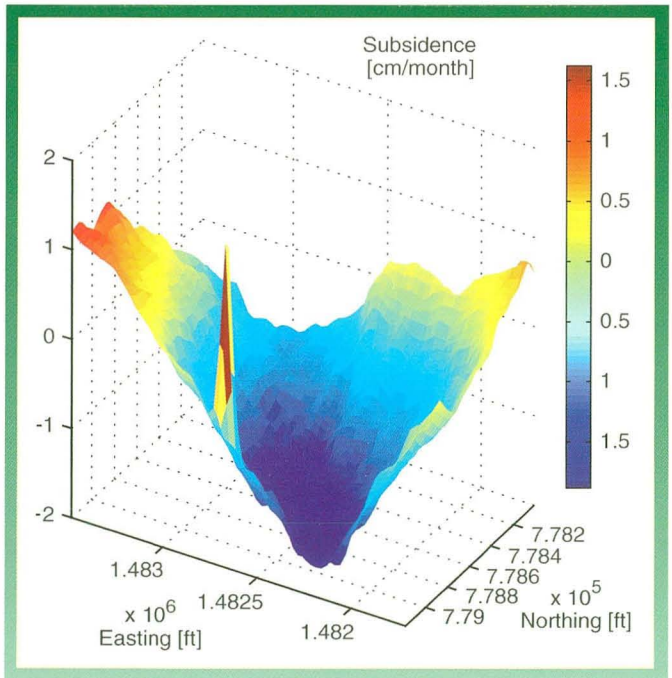

Figure 1. Monthly subsidence bowl in cm/month, Lost Hills, CA, 1999; Sections 4, 5, 29, 32, and 33

SIGNIFICANCE OF FINDINGS

Our work, done in collaboration with Chevron and Case Services, will result in higher ultimate oil recovery and lower well losses in two giant oilfields in California. A preliminary patent application has been filed.

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GAS-PRODUCTION SCENARIOS FROM HYDRATE ACCUMULATIONS AT THE MALLIK SITE, McKENZIE DELTA, CANADA

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RESEARCH OBJECTIVES

The Mallik site represents an onshore permafrost-associated methane hydrate accumulation at the McKenzie Delta, Northwest Territories, Canada. A 1,150 m deep gas hydrate research well was drilled at the site in 1998 and led to the first significant body of field data from a natural-gas hydrate deposit (Dallimore et al., 1999). An international consortium of seven organizations from five countries is currently planning a new test well for the analysis of dissociation under field conditions. The objective of the Berkeley Lab component of this research is the analysis and evaluation of various gas production scenarios from several hydrate deposits.

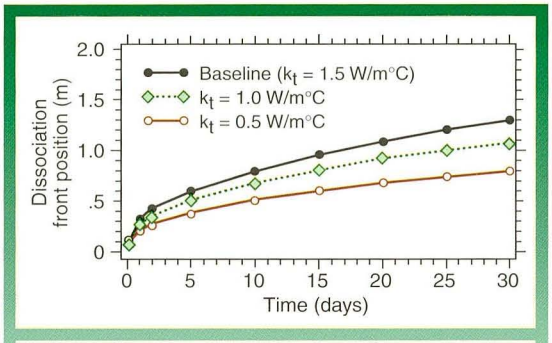

Figure 1. Sensitivity of dissociation front to the thermal conductivity

APPROACH

The analysis of several production scenarios currently under consideration was conducted using the TOUGH2 general-purpose simulator (Pruess, 1991) for multicomponent, multiphase fluid and heat flow and transport in the subsurface with the EOSHYDR2 module (Moridis et al., 1998). EOSHYDR2 is designed to model the nonisothermal CH_4 release, phase behavior, and flow under conditions typical of CH_4-hydrate deposits (i.e., in the permafrost and in deep-ocean sediments) by solving the coupled equations of mass and heat balance. The model accounts for up to four phases (gas phase, liquid phase, ice phase and CH_4-hydrate phase) and up to seven components (CH_4-hydrate, water, native methane, dissociated methane, salt, water-soluble inhibitors, and heat). The model can describe hydrate dissociation involving any combination of the possible dissociation mechanisms (i.e., depressurization, thermal stimulation, salting-out effects, and inhibitor-induced effects).

ACCOMPLISHMENTS AND SIGNIFICANCE

Early investigations indicated that production from accumulations with free gas and/or water zones underlying the hydrate deposit was not promising because of adverse conditions at the site. The study focused on accumulations with no underlying free gas or water zones, and a CH_4-hydrate saturation of at least 50% (the remainder being pore water). Thermal stimulation by circulating hot water in the well was selected as the main method of dissociation because of its effectiveness and simplicity under the conditions of the planned field test. These are significant factors in the effort to analyze field parameters of hydrate dissociation performance.

Sensitivity studies indicated that CH_4 release from the hydrate accumulations at the Mallik site increases with the CH_4-hydrate saturation, the hydrate initial temperature, the temperature of the circulating water in the well, the well boundary conditions, and the thermal conductivity of the system (Figure 1). CH_4 production appears to be less sensitive to the rock and hydrate specific heats, the permeability of the formation in the range observed at the site, and the irreducible gas saturation. A general observation of the study is that the extent of the dissociation zone appears to be limited within the short operational window of the planned test (necessitated by adverse climatic conditions at the arctic site).

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ACKNOWLEDGMENTS

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DYNAMIC RESERVOIR CHARACTERIZATION THROUGH THE USE OF SURFACE DEFORMATION DATA

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RESEARCH OBJECTIVES

The objective of this project is to develop and characterize a reservoir though the use of surface-deformation data, such as displacement and surface tilt induced by pumping or injection. Obtaining such data can be a cost-effective way of gathering information on reservoir flow geometry, which is critical for successful reservoir management.

APPROACH

When fluid is produced from or injected into a reservoir, it causes volume changes in the reservoir, which in turn induce displacements on the ground surface. If a preferential flow path such as a fault zone exists in the reservoir (which is often the case in geothermal reservoirs), flow will occur mostly along the fault. Observations of surface deformation can be used to estimate the distribution of the volume changes in the reservoir. For example, a vertical fault zone would produce a linear trough in the inverted image. The larger the volume change is at a particular location, the more likely fluid has moved in or out of the location. The distribution of volume change is tightly coupled with that of the reservoir flow properties: permeability and compressibility.

Surface expression of such reservoir dynamics can be monitored by using high-precision tiltmeters, global positioning systems, laser level gages, and InSAR (Interferometric Synthetic Aperture Radar). Monitoring of the deformation at or near the surface costs very little compared to drilling a large number of boreholes and instrumenting them with pressure sensors. This remote-sensing approach also provides independent data on reservoir dynamics that can be used to confirm or refute a reservoir model based on the borehole data alone.

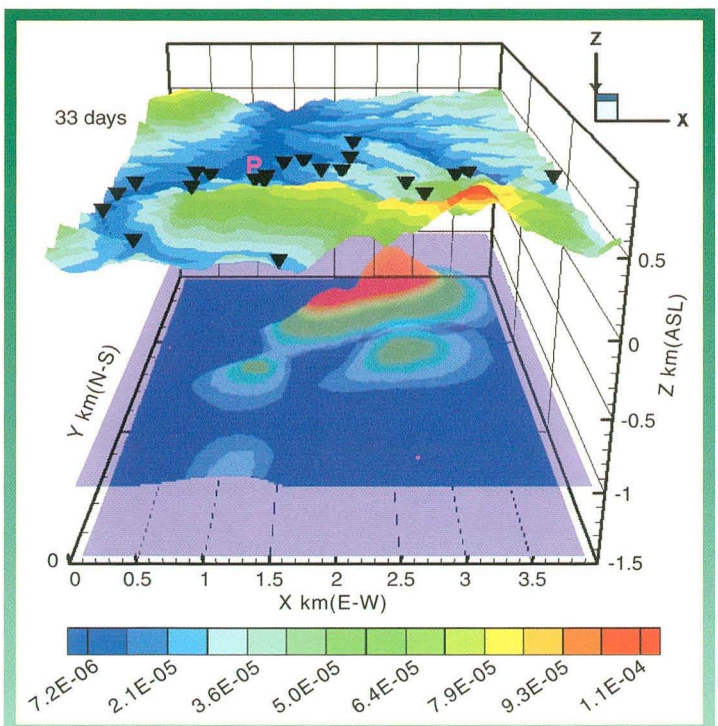

Figure 1. 3D perspective view of the inversion results. Triangles show the tiltmeter locations. The fractional volume increase at depth parallels a known fault.

ACCOMPLISHMENTS

In 2000, a total of some 24 tiltmeters were used to monitor surface tilts at the Okuaizu Geothermal Field in Japan. Monitoring was timed to coincide with a scheduled field-wide maintenance, at which time all the production and re-injection wells were shut-in. The inversion results (Figure 1) indicated that the volume change at depth parallels a known fault. We also inverted InSAR data from the Coso Geothermal Field and showed that the use of both ascending- and descending-orbit InSAR data is advantageous for obtaining better resolution of subsurface volume change.

SIGNIFICANCE OF FINDINGS

We have shown that surface deformation data such as tilt and InSAR data can be utilized to characterize the dynamics of deep reservoirs.

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REACTIVE-CHEMICAL-TRANSPORT SIMULATON TO STUDY GEOTHERMAL PRODUCTION WITH MINERAL RECOVERY

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RESEARCH OBJECTIVES

Vast reserves of dissolved minerals exist in the hypersaline brines of geothermal fields at Imperial Valley, California. Recovery of zinc from geothermal brines is taking place in this area, and recovery of silica, manganese, silver, lead, and lithium has been or is being considered. Consequently, the ability to model mineral recovery is very important in terms of economic development and resource utilization.

APPROACH

The reactive-geochemical-transport simulator TOUGHREACT (Xu and Pruess, 1998) has been used to model rock-fluid interactions during production from and injection into the hypersaline-brine geothermal system. The modeling uses published water-chemistry data from Imperial Valley and a simplified flow system intended to capture realistic features of the hydrothermal system. Simulations were performed using different production and injection rates, pH values, and silica concentrations of the injection water.

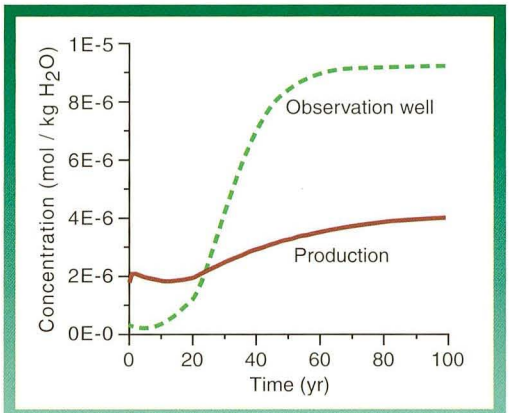

Figure 1. Evolution of aqueous zinc concentration obtained with a production/injection rate of 8 kg and an injection pH of 4

ACCOMPLISHMENTS

Results indicate that the evolution of temperature and zinc concentration depends on production and injection rate. A lower rate results in a lower temperature drop and higher zinc concentration. A low injection pH significantly enhances the dissolution of sphalerite (ZnS) in the reservoir rock, increasing aqueous zinc concentration. A higher injection silica concentration leads to silica precipitation, but decreases the reservoir porosity only slightly (even after 20 years). Simulated evolution of the aqueous zinc concentration at observation and production wells is shown in Figure 1. (The observation well is located between the injection and production wells.)

SIGNIFICANCE OF FINDINGS

This "numerical experiment" provides useful insight into the process mechanisms, conditions, and parameters controlling zinc recovery in the reservoir. This project also demonstrates that TOUGHREACT can be a useful tool for simulating these kinds of problems.

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ACKNOWLEDGMENTS

The present work was funded by the Assistant Secretary for Energy Efficiency and Renewable Energy, Office of Power Technologies, Office of Wind and Geothermal Technologies, of the U.S. Department of Energy under Contract No. DE-AC03-76SF00098. This work is a continuation of Pham et al. (2001), which is funded by California Energy Commission's Energy Innovations Small Grant Program to GeothermEx, Inc. (Grant Number 51391A/99-25).

NON-CONDENSABLE GASES: TRACERS FOR RESERVOIR PROCESSES IN VAPOR-DOMINATED GEOTHERMAL SYSTEMS

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RESEARCH OBJECTIVES

At The Geysers field, 75 miles (120 km) north of San Francisco, California, the largest known vapor-dominated geothermal system in the world, injection of water back into the reservoir began with commercial exploitation in 1960. This injection, consisting of steam condensate and available surface water, was limited to 30% of the mass extracted. In late 1997, in the steam field operated by the Northern California Power Agency (NCPA), the amount of injection essentially doubled when lake water and treated waste water from the South East Geysers Effluent Pipeline were delivered to the southern part of the system.

The purpose of this work is to update studies of steam chemistry to reflect changes resulting from the increased liquid injection, to test the applicability of geochemical analysis to steam fields with a relative high rate of injection, and to evaluate the use of non-condensable gases to identify reservoir processes.

APPROACH

The methodology used in this study is different from that of earlier work, which was based on oxygen and hydrogen isotopes. This method is no longer effective because increased injection of creek and lake water and treated waste water has lessened the isotopic contrast between reservoir steam and injectate.

We use D'Amore's (1991) gas geothermometer grids and changes in total gas contents in the steam to construct time-series diagrams for individual NCPA wells over their entire production histories. Instead of describing the grid diagram behavior of each well, the behaviors are divided into types and interpreted according to their patterns. The distribution—over space and time—of non-condensable gases in the produced steam was also analyzed.

ACCOMPLISHMENTS

Grid diagrams for nearly 70 NCPA wells were drawn by a computer program using the equations given in D'Amore and Truesdell (1985). The wells have been in production from the mid-to-late-1980s to 2000 (later data were not available).

Four types of grid diagrams were recognized (linear, hairpin, cluster, and random) by Truesdell et al. (2001). In addition, contour figures showing the distribution of total non-condensable gas in the NCPA field were developed for different years (e.g., Figure 1).

The application of gas geochemistry to detect and monitor changes over time in steam temperatures and steam fractions (from individual wells) shows that steam from wells in the center of the NCPA field originates from fairly uniform conditions produced by injection. In contrast, steam from wells in peripheral areas originates from progressively drier reservoir zones, which may return to near-original conditions depending on the characteristics of the injection operations.

Contours of total non-condensable gases show that changes in the location and amount of liquid injected have been very effective in limiting gas concentrations in the steam produced by most of the NCPA wells.

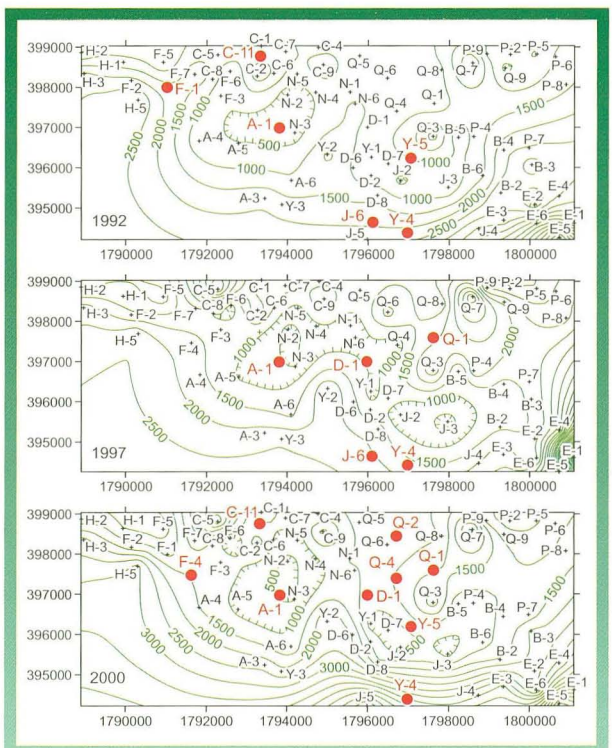

Figure 1. NCPA Geysers steam field. Contours of total non-condensable gas in the produced steam (in ppmv) for 1992, 1997, and 2000. Injection wells in use are shown as solid circles.

SIGNIFICANCE OF FINDINGS

This study confirms the usefulness of non-condensable gases to identify reservoir processes in vapor-dominated geothermal systems, particularly in The Geysers field. Variations of gas ratios in the produced steam explain processes resulting from large-scale production and from an increasing amount of injected liquid. It also illustrates that changes in the source (i.e., chemical characteristics) of the injectate are useful in detecting the various phenomena occurring in the reservoir.

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A MODEL OF THE SUBSURFACE STRUCTURE AT THE RYE PATCH GEOTHERMAL RESERVOIR BASED ON SURFACE-TO-BOREHOLE SEISMIC DATA

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RESEARCH OBJECTIVES

Berkeley Lab has cooperated with The Industrial Corporation (TIC) and Transpacific Geothermal Inc. (TGI) in studies to evaluate and apply modern seismic-imaging methods for geothermal reservoir definition under the DOE's Geothermal Program. As part of this cooperation, a 3D seismic-surface survey was acquired in 1998, at the Rye Patch Reservoir, Pershing County, Nevada, to determine the structure of the reservoir (Feighner et al., 1999). During the 3D survey, an additional experiment was conducted during which a three-component geophone was installed in a borehole at depth. This geophone recorded all seismic waves generated by the surface sources, creating a second dataset in addition to the seismic reflection data. The second dataset was used to map variations in the reservoir horizon within the area of the reservoir.

APPROACH

A high-temperature, wall-locking, three-component geophone was installed in Well 46-28 at 3,900 ft depth. The borehole geophone recorded all shots throughout the survey area, amounting to a total of 2,134 traces. The data quality is good, with a frequency content of about 25 Hz for the first arriving waves. A total of 2,005 first-arrival travel times were determined out of the 2134 possible traces. Most of the picks were reliable because the well-sampled spatial moveout across the source lines facilitated the picking.

Mapping travel-time deviations to elevation changes is a technique that has been used in seismic-refraction studies in the past. The method is an approximation that can be applied in environments where a low-velocity layer is located above a high-velocity layer or basement. Under the assumption that the ray path from source to receiver is known, any difference between the calculated and observed travel times is converted into a distance using the velocity model and applied as a deviation in the boundary between the basement and the overlaying layer. We employ the same principle in our approach and derive a velocity model of the subsurface at the Rye Patch Reservoir from a vertical seismic profile (VSP) that was conducted in 1997 (Feighner et al., 1998). Based on this velocity model, travel times are computed for each ray path from source to receiver, and the differences in the observed travel times are converted to elevation changes. In our case, we apply the total travel-time difference for each ray to the whole geologic model, thus assuming that any possible faulting affected the whole geologic sequence above the basement.

ACCOMPLISHMENTS

A mapview of the basement horizon elevation is provided in Figure 1. Three boreholes (46-28, 44-28, and 42-28) are shown for reference. It can be seen that the 0 ft elevation contour line runs through Well 46-28, which is expected since the velocity model is based on the VSP data acquired in that well. Only a small deviation between the modeled and measured data is expected at this location. The map shows the contours of an elevated structure extending from east to west across the survey area. The north-south extent of this rise reaches roughly from 2107000 (north of well 42-28) to 2102000 (between Wells 46-28 and 44-28), while the east-west extension seems to reach beyond the boundaries of the survey area (Figure 1). The elevation in the reservoir could be described by a horst or a ridge structure bound by two east-west trending faults to the north and south. The interpretation of an elevated basement with an east-west trend, bounded by linear features towards the northern and southern extension, is in agreement with 2D tomographic results (Feighner et al., 1999) and possibly with geophysical investigations undertaken in a previous study (Teplow, 1999).

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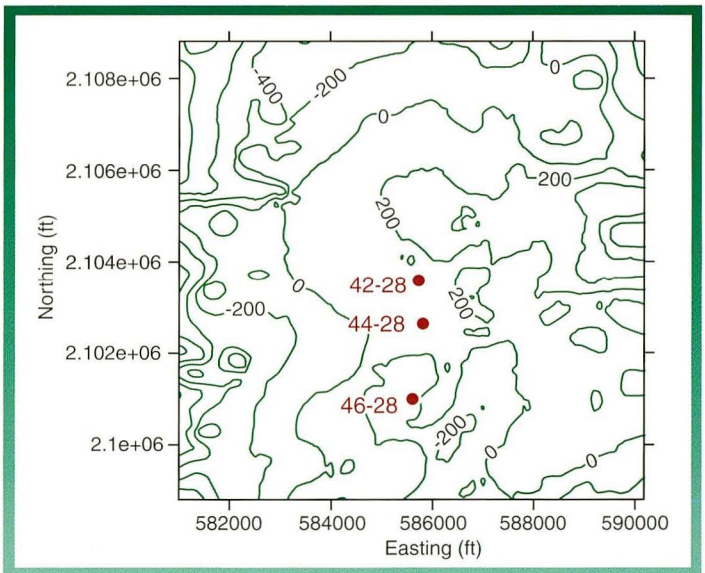

Figure 1. Contour map of the variations in elevation of the basement interface at the Rye Patch Geothermal Reservoir. The boreholes are indicated for reference.

ELECTROMAGNETIC METHODS FOR GEOTHERMAL EXPLORATION

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RESEARCH OBJECTIVES

The objective of the proposed research is to develop efficient numerical codes for mapping high-permeability zones, using single-hole electromagnetic (EM) data. These codes retain a reasonably high resolution, are simple to use, and do not require major computational resources. The work is in conjunction with the rapid development in instrumentation used for borehole EM surveys in producing geothermal fields. Mapping of fractures and other high-permeability zones are critically important because they play a very important role in developing and producing geothermal reservoirs.

APPROACH

A simple 2D inversion code for analyzing data obtained in single-borehole configurations was developed for laboratory use in FY00. The numerical method adopted is the integral equation, based on a modified Born approximation. The medium of interest is cylindrically symmetric in this case, and the resulting inversion algorithm will be simple enough to be implemented on PCs operated in the field. In FY01, the 2D inversion code development will be completed and field-tested for routine on-site use. In the next 3 years (FY02–FY04) the algorithm will be extended to investigate 3D electrical structures in the vicinity of boreholes. The medium will be divided azimuthally and radially to confirm cylindrical structure, but each element will be assigned different electrical conductivity.

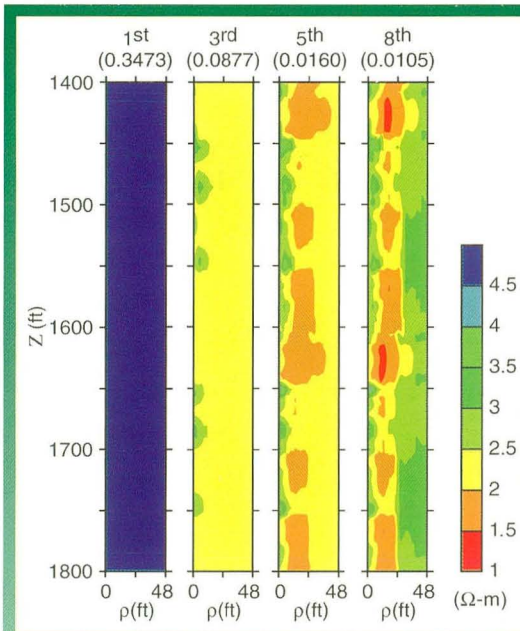

Figure 1. Conductivity imaging derived from the 2D inversion of data obtained from Chevron USA. The model started with uniform conductivity (far left) of 4 Ω-m, and after eight iterations, the misfit in terms of rms (shown as fractional numbers after the number of iterations shown at the top of each image) converged to about 1%.

ACCOMPLISHMENTS

In May 2000, Electromagnetic Instruments Inc. (EMI) conducted a field test of the newly built Geo-BILT tool (operated by Chevron USA) at Lost Hills oil field in southern California. Berkeley Lab evaluated the data for future development of the 3D approximate inversion scheme. As part of the final evaluation of 2D inversion code, we conducted a data inversion using only the Mz-Hz data. The result is shown in Figure 1.

SIGNIFICANCE OF FINDINGS

An important improvement has been implemented to the 2D inversion code developed for analyzing single-borehole EM data. The efficiency and robustness of an inversion scheme is very much dependent on the proper use of the Lagrange multiplier, which is often provided manually to achieve a desired convergence. We have developed an automatic Lagrange multiplier selection scheme. Successful application of the scheme will improve the ability of the code to handle field data.

ACKNOWLEDGMENTS

The authors would like to thank Michael Morea, Chevron USA Production Company, and the U.S. Department of Energy, National Petroleum Technology Office (Class III Field Demonstration Project DE-FC22-95BC14938) for allowing us to publish this data. This work was partially supported by the Assistant Secretary for Energy Efficiency and Renewable Energy, Office of Power Technologies, Office of Wind and Geothermal Technologies, of the U.S. Department of Energy under Contract No. DE-AC03-76SF00098.

THE YANGBAJING GEOTHERMAL FIELD, TIBET: HEAT SOURCE AND FLUID FLOW

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PROJECT OBJECTIVES

The chemical characterization of fluids in a geothermal reservoir is essential for realizing optimum utilization of the resource. The isotopic composition of elements in fluids provides a quantitative measure of material balance, and therefore isotopes are extremely powerful in unraveling fluid histories and tracing fluid flow. In this regard, conservative elements, such as the noble gases (He, Ne, Ar, Kr, and Xe), are extremely useful because they preserve isotopic information related to initial conditions and sources.

APPROACH

The isotopes of the inert noble gases provide long-lasting tracers of fluid sources, such as large ^{3}He enrichments in deep fluids originating in the mantle and enrichments in radiogenic ^{4}He and ^{40}Ar in crustal fluids. The occurrence and mixing of these various components provide tools for identifying specific fluid sources, fluid flow paths from source to reservoir, and geothermal-reservoir characteristics as defined by mixing, fluid residence times, and chemical processes.

ACCOMPLISHMENTS

The Yangbajing geothermal field, located ~94 km northwest of Lhasa, Tibet, has an installed capacity of ~25 MWe. Production is from liquid-dominated, shallow, moderate-temperature (150–165°C) reservoirs. However, Na/K geothermometer temperatures and recent drilling in the NW sector of the field indicate the presence of a deeper, higher-temperature (~300°C) reservoir beneath the shallow reservoir.

The ^{3}He/^{4}He ratios in fluids from the Yangbajing Field were found to be low (0.26 Ra) relative to typical mantle values (8–9 Ra). Despite the discovery of the high-temperature deeper reservoir, a deep resistivity anomaly inferred to be a magma body, and long-held conceptual models for the Yangbajing Field calling on a magmatic heat source, the helium isotopic compositions suggests very little (if any) involvement of recently intruded magmas. If the heat source is a magma body, then the helium has been extensively diluted with radiogenic ^{4}He by water-rock interaction or roof foundering in the magma chamber. Alternatively, the helium isotopes may suggest that heat is mined not from a magmatic intrusion but by deep circulation of meteoric waters along the Yarlu-Zangbo suture. Variations in helium abundance and isotopic composition are consistent with the mixing of a deep-high ^{3}He/^{4}He fluid (~0.26 Ra) with the shallower overlying reservoir (<0.09 Ra) currently being produced.

SIGNIFICANCE OF FINDINGS

The helium isotopic composition of the Yangbajing geothermal fluids is inconsistent with a strong magmatic influence. In light of the helium isotopic data, the inferred significance of the resistivity anomaly should be reconsidered. Variations in helium abundance and isotopic composition support mixing between the deep and shallow reservoirs, suggesting that extensive exploitation of the deeper fluids could accelerate depletion of the shallow resource.

RELATED PUBLICATIONS

Zhao, P., B.M. Kennedy, D. Shuster, J. Dor, E. Xie, and S. Du, Implications of noble gas geochemistry in the Yangbajing geothermal field, Tibet, Proc. 10th Water-Rock Conference, 2, pp. 947–950, Villasimus, Italy, July 10–15, 2001.

Zhao, P., J. Dor, and J. Jin, A new geochemical model of the Yangajing geothermal field, Tibet, Proc. World Geothermal Congress, Kyushu-Tohoku, Japan, pp. 2007–2012, May 28–June 10, 2000.

ACKNOWLEDGMENTS

This work was jointly supported by the National Natural Science Foundation of China (Grant No. 49672168 and 49972093), the International Atomic Energy Agency (Grant No. CPR9095), and the Assistant Secretary for Energy Efficiency and Renewable Energy, Office of Power Technologies, Office of Wind and Geothermal Technologies, of the U.S. Department of Energy under Contract No. DE-AC03-76SF00098.

RESEARCH PROGRAM

Environmental Remediation Technology

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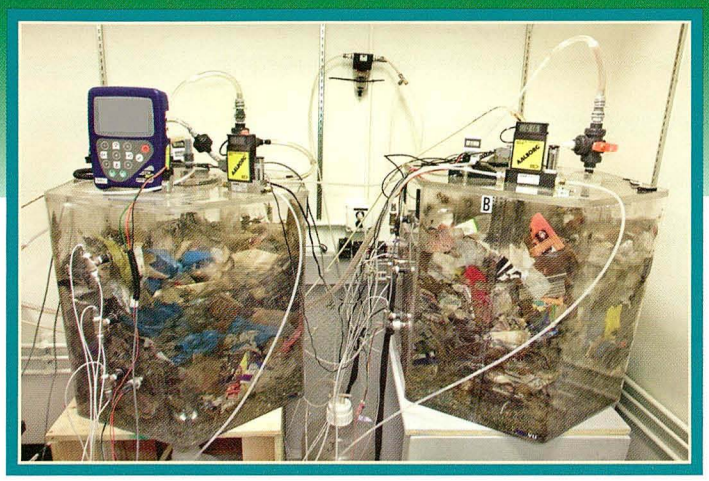

The Environmental Remediation Technology Program (ERTP) conducts multidisciplinary environmental research on characterization, monitoring, modeling, and remediation technologies. This research is directed primarily at Department of Energy and Department of Defense waste site problems. Since many of the contaminants or closely related compounds found at these sites are also dominant at industrial waste sites, much of this research is also applicable to problems faced by the private sector and other government agencies. These projects are both basic and applied, and include everything from molecular studies to full-scale field deployments in all types of media (gas, water, sediment) in all types of environments (wetlands to deserts). This year's major customers have been DOE Office of Environmental Management, DOE Office of Science, Work for Others-DOD, and Work for Others (Industry and Other Government Agencies).

DEMONSTRATIONS AND DEPLOYMENT

ERTP supports DOE's Office of Environmental Management in both the areas of Environmental Restoration (EM40) and the Office of Science and Technology (EM50). Earth Science Division (ESD) scientists directly supervise characterization, remediation and monitoring, and provide regulatory and permitting support to Berkeley Lab's Environmental Health and Safety Department for all environmental problems on site. During this past year, the program demonstrated and deployed technologies for bioventing/soil vapor extraction of volatile organic compounds (VOCs) and air sparging of solvent-contaminated groundwater.

ERTP research on viscous liquid barriers for containment (patent issued) provides a great opportunity for containing and controlling solvent, metal, and radionuclide contamination at waste sites, DOE's greatest environmental cleanup problem. Indeed, this technology was deployed at Brookhaven National Laboratory this year to contain radionuclide contamination in the subsurface at one of their facilities.

This year ERTP, in partnership with the Savannah River Technology Center and Florida State University, assisted the Institute for Ecology of Industrial Areas in Poland in completing a full-scale demonstration of biopile (aeration) technologies for cleanup of a petroleum-refinery waste lagoon. The demonstration has shown that both passive and active aeration strategies can meet cleanup standards for polycyclic aromatic hydrocarbons in the soil and that active aeration cuts the remediation time in half. This demonstration has been so successful that the petroleum refinery is commercializing the process for other refineries and fuel stations in Poland.

ERTP also supports EM50 with technical expertise via the Strategic Laboratory Council, the Oakland Site Technology Coordination Group, the multi-agency DNAPL Technology Advisory Group, the Subsurface Contaminant Focus Area (SCFA) Vadose Zone Book, the Lead Lab Council for SCFA, and the Hanford Vadose-Groundwater-River Integrated Program.

FIELD AND LABORATORY STUDIES

DOE's Office of Science provides funding for several ERTP projects. The basic research projects funded in this area take advantage of the unique facilities at Berkeley Lab, such as the Advanced Light Source, where researchers look at the interactions between contaminants, water, and minerals at the microscale. ERTP has a project funded in the Natural and Accelerated Bioremediation Research (NABIR) program, which looks at mesoscale biotransformation dynamics as the basis for predicting core-scale reactive transport of chromium and uranium.

FIELD DEMONSTRATIONS FOR DOD

Field tests at McClellan Air Force Base, Sacramento, California, for the Department of Defense have shown that Vadose Zone Monitoring Systems (VZMS)—instrument packages consisting of tensiometers, suction lysimeters, gas samplers, pressure transducers and thermistors—permanently installed at multiple levels provide better monitoring of contaminants at waste sides. The field tests at McClellan AFB allowed identification of significant shallow sources of contamination.

DEMONSTRATIONS AND TECHNICAL ASSISTANCE FOR INDUSTRY/OTHER AGENCIES

ERTP has researched selenium transport in the Grassland Water District, California, for many years. Recent research has focused on better methods for compliance monitoring and management. The U.S. Bureau of Reclamation has sponsored this work in an effort to better manage selenium loading in the agricultural waste water of the San Luis Drain. Microbial studies this year have shown that selenium in-transit losses occur and that the fate of this selenium is sediment beds. Manipulation of the microbial ecology of the Drain may stimulate the bioremediation of selenium from the water, thereby reducing the mass loading of selenium to the San Joaquin River.

ERTP also provides technical consultation to private industry and other government agencies on implementing Berkeley Lab- and DOE-patented technologies at private and government-owned sites. Private industry must have a license to the technology for use at private sites, and all ERTP expenses are reimbursed by the company or another agency. Several contracts this year were executed for consultation regarding bioremediation and characterization.

ERTP also provides technical advisory support for the Bay Area Defense Conversion Action Team (BADCAT) and the California Environmental Business Council (CEBC).

NABIR PROGRAM OFFICE

ERTP continued to be the NABIR Program Office for the Office of Science. The NABIR Program Office maintains the dynamic NABIR Web home page (www.lbl.gov/NABIR/) with links to investigators, program element managers, science team leaders, recent publications, annual meeting registration, calls for proposals, review documents, and other Web sites. In addition, the NABIR Program Office also organizes the NABIR annual investigators meeting, with more than 150 participants and sessions for posters, presentations, and breakout sessions. The NABIR Program Office is also producing a new NABIR Bioremediation Primer that will be available to the public in print or electronically on the NABIR home page. The NABIR program office also assisted DOE-HQ in reviewing, evaluating and starting up the Field Research Center for the NABIR program at Oak Ridge National Laboratory.

PARTNERS AND FUNDING

ERTP receives support from DOE programs in the Offices of Science and Environmental Management (EM). The EM programs include the Environmental Management Science Program; the Subsurface Contaminants Focus Area; and the Characterization, Monitoring, and Sensor Technology Crosscutting Program. The Office of Science funds the NABIR Program Office at Berkeley Lab, and the Office of Science, Office of Biological and Environmental Research funds two environmental remediation projects. Support is also received from DOD, Cal-EPA, other DOE Labs, the University of California at Berkeley, and U.S. Bureau of Land Management. Other supporters in 2000 include: Pacific Northwest National Laboratory, Radian International, Earthtech, Woodward & Clyde, Florida State University, and IT Corporation. Partners include UC-Berkeley, Stanford University, Westinghouse Savannah River Company, Idaho National Engineering Laboratory, Lawrence Livermore National Laboratory, Pacific Northwest National Laboratory, Utah State University, University of Nevada, and University of Illinois.

ISOTOPE TRACKING OF WATER INFILTRATION THROUGH THE UNSATURATED ZONE AT HANFORD

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RESEARCH OBJECTIVES

Significant amounts of radioactive waste were generated by the production of fuel for nuclear weapons at the Hanford site in Washington. High-level waste is currently stored in tanks, some of which are known to be leaking. In addition, large quantities of low-level waste were discharged directly to the ground. As a result of these practices, radionuclide contamination has been detected in the groundwater at the site and poses a significant threat to the nearby Columbia River. To examine the pathways of fluid and contaminant transport through the vadose zone, we undertook an isotopic and chemical study of pore-water samples from a borehole through the unsaturated zone.

APPROACH

The stable hydrogen and oxygen isotope compositions of water provide natural labels for different water sources. Further, evaporation modifies the isotopic signature of water, producing a distinctive signal that can be used to identify affected fluids. In the area of the borehole, the potential inputs to the vadose zone (local precipitation, process waters derived from the Columbia River) have isotopic compositions in the same range as the groundwater. However, evaporation appears to have significantly affected most of the vadose zone waters in the area. To quantify these effects, the isotopic compositions of 32 samples of pore water that were vacuum-distilled from vadose zone core samples have been analyzed. The chemical compositions of the pore waters were also measured by analyzing 1:1 de-ionized water leaches of the core material.

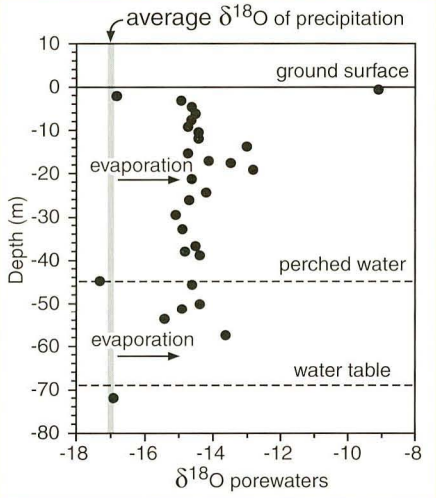

Figure 1. Oxygen isotope compositions of pore water samples distilled from a borehole drilled through the Hanford unsaturated zone

ACCOMPLISHMENTS

Most of the measured isotopic compositions of the pore-water samples were shifted by evaporation. The oxygen isotope compositions of the pore-water samples are plotted versus depth on Figure 1. The $\delta^{18}O$ value of the shallowest sample (taken at ~0.5 m depth) is much higher than either local precipitation or process water derived from the Columbia River (the two potential sources of surface water), signifying that it is strongly evaporated. This is typical of near-surface soil waters, especially in arid and semi-arid environments. At 2 m depth, the $\delta^{18}O$ value of the pore water is equal to the average value of precipitation/Columbia River water. Beneath 2 m, however, most of the pore waters are shifted to higher $\delta^{18}O$ values, indicating that they have also evaporated. Two pore-water samples from the deeper part of the core did not have an evaporated signal (the 44.7 and 71.8 m samples). The deeper sample is from the saturated zone and reflects the isotopic composition of the groundwater. The other sample is from a perched water zone above a caliche layer in the core. This perched water sample was the only pore-water sample with significantly elevated concentrations of several contaminants (Se, Mo, Cr, U, NO_3^-, SO_4^{2-}, and possibly ^{99}Tc).

SIGNIFICANCE OF FINDINGS

Two key aspects of these data have significant implications for fluid infiltration at Hanford:

- The 2–4% shift in the oxygen isotope composition of most of the pore-water samples indicates that they have undergone 20–35% evaporation. This has important implications for natural infiltration rates at the site. No detailed model is currently available for translating the average oxygen isotope shift to an infiltration flux. However, to first order, it can be reasoned that the changes observed in these samples correspond to infiltration rates of approximately 2.5–6.0 cm/yr.
- The isotopic composition of the perched water sample is clearly distinct from the pore water above and below this horizon, indicating that it was not derived from direct, vertical infiltration. Further, the elevated levels of contaminants in the perched water imply that this water was partially derived from Hanford operations. The most likely source of this water is a set of surface holding ponds that were located ~50 m from the borehole, although it is also possible that there could be some input from a tank farm further up gradient.

ACKNOWLEDGMENTS

This work has been supported by the Assistant Secretary of the Office of Environmental Management, Office of Science and Technology, Environmental Management Science Program of the U.S. Department of Energy, under Contract No. DE-AC03-76SF00098.

FUZZY-SYSTEMS MODELING OF *IN SITU* BIOREMEDIATION OF CHLORINATED SOLVENTS

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RESEARCH OBJECTIVES

We seek to evaluate the *in situ* remediation of chlorinated solvents carried out at the Savannah River Site in 1992–93, using fuzzy-systems modeling. This kind of modeling is well suited to the analysis of imprecise and uncertain concentration measurements in monitoring wells. We hope by this work to determine what further applications of this modeling technique would be useful for remediation.

APPROACH

In 1992–93, a large-scale vadose zone-groundwater vapor stripping and bioremediation demonstration was conducted at the Savannah River Site. Bioremediation was carried out by injecting several types of gases (ambient air, methane, nitrous oxide and triethyl phosphate mixtures) through a horizontal well in the groundwater at a depth of 175 ft. Simultaneously, soil gas was extracted through a horizontal well in the vadose zone at a depth of 80 ft (Hazen et al., 1997). Because of the natural heterogeneity of soils and complex lithological and hydrogeological conditions, significant spatio-temporal variations of volatile organic compounds (VOCs), enzymes, and biomass in 11 groundwater-monitoring wells were observed over the field site. Such variations in concentrations make some of the results seem ambiguous and difficult to use for describing bioremediation processes.

One of the most powerful modern approaches for analyzing such uncertain and imprecise data is fuzzy-systems modeling. One of the main advantages of the fuzzy-logic approach is the use of the intuitive human ability to conceptualize imprecise properties of an object using the concept of a fuzzy number. The fuzzy number is a function between the variable and the continuous fuzzy membership function (FMF), which varies from 0 to 1. Concentration FMFs were determined for each remediation campaign (from the probability density function [PDF] for a real [nominal] data set) by normalizing the PDF to the maximum value of the PDF.

ACCOMPLISHMENTS

Comparison of FMFs for trichloroethylene (TCE) and pentachloroethylene (PCE) mineralizations indicated that (a) air stripping led to an initial decrease in the TCE mineralization potential, but an increase in PCE mineralization potential over the field scale, and (b) bioremediation by injecting a methane, air, nitrous oxide, and triethyl phosphate mixture was very effective in wells located close to the injection well. We also determined fuzzy relationships between the methanotroph densities and TCE concentration by creating a set of continuous FMFs and simple fuzzy logic if-then rules.

SIGNIFICANCE OF FINDINGS

The fuzzy-systems modeling approach clarified that injecting a balanced mixture of air, methane, nitrous oxide, and triethyl phosphate into the groundwater was the most effective bioremediation method. Fuzzy modeling can be used to supplement the conventional statistical and numerical analyses of bioremediation for obtaining a better understanding of the volume-averaged solvent concentrations over the field scale. Future research using these methods could also involve developing fuzzy-ruled methods to aid in managing remediation activities, predictions, and risk assessment.

RELATED PUBLICATION

Hazen, T.C., K.H. Lombard, B.B Looney, M.V. Enzien, J.M. Dougherty, C.B. Fliermans, J. Wear, and C.A. Eddy-Dilek, Full scale demonstration of *in situ* bioremediation of chlorinated solvents in the deep subsurface, using gaseous nutrient biostimulation, in Progress in Microbial Ecology, M.T. Martins et al., eds., pp. 597–604, 1997.

ACKNOWLEDGMENTS

The work was partially supported by Assistant Secretary of the Office of Environmental Management, Office of Science and Technology, Environmental Management Science Program of the U.S. Department of Energy, under Contract No. DE-AC03-76SF00098.

EXPERIMENTAL INVESTIGATION OF AEROBIC LANDFILL BIODEGRADATION

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RESEARCH OBJECTIVES

The United States produces approximately 200 million tons of municipal solid waste annually, 57% of which is disposed of in municipal landfills. With increasing costs and difficulties in permitting new landfill sites, existing landfill space is becoming a valuable commodity. Current regulations require capping of landfills to isolate waste from incoming rainwater and collection of leachate for treatment prior to release to the environment, creating what is termed a "dry tomb" landfill. Restricting exposure of air and water to the refuse slows biodegradation rates and increases the time required for landfill stabilization. The objective of this project is to develop data to support the concept of Aerobic Landfill Bioreactors. In these systems, the refuse mass is kept wet and aerobic, thereby greatly increasing the biodegradation rate. The increased rate of biodegradation results in faster stabilization and increased settling, which would allow for input of additional refuse or faster land reuse. In addition, aerobic systems do not produce noxious odors or methane, a powerful greenhouse gas.

APPROACH

In this study, rates of settling and biodegradation are measured in large laboratory-scale bioreactors. Three treatments are being applied to the bioreactors: (a) aerobic landfill (air injection with water addition and recirculation), (b) dry, anaerobic landfill (no air injection or leachate recirculation), and (c) wet, anaerobic landfill (no air injection, but water addition and recirculation). The three bioreactors consist of 55 gal. clear acrylic tanks instrumented to monitor pressure, temperature, moisture, humidity, and gas and leachate composition and flow rates. All tanks contain 10 cm of gravel at the bottom, overlain by a sample of typical municipal waste. Air is injected into the bottom of the tanks, and gas is vented out the top. Leachate is collected at the bottom of the tanks, recirculated, and sprinkled over the top of the refuse. A neutron probe is used to monitor the average moisture content of the refuse.

Relative degradation rates between the tanks are monitored by CO_2 and CH_4 production rates. Respiration tests were also conducted in the aerobic tank by ceasing air injection and monitoring the rate of oxygen consumption. The leachate is sampled regularly and monitored for biological activity and chemical composition.

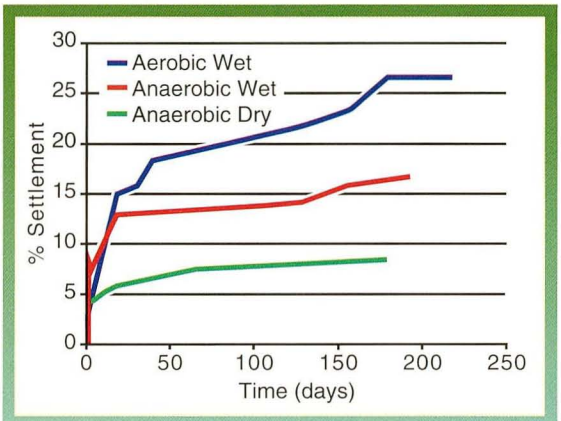

Figure 1. Settling of the refuse mass over time by type of treatment

ACCOMPLISHMENTS

Over the test period, the aerobic landfill bioreactor has shown significantly more settling than the anaerobic reactors (see Figure 1). The leachate from the aerobic bioreactor has maintained a neutral pH and has shown low levels of all measured parameters (metals, nitrate, phosphate, and total organic carbon). Respiration tests in the aerobic reactor have demonstrated a dependence on refuse age, temperature, and moisture content. Live/dead cell counts have also shown a decrease in biological activity over the same period. The wet, anaerobic bioreactor has shown high levels of all measured chemical parameters in the leachate and has required buffering to adjust the pH to neutral levels. The dry, anaerobic reactor did not produce any leachate, and showed a lower settling rate and CO_2 rate than the wet, anaerobic reactor. Neutron-probe measurements have proven to be a reliable method for monitoring average moisture content within the tanks.

SIGNIFICANCE OF FINDINGS

This study demonstrates that maintaining the refuse as an aerobic bioreactor increases the rates of settling and stabilization as well as producing less odor and less hazardous leachate. Ongoing work includes investigation of the effect of nutrient addition on activity and further investigation of the effect of moisture and air addition on biodegradation rates. A recently developed code for numerical simulation of landfill bioreactors (T2LBM) will also be used to model biodegradation in the reactors. See a related report in this publication for details on the T2LBM landfill biodegradation model.

RELATED PUBLICATIONS

Borglin, S., T. Hazen, C. Oldenburg, and P. Zawislanski, Laboratory investigation of the aerobic biodegradation of municipal landfill materials, Berkeley Lab Report LBNL-47979, 2001.

Oldenburg, C.M., T2LBM: Landfill bioreactor model for TOUGH2, Version 1.0, Berkeley Lab Report LBNL-47961, 2001.

ACKNOWLEDGMENTS

This work has been supported by the Laboratory Directed Research and Development Program of Berkeley Lab, provided by the Director, Office of Science, of the U.S. Department of Energy under Contract No. DE-AC03-76SF00098.

SUBSURFACE IMAGING FOR CHARACTERIZING HETEROGENEITY AFFECTING MICROBIAL-TRANSPORT PROPERTIES IN SEDIMENTS

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OBJECTIVE

Although heterogeneity occurs at almost every scale, it is not known how key physical and chemical parameters affect microbial behavior at different scales in a natural environment. A primary goal is to relate physical and chemical parameters—using geophysical methods (i.e., parameters that we have experience measuring *in situ*)—to significant microbial properties and thus predict their behavior in the subsurface.

APPROACH

This research involves an integrated approach to characterizing and identifying the fundamental properties and scales necessary to image heterogeneities, using geophysical methods that may control transport in near-surface sedimentary media. Particular emphasis is placed on understanding transport behavior relative to understanding subsurface microbial behavior.

This approach uses controlled small-scale field sites and supplementary laboratory information to characterize the properties affecting chemical and bacterial transport, which can be imaged with *in situ* characterization methods. Efforts in this research have been made toward defining the hierarchy of physical characteristics that control transport and geophysical properties at the laboratory and field scale. Also, several other imaging techniques (radar, self potential, DC resistivity) are being used to obtain a more direct measure of physical, microbial, and chemical properties.

ACCOMPLISHMENTS

Work in the past year at the Oyster Site in Virginia (as part of the Department of Energy's NABIR program) has focused on correlating seismic-imaging and radar results to hydrologic and chemical properties. Such work will aid in the understanding of bacterial transport properties. In addition, geophysical properties are being correlated to flow and transport properties affecting flow through a geostatistical approach. Also being investigated is the possibility of direct detection of microbes using geophysical methods. Experiments in the lab and field have indicated that both electrical properties and seismic properties will be affected by the presence of microbes. The charac- terization at this site is fully described at http://www.esd.lbl.gov/people/shubbard/web_page.

RELATED PUBLICATIONS

Chen, J., Y. Rubin, and S. Hubbard, Estimating hydraulic conductivity at the South Oyster Site using geophysical tomographic data, Water Resour. Res., 2001 (in press).

Hubbard, S., and Y. Rubin, A review of selected estimation techniques using geophysical data, Journal of Contaminant Hydrology, 45, 3–34, 2000.

Hubbard, S., J. Chen, J. Peterson, E. Majer, K. Williams, D. Swift, B. Mailliox, and Y. Rubin, 2001, Hydrogeological characterization of the D.O.E. Bacterial Transport Site in Oyster Virginia, using geophysical data, Water Resour. Res., 2001 (in press).

ACKNOWLEDGMENTS

This work has been supported by the Director, Office of Science, Office of Biological and Environmental Research, Environmental Sciences Divison, Natural and Accelerated Bioremedation Research Program under Contract No. DE-AC03-765F0098.

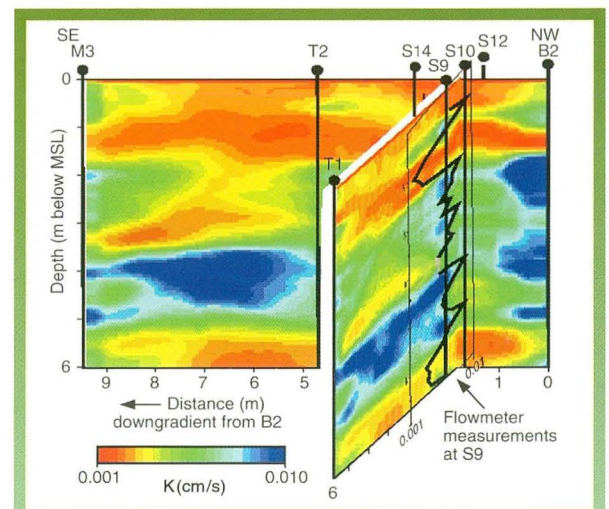

Figure 1. An example of hydraulic-conductivity estimates obtained using radar and seismic tomographic data at the DOE Bacterial Transport Site in Oyster, VA. Note the good correlation with the actual flow measurements (Chen et al., 2001; Hubbard et al., 2001).

HIGH-RESOLUTION IMAGING OF VADOSE ZONE TRANSPORT USING CROSSWELL RADAR AND SEISMIC METHODS: RESULTS OF TESTS AT THE HANFORD (WASHINGTON) SISSON AND LU SITE

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RESEARCH OBJECTIVES

At the DOE Hanford site, heterogeneities of interest can range from localized phenomena (such as silt or gravel lenses, fractures, and clastic dikes) to large-scale lithologic discontinuities. These features have been suspected of leading to funneling and fingering, additional physical mechanisms that could alter and possibly accelerate the transport of contaminants to underlying groundwater. Understanding of contaminant migration through the vadose zone has not only been hampered by inadequate conceptual models, but has also suffered from inadequate monitoring technologies. Over the last few years, however, crosswell radar and seismic imaging have emerged as possible monitoring solutions.

The main questions addressed with crosswell methods are:

- What parts of the vadose zone-groundwater system control flow geometry?
- What physics controls flow and transport in unconsolidated soils of the vadose zone?
- What is the optimum suite of field tests and laboratory studies to provide information for predicting flow and transport behavior?
- How can the information obtained during site characterization be used for building confidence in predictive numerical models?

The primary purpose of crosswell radar and seismic imaging at Hanford is to provide detailed information on the lithology and structure (25 cm or less resolution) as well as provide the same level of detail on the location of the fluid transport. A second purpose is to evaluate these methods and/or modification of the methods to determine their use at the tank-farm scale.

APPROACH

Tests were conducted at an infiltration site where there were four PVC-lined holes spaced 3 to 5m apart spanning the injection zone. The ground penetrating radar (GPR) work consisted of repeated crosswell tomographic data sets that were collected between the six possible well pairs at the Sisson-Lu site before, during, and after infiltration tests using fresh water. A total of four data collection visits were made to the site, with three of the visits consisting of exactly the same data sets being collected. The crosswell seismic imaging data were collected after all of the infiltration tests were completed because the wells used for the crosswell seismic had to be filled with water. The piezoelectric source emitted energy from 1 to 10 kHz.

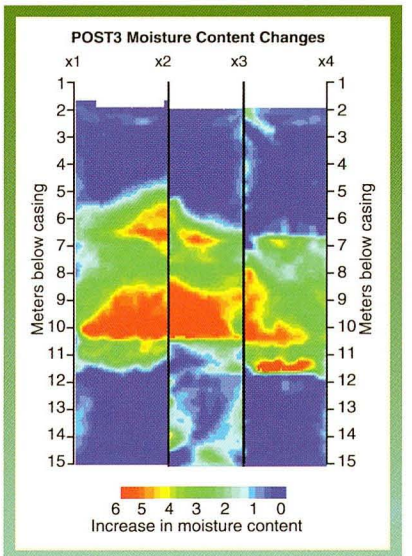

Figure 1. Moisture changes from the time-lapse radar data

ACCOMPLISHMENTS

In general, the radar and seismic results were excellent. At the time of the experiment's design, we did not know how well these two methods could penetrate or resolve the moisture content and structure. It now appears that the radar could easily go up to 5, even 10 m between boreholes at 200 MHz, and even farther (up to 20 m) at 50 MHz. The seismic-imaging results indicate that at several-hundred-hertz propagation of 20 to 30 m, high resolution is possible. One of the most important results, however, is that together, seismic and radar are complementary in their properties estimation. The radar was sensitive primarily to changes in moisture content, while the seismic imaging was sensitive primarily to porosity. In a time-lapse mode, the radar can show moisture-content changes to a high resolution (see Figure 1), with the seismic imaging providing high-resolution lithology. At this time, the two different data sets have not been merged or jointly interpreted with each other or with other data sets, but the potential for providing information on fluid flow through vadose zone environments is very good.

ACKNOWLEDGMENTS

This work was funded by Assistant Secretary of the Office of Environmental Management, Office of Science and Technology, Environmental Management Science Program of the U.S. Department of Energy, through the Science and Technology Program at PNNL. We would like to thank Glendon Gee and Andy Ward for their efforts.

EX SITU TREATMENT OF MTBE-CONTAMINATED GROUNDWATER IN FLUIDIZED BED REACTORS

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RESEARCH OBJECTIVES

Contamination of groundwater by methyl *tert*-butyl ether (MTBE) is a problem throughout the United States because of its extensive usage as a gasoline oxygenate. Few technologies exist for treatment of MTBE-impacted water. *Ex situ* treatment of groundwater with granular activated carbon (GAC) is generally regarded as the only proven method for MTBE-contaminated groundwater remediation. However, the cost of replenishing GAC and treating the spent GAC is prohibitively high. More cost-effective and efficient treatment technologies are desperately needed.

The objective of this research is to understand the biological treatment process of MTBE in fluidized-bed bioreactors and to develop a reliable *ex situ* MTBE treatment technology in fluidized-bed bioreactors that use GAC.

APPROACH

Biological treatment of MTBE-impacted groundwater poses many problems because of the lack of basic knowledge about MTBE biodegradation. Typically, MTBE treatment systems have start-up problems with poor process control, and they become unmanageable when they fail. Contributing factors to these problems are slow growth rate, low biomass yields, and instability of the degrading cultures when MTBE serves as the sole substrate. On the other hand, co-metabolic MTBE degradation has the advantage of being inducible by co-substrates, such as iso-pentane (IP) and propane. The process also has some limitations, however, including possible failure caused by the depletion of co-substrate and competitive inhibition between MTBE and the co-substrate.

ACCOMPLISHMENTS

These metabolic processes were simulated in two laboratory-scale fluidized-bed bioreactors, using fresh GAC saturated for a week with high concentrations of MTBE (>20,000 mg/L). Under the same starting conditions and treatments, Reactor 1 removed 99.9% of MTBE over the first 80 days, suggesting that MTBE was being utilized as the sole substrate, while Reactor 2 failed to show significant MTBE treatment. An IP degrading mixed culture (with IP at 583 mg/L reactor/day) was then provided for Reactor 2, and MTBE treatment in Reactor 2 began to improve. Within a month, MTBE treatment efficiency was more than 99.9%, and IP addition was terminated. The reactor maintained MTBE removal efficiency without further IP addition.

As shown in Figure 1, treatment efficiency in both reactors transiently dropped and then rebounded to 99.9% when the MTBE loading rate was increased up to 700 mg/L reactor/day. However, the reactors showed different responses to the changing loading rate. The changing loading rate had little impact on Reactor 1, whereas Reactor 2 took much longer to recover to the previous treatment level.

SIGNIFICANCE OF FINDINGS

These results show that MTBE treatment in fluidized-bed bioreactors can be achieved, either through growth-based metabolism or co-metabolism using iso-pentane- degrading microorganisms. Also, these studies demonstrated that the biological removal of MTBE-impacted groundwater is a highly feasible treatment technology at contaminated sites and that MTBE degradation can be initiated in treatment systems at these sites by adding iso-pentane at proper concentrations.

RELATED PUBLICATION

Oh, K.-C., and W.T. Stringfellow, Treatment of MTBE in a fluidized-bed bioreactor using iso-pentane as a co-substrate, 6th Battelle Symposium, San Diego, California, June 3–7, 2001.

ACKNOWLEDGMENTS

This work has been supported by Kinder Morgan Energy Partners and Envirex/U.S. Filter, under Berkeley Lab Work For Others Agreement No. BG99-035(00).

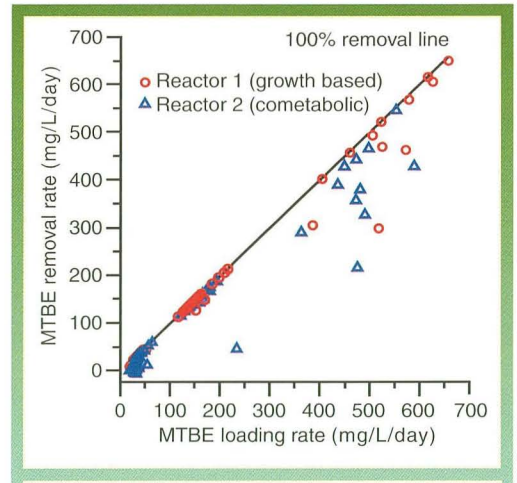

Figure 1. MTBE loading rate vs. MTBE removal rate in Reactors 1 and 2

NUMERICAL SIMULATION OF LANDFILL BIODEGRADATION PROCESSES

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RESEARCH OBJECTIVES

The need to control gas and leachate production while minimizing refuse volume in municipal solid waste (MSW) landfills has motivated the development of landfill simulation models that can be used by operators to predict and design optimal treatment processes. Prior models of landfill processes are either batch models (zero-dimensional), multilayer batch models (one-dimensional), or do not consider gas production as part of biodegradation. The objective of this research is to develop fully three-dimensional numerical simulation capabilities for landfill biodegradation processes, including gas production. In this effort, we have developed T2LBM, a module for the TOUGH2 simulator. This module implements a landfill bioreactor model to provide simulation capability for the processes of aerobic or anaerobic biodegradation of municipal solid waste and the associated flow and transport of gas and liquid.

APPROACH

Biodegradation and gas production in MSW landfills is an enormously complex and variable process. To make progress in the simulation of landfill processes, simplifications must be made. The approach chosen for T2LBM couples the process modeling of the flow and transport of gas and aqueous phases inherent in TOUGH2, with biodegradation and gas-generation processes. For simplicity, T2LBM models the biodegradation of a single substrate component (acetic acid, CH_3COOH) as a proxy for all of the biodegradable fractions in MSW. T2LBM includes six chemical components (H_2O, CH_3COOH, CO_2, CH_4, O_2, N_2) and heat distributed in gaseous and aqueous phases with partitioning by Henry's law. This approach assumes implicitly that hydrolysis reactions occur to produce acetic acid and places the model focus on biodegradation and associated gas production, along with flow and transport processes (including non-isothermal effects).

ACCOMPLISHMENTS

We have developed T2LBM and verified its performance against results from published laboratory studies of aerobic and anaerobic biodegradation. In addition, we have simulated a hypothetical MSW landfill with leachate recirculation and subsequent air injection into the bottom of the landfill. Shown in Figure 1 are four panels representing liquid saturation, temperature, acetic acid mass fraction, and aerobicity for the sample problem after one day. At this time, liquid saturation is variable, corresponding to the heterogeneous permeability field as shown in the upper-left panel. The temperature field (upper-right panel) reflects the heating caused by aerobic biodegradation as oxygen in the ambient air is consumed. The low-temperature region in the right-hand side of the domain corresponds to the high-liquid saturation region, where there is less ambient air and more liquid to be heated. At this location, anaerobic conditions prevail, with correspondingly smaller heat production. The mass fraction of acetic acid shown in the lower-left panel reveals that the anaerobic reaction has biodegraded more acetic acid than the aerobic reaction. In the final panel, the quantity called aerobicity is shown, in which aerobicity equal to one indicates aerobic conditions, and aerobicity equal to zero indicates anaerobic conditions. Most of the domain is weakly aerobic as oxygen in the ambient air is still being consumed, while in the low-permeability, high-liquid saturation region, conditions have already become anaerobic. Methane and CO_2 mass fractions in the gas (not shown) confirm these interpretations.

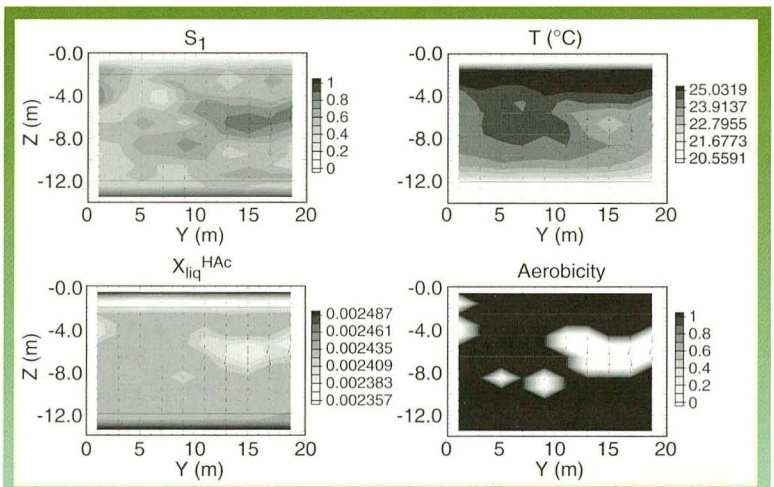

Figure 1. Liquid saturation (S_l), temperature (T), mass fraction acetic acid (X^{HAc}_{liq}), and aerobicity with liquid velocity vectors at $t = 1$ day

SIGNIFICANCE OF FINDINGS

Our simulations to date point out the complexity of landfill biodegradation processes and demonstrate that numerical simulation of these processes is possible. Application of T2LBM is ongoing and aimed at simulating results of laboratory experiments and field tests of landfill biodegradation processes.

RELATED PUBLICATION

Oldenburg, C.M., T2LBM: Landfill bioreactor model for TOUGH2, Version 1.0, Berkeley Lab Report LBNL-47961, 2001.

ACKNOWLEDGMENTS

This work has been supported by the Laboratory Directed Research and Development Program of Berkeley Lab, provided by the Director, Office of Science, of the U.S. Department of Energy under Contract No. DE-AC03-76SF00098.

WATER-TABLE RISE CORRELATES WITH TCE INCREASE AT A CONTAMINATED SITE

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RESEARCH OBJECTIVES

The objective of this study is to correlate water-table elevation changes with contaminant concentration changes in monitoring wells. The study site is Operable Unit 1 (OU1) at the former Fort Ord Army Base, along the central California coast, where the unconfined A-aquifer (saturated thickness ~8 m) exists in unconsolidated dune sands above a thick sequence of clays known locally as the Fort Ord-Salinas Valley Aquiclude (FO-SVA). This work is part of a larger effort to understand the groundwater flow and contaminant transport in the layered sands and clays at a depth of 30 m (100 ft) downgradient from OU1. Historically, solvents and fuels were used at OU1 for firefighter training, resulting in groundwater contamination consisting of volatile organic compounds (VOCs), primarily trichloroethylene (TCE). Groundwater extraction and treatment from the A-aquifer has been underway since 1988. Water-table elevation readings and groundwater chemical analyses are carried out quarterly in nearby monitoring wells.

APPROACH

Approximately 8 Mb of quarterly data on contaminant chemistry and water-table elevations provided by Harding ESE have been entered into the database management system GIS/KEY®. This system is useful for displaying spatial and temporal data relevant to the site. The maps created using GIS/KEY® have enabled us to correlate water-table rise with TCE concentration increases and to observe the downgradient propagation of pulses containing TCE-contaminated water.

ACCOMPLISHMENTS

Figure 1 shows a map of three representative wells near the burn pit at OU1. The three superimposed graphs are plots of the temporal changes of the water-table elevation in feet above mean sea level (in blue) and the TCE concentration in mg/L (in green). The vertical dashed green line is a reference line positioned in the first quarter of 1998 in each graph. These three graphs show that the timing, rate, and magnitude of the water-table rise that began in 1998 were similar in all three wells, whereas the timing of the TCE concentration increase varied. The TCE concentration increased as the water table rose near the burn pit (well MW-OU1-06-A), but the corresponding TCE concentration increases were delayed in the downgradient wells by 3 to 6 months for the near well (MW-OU1-05-A) and 6 to 12 months for the more distant well (MW-OU1-20-A).

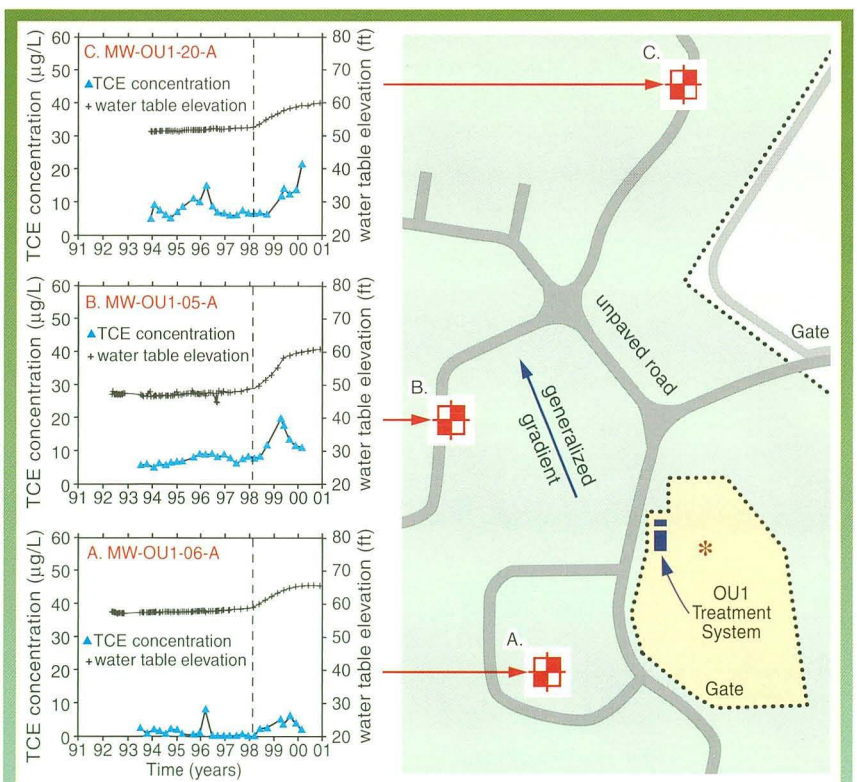

Figure 1. Temporal evolution of the water table elevation and TCE concentration in groundwater for three wells near the burn pit area of OU1.
(* Approximate location of former burn pit)

SIGNIFICANCE OF FINDINGS

This delay suggests that pulses of TCE contamination released from the source area are mobilized by water-table rise and then advected downgradient. These water-table excursions and subsequent TCE increases are likely caused by TCE-contaminated water held in a smear zone between the saturated and vadose zones near the source area. The GIS/KEY® system allowed us to extract and display these useful data from the full set of monitoring data gathered from 56 wells at OU1.

ACKNOWLEDGMENTS

We thank Buck King, Larry Friend, and Ed Heistand of Harding ESE for providing data for OU1. This work was supported by the U.S. Army Industrial Ecology Center through the Concurrent Technologies Corporation Contract No. DAAE30-98-C-1050, Task No. 281, CRDL No. B009, administered by the University of California, Santa Cruz, and by Berkeley Lab under U.S. Department of Energy Contract No. DE-AC03-76SF00098.

FLUID FLOW, HEAT TRANSFER, AND SOLUTE TRANSPORT AT HANFORD TANK SX-108: A SUMMARY REPORT ON MODELING STUDIES

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RESEARCH OBJECTIVES

Of the 15 single-shell tanks at the Hanford 241-SX tank farm, ten are known leakers. Fluid flow and solute transport in the unsaturated zone surrounding the tanks is affected by radioactive decay heat and by chemical interactions between fluids and sediments. Multiphase processes near the tanks include flow of aqueous and gaseous phases, boiling and condensation, migration of solutes, precipitation and dissolution, and vapor-liquid counterflow. Additional effects arise from variable solute concentrations in the aqueous phase, heat generation from leaked radioactive fluids, interference between the heat load and fluid leaks of different tanks, and suspected (but poorly constrained) water-line leaks.

The purpose of the studies reported here is to develop a better understanding of the unique hydrogeologic system created by the Hanford tanks through detailed mechanistic modeling of fluid flow, heat transfer, and mass transport. Our aim is to provide support and guidance for performance assessment, field characterization, and decision-making on remedial measures.

APPROACH

We focus especially on Tank SX-108, which is one of the highest heat-load tanks in the 241-SX tank farm and a known leaker. A realistic quantitative model of mass and energy transport near the tanks requires:

- Comprehensive treatment of all significant physical and chemical processes
- Accurate representation of hydrogeologic conditions at the site
- Realistic parameters for fluids and sediments, and for temperature and leak history of the tanks

These are ambitious goals that can only be achieved through a process of iterative refinement, starting from relatively simple models. The initial emphasis of the work reported here is on process issues, focusing on the extent to which various multiphase and nonisothermal processes may impact the migration of moisture and aqueous solutes. The Hanford sediments are represented as layer-cake stratigraphy, and actual measured temperatures are used to specify the tank heat source. Berkeley Lab's general-purpose fluid- and heat-flow simulator TOUGH2 is used in this work.

ACCOMPLISHMENTS

A series of two-dimensional radially symmetric models was developed to probe different processes and mechanisms to determine what processes are important for contaminant behavior and how they can be modeled effectively. Figure 1 shows the simulated distribution of a conservative solute resulting from a tank leak in 1966 estimated at 50,000 gallons. Our simulations show strong vapor-liquid counterflow effects (heat pipe) in the region surrounding the tank during the period of above-boiling tank temperatures (1956–1967). These effects provide a very efficient mechanism for (1) heat transfer away from the tank and (2) solute transport towards the tank. Aqueous solutes are predicted to concentrate and eventually precipitate near the tank.

ACKNOWLEDGMENTS

This work was supported by the Assistant Secretary of the Office of Environmental Management, Office of Science and Technology, of the U.S. Department of Energy, under Contract No. DE-AC03-76SF00098 through Memorandum Purchase Order 248861-A-B2 between Pacific Northwest National Laboratory and Berkeley Lab.

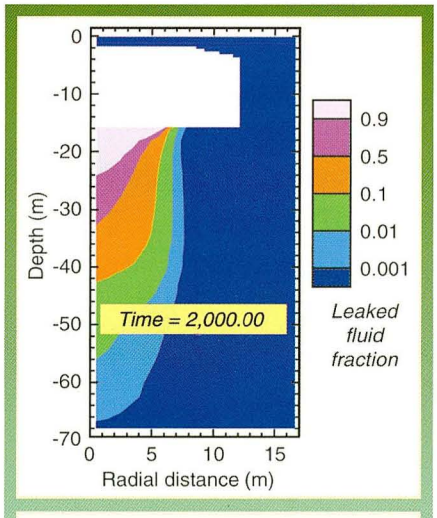

Figure 1. Model domain showing leaked fluid distribution following a 50,000-gallon leak in 1966

A DECISION SUPPORT SYSTEM FOR ADAPTIVE REAL-TIME MANAGEMENT OF SEASONAL WETLANDS IN CALIFORNIA

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RESEARCH OBJECTIVES

This project describes the planned application of a decision support system (DSS) and the development of a comprehensive flow and salinity monitoring program to improve management of seasonal wetlands in the San Joaquin Valley of California. The Environmental Protection Agency is in the process of regulating salinity discharges from nonpoint sources to the San Joaquin River. This project is seen as a proactive initiative to develop new management strategies and gather data to demonstrate the likely impact of regulation on the long-term health and function of wildfowl habitat.

APPROACH

Seasonal wetlands in the Grassland Water District (GWD) are flooded in the fall and drained in the spring to provide habitat for migratory waterfowl, shorebirds, and other wetland-dependent species. The spring draining period is timed to correspond with optimal germination conditions (primarily optimal soil temperature) for growing naturally occurring moist-soil plants and to make seed and invertebrate resources available to migrating birds. Improved coordination of wetland releases with east-side reservoir releases in the San Joaquin Basin has been suggested as a means of improving compliance with San Joaquin River water-quality objectives.

Flow transducers and electrical conductivity sensors have been placed at control structures within the GWD. These devices take measurements every 15 minutes to provide an accurate measurement of salt loads imported and exported from the GWD. Data logged at each site is telemetered to Berkeley Lab. Daily salinity loading is calculated from the daily mean values, which are compared with daily assimilative capacity determinations (made using data available from the river monitoring stations). Wetland discharge opportunities during the spring months will be evaluated weekly by the project team in collaboration with the district water master.

Salinity balances are calculated at two scales—the district scale (90,000 acres) and the individual duck club scale (640 acres). A DSS is under development to assist in computing GWD wetland water requirements, estimating wetland salinity loads in seasonal wetlands, and selecting the best management practices.

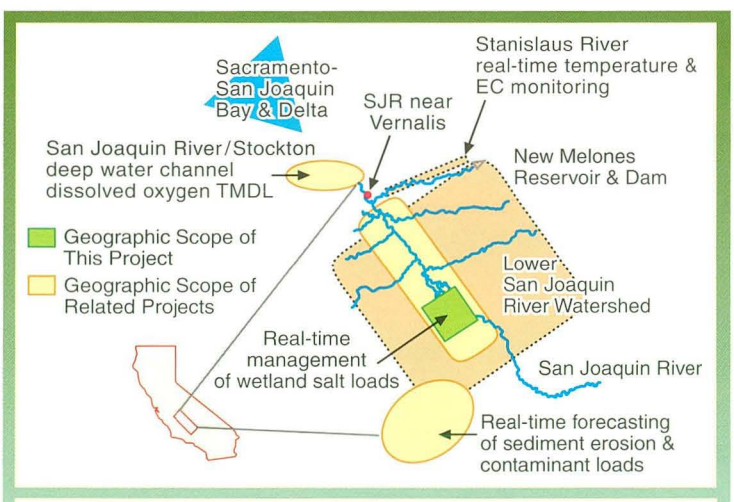

Figure 1. Geographical nexus of CALFED-sponsored real-time flow and water-quality monitoring and management projects

ACCOMPLISHMENTS

Real-time flow, electrical conductivity, and temperature data from the GWD is provided by e-mail and through a Web site (http://socrates.berkeley.edu/%7eph299/Grassland_Realtime/Hanna-Grass/RTWQGWD/) as input to the real-time water-quality forecast model of the San Joaquin River (operated by the San Joaquin River Management Program Water Quality Subcommittee). This is one of a number of real-time monitoring and management projects in the San Joaquin Basin (Figure 1). Agencies such as the U.S. Bureau of Reclamation use the San Joaquin River Management Project Web-posted forecasts of river water quality during periods when water quality in the San Joaquin River is impaired.

SIGNIFICANCE OF FINDINGS

Information obtained through this project will likely be transferable and significantly valuable to all wetlands in the Grassland Ecological Area, including those wetlands managed by state and federal wildlife agencies. Successful implementation of this combined monitoring, experimentation, and evaluation program will provide the basis for adaptive management of wetland drainage throughout the entire 70,000 hectare Grassland Ecological Area. The project involves local landowners, duck club operators, and managers of state and federal refuges in the Grassland Basin.

RELATED PUBLICATION

Quinn, N.W.T, A Decision Support System for real-time management of water quality in the San Joaquin River, California, Environmental Software Systems, Environmental Information and Decision Support (R. Denzer, D.A. Swayne, M. Purvis, and G. Schimak, eds.), Kluwer Academic Publishers, Massachusetts, 1999.

ACKNOWLEDGMENTS

This project is supported by a CALFED grant through the Grassland Water District, Contract No. 0041000.

A NEW METHOD OF WELL-TEST ANALYSIS USING OPERATIONAL DATA

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RESEARCH OBJECTIVES

A pumping or injection well test is common practice in hydrology and petroleum engineering. It is performed to estimate formation hydraulic properties in the vicinity of the well. Normally, such a test requires either maintaining a constant pumping rate or a full shut-in of the well for a substantial period of time at the beginning of the test. We propose to use regular monitoring data (from a production or injection well) for estimating the formation properties without interrupting the operations. Thus, instead of shutting-in the well for a substantial time period, we propose to select a portion of the pumping data over a certain time interval and then derive our conclusions from these data.

APPROACH

A distinctive feature of our approach is that we introduce an additional fitting parameter, an effective pre-test pumping rate, to account for the nonuniform pressure distribution at the beginning of the testing time interval. We derive our model from the same assumptions as in a standard pressure-drawdown or pressure-buildup test analysis. The effective pumping rate prior to the test is a parameter of crucial importance for our procedure because no shut-in period precedes the test during regular operations. We seek to show that accounting for this parameter improves the analyses of traditional pressure-drawdown or pressure-buildup tests.

ACCOMPLISHMENTS

Traditional methods of well-test analysis assume uniform initial pressure distribution near the wellbore. But this assumption did not hold true when regular pumping data were analyzed. (Moreover, using rigorous residual term estimates, we demonstrated that it may be inaccurate even for a traditional well test.) Based on this finding, we proposed a modified initial condition involving an effective pre-test pumping rate as an additional parameter. We then demonstrated that the recovered value of the effective pre-test pumping rate approximates the actual pre-test pumping rate with remarkable accuracy.

From this, we have developed an efficient estimation method, combining analytical calculations with numerical minimization of a function of one variable. As shown in Figure 1, data points very accurately match the fitting curve.

Along with this new method, we have developed a procedure for estimating ambient reservoir pressure and dimensionless wellbore radius. For this procedure, a well test was simulated, using the parameter estimated by the optimization procedure mentioned above. In this part of our analysis, we used only the simulated data; consequently, no special operations at the well were required.

The new estimation method was implemented in a code operational data analysis (ODA). This code incorporates a special curve-fitting procedure, which we designed to significantly simplify the problem and reduce the amount of computations. The code has a user-friendly interface, and a beta version of it is available for testing and evaluation.

SIGNIFICANCE OF FINDINGS

We have demonstrated that accounting for pumping that occurred before the test may be important even in a traditional well-test analysis. Our method produces results that are stable with respect to variations in the selection of specific test periods and also yields more accurate estimates of the aquifer's hydrological parameters. Moreover, our approach requires a shorter test time interval and less frequent measurements during this interval. Estimation of the initial aquifer pressure and effective radius of influence does not require any field operation and does not impose any additional cost.

RELATED PUBLICATIONS

Silin, D.B., and C.-F. Tsang, Estimation of formation hydraulic properties accounting for pre-test injection or production operations, Journal of Hydrology, 2001 (submitted).

Silin, D.B., and C.-F. Tsang. Estimation of formation hydraulic properties from analysis of regular operations data, SPE 68780, 2001.

ACKNOWLEDGMENTS

This research has been supported by the U.S. Environmental Protection Agency, Office of Ground Water and Drinking Water, Underground Injection Control Program, under an Interagency Agreement with the U.S. Department of Energy under Contract No. DE-AC03-76SF00098.

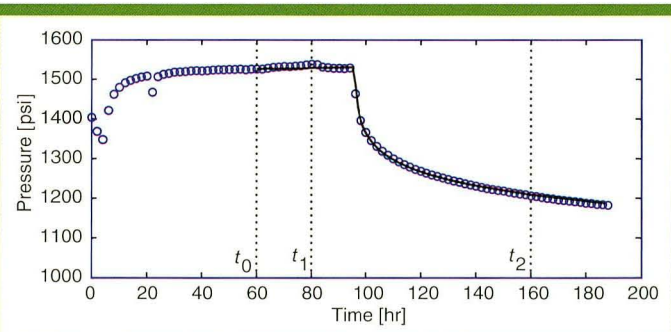

Figure 1. Well-test data matching, including the effect of injection prior to the test. The data points are plotted as circles; the solid line is the fitting curve produced by ODA.

FAST FLOW IN UNSATURATED COARSE SEDIMENTS

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OBJECTIVES

Some highly contaminated unsaturated sediments contain substantial fractions of coarse sands and gravels. Very coarse-textured (>1 mm grain-size) media can sustain high flow rates at relatively low saturations, doing so by film flow rather than by flow through an interconnected network of saturated pores. Thus, the physics of fast-flow processes in unsaturated, very coarse media is fundamentally different from that traditionally recognized in finer textured sediments (Figure 1). Our objectives are (1) to quantify the macroscopic hydraulic properties of very-coarse-textured sediments in the near-zero (–5 to 0 kPa) matric potential region and (2) to determine the microscale basis for fast unsaturated flow.

APPROACHES

Studies are being conducted to quantify macroscopic and microscopic (grain-film scale) hydraulic properties and processes in coarse sands and gravels. To obtain results that are directly relevant to the DOE, most of our efforts focus on sediments from the Hanford Site (Hanford formation, with grain-sizes ranging from 0.1 to 50 mm). Additional tests are being done on quartz and tuff gravels. The 0 to –5 kPa region is a difficult energy range to study because of extreme changes in saturation and conductance that take place in coarser-textured media. We have developed new methods for bulk measurements of unsaturated potential-saturation-conductance relations on coarse sediments. These methods are variations on suction-plate equilibration, unit-gradient infiltration, and steady-flux techniques. Other methods (pressure- plate and vapor-pressure equilibration) are used on the same sediments to characterize potential-saturation-conductance relations over the full range of environmentally relevant conditions.

ACCOMPLISHMENTS

The experiments on macroscopic hydraulic characteristics focus on the near-zero matric potential range where gravel pores are drained. This energy range was identified from capillary drainage calculations and from measured saturations. Under conditions of drained pores, the measured unsaturated hydraulic conductivity is film-controlled. Moisture characteristics (matric potential versus saturation) and unsaturated hydraulic conductivities are being obtained on Hanford formation gravels at the column scale. These column-scale hydraulic properties are being compared with grain-film hydraulic properties to explain macroscale flow and transport through tested microscale concepts. Initial experiments on film hydraulic properties have been completed, with results similar to those obtained in our previous work on transient film flow (Tokunaga et al., 2000). Tests at very negative matric potentials show that the Hanford gravels have substantial intragranular porosity and surface area.

SIGNIFICANCE OF FINDINGS

Our analyses of unsaturated flow in coarse sediments are showing that at near-zero matric potentials, fast film flow is possible. Magnitudes of fast, unsaturated flow in gravels at near-zero matric potentials are consistent with direct measurements of film hydraulic properties. Findings of high intragranular porosity and surface area are important for understanding contaminant transport at Hanford.

RELATED PUBLICATIONS

Tokunaga, T.K., J. Wan, and S.R. Sutton, Transient film flow on rough fracture surfaces, Water Resour. Res. 36, 1737–1746, 2000.

Tokunaga, T.K., and J. Wan, Approximate boundaries between different flow regimes in fractured rocks. Water Resour. Res., 2001 (in press).

ACKNOWLEDGMENTS

This study is funded by the Assistant Secretary of the Office of Environmental Management, Office of Science and Technology, under U.S. Department of Energy (DOE) Contract No. DE-AC03-76SF0098. We thank Andrew Mei and Robert Conners of Berkeley for technical support and John Zachara, Robert Lenhard, Steve Smith, and Bruce Bjornstad of Pacific Northwest National Laboratory for samples of Hanford formation sediment. We thank the DOE, Office of Science, Office of Basic Energy Sciences, Division of Chemical Sciences, Geosciences, and Biosciences for support of our related studies on unsaturated flow in fractured rock.

DIFFUSION-LIMITED BIOTRANSFORMATION OF METAL CONTAMINANTS IN SOIL AGGREGATES: CHROMIUM

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OBJECTIVES

Understanding transport and reactions of metal contaminants (such as chromium [Cr]) in soils is complicated by small-scale variations in physical, chemical, and microbiological characteristics. The fate of elements with redox-dependent solubilities can be complex because strong redox potential gradients can develop over very short distances. In nature, Cr exists in the III and VI oxidation states, with the majority of the former species being stable solids and the majority of the latter being more soluble and mobile. Transport and reactions of chromium in soils are critical concerns because of the carcinogenic effects of Cr(VI). Chromium reduction rates reflect interdependent influences of physical, geochemical, and microbial processes. In this study, this interdependence is examined for Cr(VI) contamination of soil aggregates (cohesive structural units comprised of many primary mineral particles).

APPROACH

Possible Cr redox zonation during contamination of large (90 to 150 mm diameter) soil aggregates was tested. Solutions containing up to 800 ppm carbon as tryptic soy broth were used to wet these soil aggregates. Following 17 days of incubation, these aggregates were exposed to Cr(VI) solutions (1,000 ppm initial Cr) for three days, representing an episodic contamination event (Figure 1a). Aggregates were then either frozen or incubated for an additional 31 days (room T), resin-fixed, cut to obtain cross sections (Figure 1b), and scanned for mapping Cr distributions (using an X26A x-ray microphobe at the National Synchrotron Light Source, Brookhaven National Laboratory). Another set of aggregates was cored to characterize profiles of microbial communities (through phospholipid fatty acid analyses, enzyme analyses, and measurement of microorganism density and activity).

ACCOMPLISHMENTS

Aggregates with higher available organic carbon took up higher amounts of Cr(VI), and reductively precipitated Cr(III) within shorter distances (Figure 1c). Micro x-ray absorption spectroscopy showed that transported Cr was largely reduced to Cr(III), with only 23, 11, and 4% remaining as Cr(VI) in the +0, +80, and +800 ppm organic carbon systems, respectively. Chromium diffused into 100%, 80%, and 50% of the available soil volume in the aggregates with 0, +80 ppm, and +800 ppm organic carbon, respectively. Chromium concentrations increased by 212, 406, and 1,350 ppm Cr, in the contaminated regions of the 0, +80 ppm, and +800 ppm organic carbon aggregates, respectively.

SIGNIFICANCE OF FINDINGS

These results show the importance of intra-aggregate spatial relations for redox-sensitive contaminants as well as for the microbial communities responsible for redox gradients and reductants. Similar stratification of redox potentials, metal contaminants, and microbial communities might occur within larger sediment blocks deeper in the subsurface. In soils and sediments comprised of aggregates or blocks that support internal redox gradients, bulk characterization of chemical and microbiological conditions does not allow mechanistic understanding of biogeochemical processes controlling the fate and transport of contaminants.

ACKNOWLEDGMENTS

This work has been supported by the Director, Office of Science, Office of Biological and Environmental Research, Environmental Sciences Division, Natural and Accelerated Bioremediation Research Program of the U.S. Department of Energy under Contract No. DE-AC03-76SF0098. Use of the Advanced Photon Source was supported by the U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences.

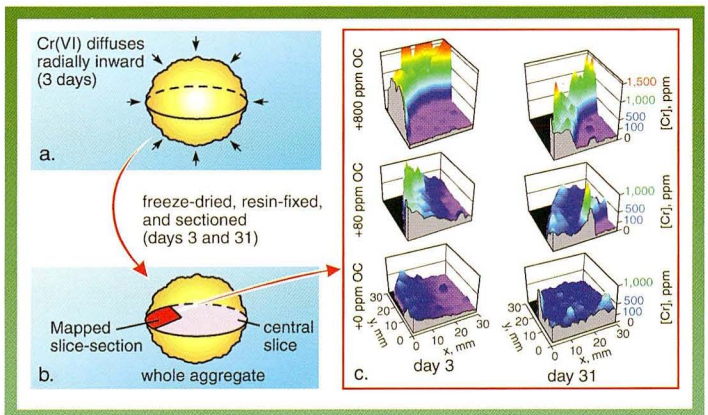

Figure 1. Synchrotron x-ray microprobe maps of total Cr in sections from six soil aggregates. Each aggregate was incubated with either +0, +80, or +800 ppm organic carbon solutions, then exposed to 1,000 ppm Cr(VI) solutions. The black region is outside of the aggregate. The more reducing conditions established in the higher organic carbon aggregates result in a more rapid Cr(VI) reduction at shorter distances, higher diffusion uptake of Cr, and sharply terminated contaminant fronts. Thus, highly contaminated and uncontaminated regions can coexist within aggregates and sediment blocks at contaminated sites.

COLLOID FORMATION DURING LEAKAGE OF HANFORD TANK-WASTE LIQUID INTO UNDERLYING VADOSE ZONE SEDIMENTS

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OBJECTIVES

Leakage of underground tanks containing high-level nuclear waste solutions has been identified at various DOE facilities. The Hanford Site is the main facility of concern, with about 2,300 to 3,400 m^3 of waste liquids leaked. Radionuclides and other contaminants have been found in elevated concentrations in the vadose zone and groundwater underneath single-shell tank farms. We do not yet know the nature of pathways and mechanisms responsible for deep vadose zone contaminant transport, and such understanding is urgently needed for future remediation. It is often speculated that colloid-facilitated contaminant transport is a major mechanism contributing to rapid contaminant migration. Because of the extreme chemical conditions of most of these tank waste solutions (very high pH, aluminum concentration, and ionic strength), understanding interactions between the highly reactive waste solutions and sediments becomes crucial for predicting contaminant migration through the deep vadose zone. The objectives of this research are to identify the key processes occurring at the contaminant reaction front, including reaction products, kinetics, colloid generation, and permeability reduction.

APPROACHES

The process of leaking tank-waste solution interacting with the underlying sediments was simulated through infiltrating simulated redox tank-waste solutions into columns packed with Hanford vadose zone sediments. Since the sediments immediately underlying some single-shell tanks experience elevated temperatures from heat released by reactions within tanks, experiments were conducted at elevated (70°C) and room temperatures. Effluents from columns were collected with fraction collectors and analyzed for turbidity, pH, and chemical composition. Secondary colloids collected from effluents were characterized for their major elements using an electron microprobe, and mineralogy was determined by x-ray diffraction. The morphology of the particles was studied using a scanning electron microscope. Changes in major elemental composition within the sediment columns were measured using x-ray fluorescence.

ACCOMPLISHMENTS

A large quantity of secondary colloids formed because of the waste solution and sediment interactions. The secondary colloids formed at different infiltration stages (see Figure 1) possess different chemical composition and mineralogy. At the moving front of the tank waste plume, amorphous silica, calcite, and bayerite are the major phases. Within the waste plume stage, zeolite minerals are dominant. During the dilution stage, bayerite is abundant. The majority of precipitates collected from effluents were submicron to micrometer sized. Maximum particle formation occurred at the leading edge of the waste plume, owing to maximum geochemical disequilibrium. Maximum transport of the secondary colloids also occurred at the leading edge, when and where pores have not yet been plugged by particle production and new colloids have not yet attached to primary grain surfaces.

SIGNIFICANCE OF FINDINGS

Our laboratory studies revealed the complex processes of reaction-dependent colloid generation/release, permeability change, and flow pathway alteration that can strongly influence flow and transport of redox tank contaminants in the Hanford vadose zone. In comparison to the large quantity of secondary colloids, the inventory of indigenous colloids is often small. Evaluating their carrying capacity of contaminants, degree of release, and transport is a critical issue for understanding highly sorptive contaminant transport at Hanford and other sites.

ACKNOWLEDGMENTS

This work is funded by the Assistant Secretary of the Office Environmental Management, Office of Science and Technology of the U.S. Department of Energy, under contract No. DE-AC03-76SF-00098.

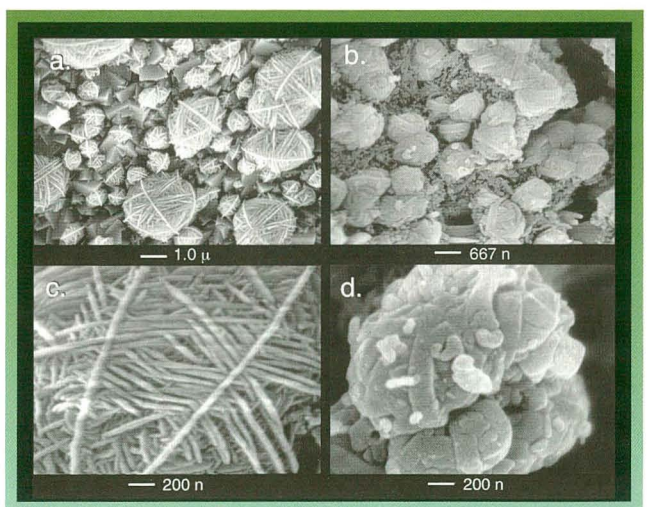

Figure 1. Single crystals of zeolites, cancrinite type, $Na_8(Al_6Si_6O_{24})(NO_3)_2 \cdot 4H_2O$, formed during the waste-plume stage.

LAND DISPOSAL OF SELENIFEROUS SEDIMENTS: A PILOT-SCALE TEST

Peter T. Zawislanski, Sally M. Benson, Robert TerBerg, and Sharon E. Borglin
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RESEARCH OBJECTIVES

A pilot-scale land disposal test for selenium (Se) enriched sediment is being conducted in the San Joaquin Valley, California. Agricultural drain water from surrounding areas in the Grasslands Water District is channelled via the San Luis Drain (SLD) toward the San Francisco Bay Delta. The drain water carries with it and subsequently deposits Se-rich sediments, which are further Se-enriched through biogeochemical processes. The need to periodically dredge and remove the sediments has prompted research into alternative means of disposal. Berkeley Lab's Earth Sciences Division, in collaboration with the U.S. Bureau of Reclamation and local water districts, is conducting pilot-scale tests on the viability of low-cost land disposal of the sediments.

To assess the long-term environmental safety of SLD-sediment land disposal, Berkeley Lab researchers are working to answer the following specific questions:

- Under the given geological conditions, will Se move downward in the soil profile and result in groundwater contamination?
- Will Se remain geochemically stable under surface conditions, such that its solubility and mobility do not significantly increase over time?
- To what degree will Se be taken up by plants?
- Will increased Se levels in soil reduce crop yields?

APPROACH

Two field experiments are currently underway. In one experiment, 10 cm of dredged sediments from the SLD were applied to the adjacent embankment. In the second experiment, 10 cm of sediments were placed on top of, and blended with, 75 cm of agricultural soils in a nearby cultivated farm plot. Soils and sediments down to the shallow water table were sampled once before application and several times afterwards. Surface soils were fractionated with respect to Se using a sequential extraction procedure as well as x-ray spectroscopy. Soil water and groundwater were periodically sampled and moisture conditions were measured. Plants were identified, sampled, and analyzed for Se. In the farm plot, planted cotton was sampled and analyzed at different stages, including at harvest, when biomass was measured.

ACCOMPLISHMENTS

Selenium in the applied sediment has been relatively geochemically stable. Although slow oxidation of the Se pool has occurred, the majority (>90%) is in insoluble forms, dominated by elemental Se and organo-Se. Because of the low permeability of underlying sediments, particularly in the embankment plots, concentrations of dissolved Se in the sediment profile and groundwater remain at background levels (Figure 1). As a result of tillage and irrigation, subsurface Se concentrations in the farm plots are higher, but in neither case was a significant effect on groundwater observed. Analysis of plants from the embankment plots has not shown Se enrichment, with plant-tissue Se around 1μg g-1. In the farm plots, cotton yields were comparable to the control area, despite enrichment with Se to values ranging from 5 to 20 $\mu g\ g^{-1}$, relative to the background value of 1$\mu g\ g^{-1}$.

SIGNIFICANCE OF FINDINGS

The findings of this study support the use of land disposal for Se-enriched sediments in the San Luis Drain. Long-term Se leaching will be limited by slow Se oxidation and the low permeability of underlying sediments. Plant uptake of Se on the embankment appears negligible. Uptake of Se by cotton plants did not affect cotton productivity or quality.

RELATED PUBLICATION

Zawislanski, P.T., S.M. Benson, R. TerBerg, and S.E. Borglin., Land disposal of San Luis Drain sediments, Progress Report, October 1998–November 2000, Berkeley Lab Report LBNL-47861, 2001.

ACKNOWLEDGMENTS

This work was supported by the U.S. Bureau of Reclamation, under U.S. Department of Interior Interagency Agreement 99AA200176, through U.S. Department of Energy Contract No. DE-AC03-76SF00098.

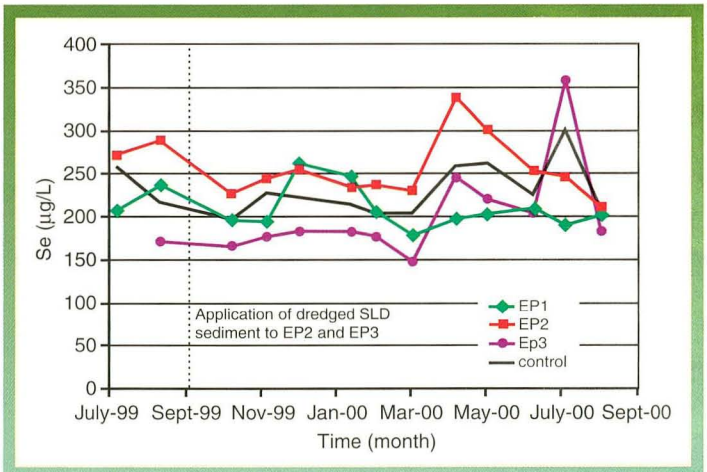

Figure 1. Selenium in groundwater underlying the embankment plot. Aside from small seasonal fluctuations, no changes in Se concentrations were observed relative to the control wells.

RESEARCH PROGRAM

Climate Variability and Carbon Management

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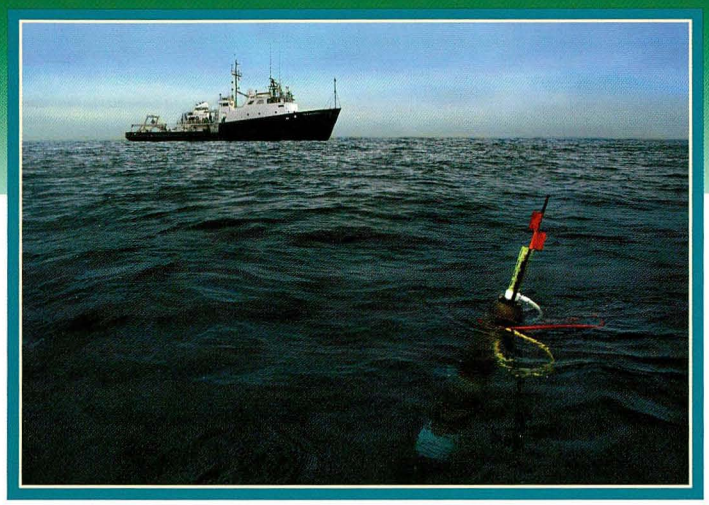

Climate variability and carbon management research is a new and fast-growing program in the Earth Sciences Division. It contains research programs and DOE centers focusing on regional climate and hydrology, and the biogeochemistry and carbon sequestration of geologic, oceanic, and terrestrial systems. Over the past four years, we have added new staff with expertise in global- and regional-scale climate modeling, ecosystem modeling, marine geochemistry, and the carbon and water cycles to provide a strong scientific foundation for addressing concerns related to carbon emissions and climate variability.

We have also expanded the research focus of our existing staff to include issues related to deciphering the isotopic composition of ice cores, developing methods for modeling production of methane from hydrate formations, geophysical monitoring of underground CO_2 injection, and predicting the reactivity of CO_2 in deep geologic formations. Central to making an important scientific contribution in these important areas is a strong link to the Center for Atmospheric Sciences at UC Berkeley.

Last year, we made progress on several initiatives, including NASA/RESAC (California Water Resources Research and Applications Center) and DOCS (the DOE Ocean Carbon Sequestration Center). In addition, we have new initiatives: the GEO-SEQ project for geologic sequestration of CO_2 and the ARM Carbon project, which involves adding carbon and water-cycle monitoring to DOE's Atmospheric and Radiation Measurements Program (ARM).

Berkeley Lab's RESAC team has continued to produce Regional Climate System Model (RCSM) short-term weather and stream-flow predictions, seasonal climate and stream flow predictions, long-term climate variability and impact assessments, and model evaluations. The team has maintained a two-way flow of information between RESAC and users, has become a member of the Earth Science Information Partnership as an ESIP 2, contributed to the 2000 Intergovernmental Panel on Climate Change (IPCC) and the U.S. National Assessment, and participated in numerous outreach activities. In addition to RESAC activities, climate variability scientists have also completed a number of water-quality and sediment-related research projects .

One of the strengths of the Climate Variability and Carbon Management Program is its active partnerships with researchers in universities, industry, and other research laboratories. As a DOE Center and Berkeley Lab research enterprise, the ocean research group links with Scripps Institution of Oceanography, Massachusetts Institute of Technology, Stanford University, UC Irvine, WETLabs Inc., Moss Landing Marine Labs, Monterey Bay Aquarium Research Institute, Rutgers University, and Lawrence Livermore National Laboratory. The Berkeley Lab ocean biogeochemistry group achieved an important scientific breakthrough this year by launching robotic floats that measure organic carbon in the ocean and communicate via satellite telemetry. The DOCS Center (and the ocean biogeochemistry group) will also participate in an advanced iron-fertilization experiment near Antarctica in late 2001/early 2002.

The GEO-SEQ project is a public-private partnership to develop the information and technology needed for CO_2 geologic sequestration by 2015. Partners include Lawrence Livermore and Oak Ridge National Laboratories, Stanford University, Texas Bureau of Economic Geology, the Alberta Research Council, the U.S. Geological Survey, and five private partners: BP, Chevron, Pan Canadian Resources, Texaco, and Statoil. This wide set of partners is essential for the project to achieve its highly applied goals. GEO-SEQ will develop methods to co-optimize value-added sequestration, procedures for lowering the cost of sequestration, monitoring technologies for oil, gas, brine, and coal formations, and the methodology and information for assessing capacity and predicting performance of these formations.

The carbon cycling and terrestrial biogeochemistry group has collaborated with universities and research institutes in progressing on three main fronts: impacts of climate change and land use, sequestration, and modeling ecosystem-atmosphere interactions. The ARM Carbon project has installed a suite of instrumentation in the Southern Great Plains (SGP), making it

(when complete) the first site in the world to have carbon and carbon-isotope monitoring simultaneously from fields, tall tower, and regular plane flights. The project is dovetailed with the ARM-based Water Cycle Initiative Pilot. The water-cycle pilot is using an integration of modeling, field measurements, and specialized isotopic measurements to improve our ability to predict and budget water cycling in the SGP.

The Climate Variability and Carbon Management Program's research areas are highly relevant to current and emerging policy issues, such as climate change and carbon sequestration, and contribute to many agency missions and initiatives. This has been a very productive year for research and program-building, and we believe that this area will continue to grow into one of ESD's major research activities in the years and decades to come.

FUNDING

Climate Variability and Carbon Management Program research is funded by the U.S. Department of Energy's Office of Basic Energy Sciences, Office of Fossil Energy, Office of Geological and Environmental Research, Office of Biological and Environmental Research; the U.S. Department of Commerce, National Oceanic and Atmospheric Administration; the National Aeronautics and Space Administration; the National Science Foundation; and the Office of Naval Research.

THE GEO-SEQ PROJECT

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RESEARCH OBJECTIVES

The GEO-SEQ Project is a public-private applied R&D partnership, founded with the goal of developing the technology and information needed to enable safe and cost-effective geologic sequestration of CO_2 by the year 2015. The goals of the project are to:

- Lower the cost of geologic sequestration by (1) developing innovative optimization methods for sequestration technologies, with collateral economic benefits such as enhanced oil recovery (EOR), enhanced gas recovery (EGR), and enhanced coalbed methane production, and (2) understanding and optimizing trade-offs between CO_2 separation and capture costs, compression and transportation costs, and geologic-sequestration alternatives.
- Lower the risk of geologic sequestration by (1) providing the information needed to select sites for safe and effective sequestration, (2) increasing confidence in the effectiveness and safety of sequestration by identifying and demonstrating cost-effective monitoring technologies, and (3) improving performance-assessment methods to predict and verify that long-term sequestration practices are safe, effective, and do not introduce any unintended environmental impact.
- Decrease the time to implementation by (1) pursuing early opportunities for pilot tests with our private sector partners and (2) gaining public acceptance.

APPROACH

The GEO-SEQ Project consists of four coordinated and interrelated tasks carried out by a multidisciplinary team from eight research organizations: Berkeley Lab (Sally Benson, Larry Myer, Curt Oldenburg, Karsten Pruess, Mike Hoversten, Ernie Majer, Chin-Fu Tsang, Christine Doughty); Lawrence Livermore National Laboratory (Kevin Krauss, Jim Johnson, Carl Steefel, Robin Newmark); Oak Ridge National Laboratory (David Cole, Gerry Moline, Katherine Yuracho); Stanford University (Franklin Orr, Anthony Kovscek); Texas Bureau of Economic Geology (Susan Hovocks, Paul Knox, and T. Trembly); U.S. Geological Survey (Robert Burress); Alberta Research Council (Bill Gunter, David Low); and NITG-TNN, The Netherlands (Bert van der Meer).

The research is conducted with the participation, advice, and cooperation of DOE's National Energy Technology Laboratory and five industry partners: Chevron, Texaco, Pan Canadian Resources, British Petroleum, and Statoil. In addition, through ongoing collaborations and our advisory committee, the team extends to include other universities and a number of public and private research organizations.

ACCOMPLISHMENTS

Highlights of the research conducted to date include:

- Screening criteria for selection of oil reservoirs that could be candidates for co-optimizing CO_2-EOR and CO_2 sequestration were developed.
- Numerical simulations based on a conceptual model of the Rio Vista Gas Field, in California, suggest that it is feasible to inject CO_2 into depleted natural gas reservoirs to sequester carbon and enhance methane recovery.
- Numerical simulations have been carried out to show changes in mineralogy and porosity in a brine-saturated sandstone formation resulting from injection of impure (i.e., containing SO_2, NO_2, and H_2S) CO_2 waste streams.
- Software tools that combine the output of reservoir simulators with forward and reverse geophysical modeling were demonstrated on a generic conceptual model to show that gravitational, seismic, and crosswell electromagnetic techniques could be used to track CO_2 subsurface migration.
- Field trails of crosswell seismic and EM for monitoring of CO_2 migration were carried out at the Chevron Lost Hills CO_2 EOR pilot.
- Effects of hydrocarbon and clay on isotopic compositions need to be taken into account in using isotopic tracers for monitoring reservoir processes.
- State-of-the-art coalbed methane numerical simulators were compared, using a test model of CO_2 injected into a coal bed from a single well.
- A set of benchmark problems was developed and distributed as a basis for an international comparison study of reservoir simulators for oil, gas, and brine formations.
- An assessment of the capacity for sequestration of all the CO_2 generated from fossil-fuel-fired power plants in California suggests that oil reservoirs, gas fields, and brine formations could be sufficient for both short- and long-term needs.

SIGNIFICANCE OF FINDINGS

The climate of the earth is affected by changes in radiative forcing caused by several sources, including greenhouse gases (CO_2, CH_4, N_2O). Energy production and the burning of fossil fuels are substantially increasing the atmospheric concentrations of CO_2. One of several proposed strategies to reduce atmospheric emissions is to capture CO_2 from fossil-fuel final power plants and sequester it deep underground. Results of the GEO-SEQ Project are providing methods and information to enable safe and cost effective geologic sequestration.

RELATED PUBLICATIONS

Publications of the GEO-SEQ Project, in addition to information about other research being conducted, can be found at http://esd.lbl.gov/GEOSEQ/.

ACKNOWLEDGMENTS

Support for this work was provided by the Assistant Secretary for Fossil Energy, Office of Coal and Power Systems and Office of Natural Gas and Petroleum Technology, through the National Energy Technology Laboratory; and by the Director, Office of Science, Office of Basic Energy Sciences, of the U.S. Department of Energy under Contract No. DE-AC03-76SF00098.

BOREHOLE SEISMIC MONITORING OF CO_2 INJECTION IN A DIATOMITE RESERVOIR

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RESEARCH OBJECTIVES

Geologic sequestration of CO_2 is one method proposed for reducing atmospheric CO_2. Ensuring long-term storage is a component of any sequestration program. Our goal is to demonstrate techniques for seismic imaging of subsurface CO_2 through field testing. These techniques can be used for monitoring geologic sequestration.

APPROACH

Previous studies in carbonate reservoirs have shown that seismic velocity changes are caused by CO_2 injection and that these changes can be spatially mapped using crosswell seismic surveys (Wang et al., 1998). The seismic velocity can change up to 10%, which is easily detectable and mappable with modern crosswell seismic surveys. Clearly, borehole seismic surveys hold great promise for mapping and long-term monitoring of sequestered CO_2.

We are using an oil field (at Lost Hills, California) currently undergoing CO_2 injection as a test site for borehole seismic monitoring. Previous crosswell and single-well seismic studies have shown the ability to detect a single gas-bearing fracture such as the CO_2-filled hydrofracture at Lost Hills (Majer et al., 1997). Berkeley Lab has collected time-lapse borehole seismic data using two observation wells, OB-C1 and OB-C2, before and after CO_2 injection. Two separate crosswell surveys used a piezoelectric source and an orbital vibrator source.

The third survey was a single-well imaging experiment (i.e., source and receivers in the same well) using the piezoelectric source and both the three-component accelerometers and hydrophone sensors. The piezoelectric source generates high-frequency data (>2000 Hz), giving wavelengths of about 1 m. The orbital vibrator source is lower frequency (70–350 Hz), providing a separate scale of investigation (wavelengths of about 6 m).

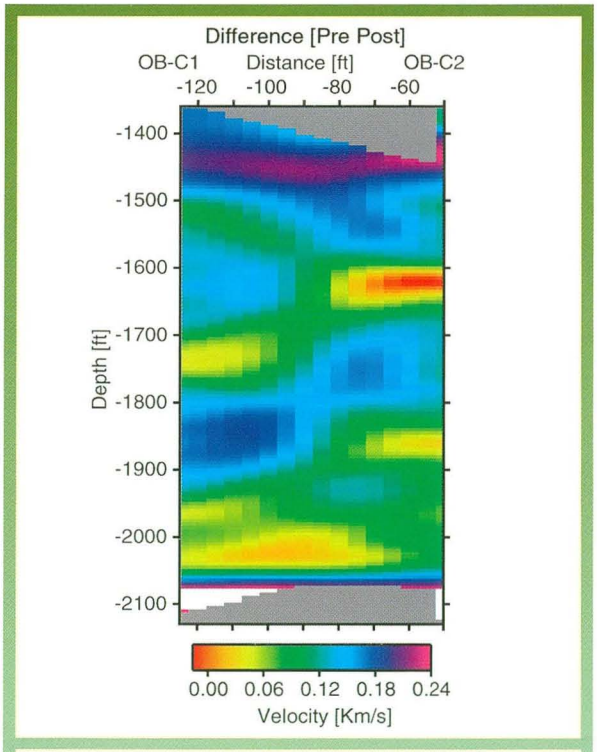

Figure 1. Time-lapse change in seismic velocity as measured by the high-frequency piezoelectric crosswell surveys at the Lost Hills CO_2 injection field site. Regions of large change (blue) indicate a decrease in velocity, indicative of CO_2 in the subsurface.

ACCOMPLISHMENTS

We have acquired three time-lapse data sets—piezoelectric and orbital-vibrator crosswell and piezoelectric single well. We also have acquired postinjection orbital vibrator single-well data as part of a tube-wave suppressor test. Analysis of the high-frequency crosswell shows clear changes in velocity (Figure 1). Analysis of single-well imaging indicates possible reflection imaging of the hydrofracture zone.

SIGNIFICANCE OF FINDINGS

Time-lapse crosswell and single-well methods hold great promise in aiding our understanding of the fundamental rock physics and wave propagation effects that will allow monitoring of CO_2 subsurface sequestration. *In situ* monitoring will likely be a part of any long-term geologic sequestration.

RELATED PUBLICATIONS

Daley, T.M., and D. Cox, Orbital vibrator seismic source for simultaneous P- and S-wave crosswell acquisition, Berkeley Lab Report LBNL-43070, 1999, Geophysics (in press), 2001.

Majer, E.L., J.E. Peterson, T.M. Daley, B. Kaelin, J. Queen, P. D'Onfro, and W. Rizer, Fracture detection using crosswell and single-well surveys, Geophysics 62(2), 495–504, 1997.

Wang, Z., M.E. Cates, and R.T. Langan, Seismic monitoring of a CO_2 flood in a carbonate reservoir: A rock physics study, Geophysics 63, 1604, 1998.

ACKNOWLEDGMENTS

This work was supported by the Assistant Secretary for Fossil Energy, Office of Coal and Power Systems and Office of Natural Gas and Petroleum Technology, through the National Energy Technology Laboratory (NETL), of the U.S. Department of Energy under Contract No. DE-AC03-76SF000098. Data processing was performed at the Center for Computational Seismology, which is supported by the Office of Basic Energy Sciences. Thanks to Mike Morea and Chevron USA Production for field information.

CAPACITY INVESTIGATION OF BRINE-BEARING SANDS FOR GEOLOGIC SEQUESTRATION OF CO_2

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RESEARCH OBJECTIVES

Geologic sequestration of CO_2 in brine-bearing formations has been proposed as a means of reducing the atmospheric load of greenhouse gases. For this procedure to have any meaningful impact on the global carbon cycle, vast quantities of CO_2 must be injected into the subsurface and isolated from the biosphere for hundreds or thousands of years. Numerous brine-bearing formations have been identified as having potential for geologic sequestration of CO_2. The objective of this research is to go beyond identification and do quantitative studies of CO_2 sequestration capacity in realistic geologic settings.

APPROACH

To evaluate CO_2 sequestration capacity, we use the numerical simulator TOUGH2, which considers all flow and transport processes relevant for a two-phase (liquid-gas), three-component (CO_2, water, dissolved NaCl) system. In particular, CO_2 may exist in a gas-like supercritical state or be dissolved in the aqueous phase.

We focus on the Frio formation of the upper Texas Gulf Coast. Key features that make the Frio formation well-suited for geologic sequestration include the existence of many localized CO_2 point sources (power plants, refineries, chemical plants), large volumes of suitable brine formations (unusable as potable water, away from petroleum resources), formations that are well characterized as a result of stratigraphically and structurally analogous petroleum reservoirs, extensive use of the Frio for deep-well injection of hazardous waste, and CO_2 injection technology developed for improved oil recovery that has been tested in analogous Gulf Coast formations.

A three-dimensional numerical model is developed of a 1 km × 1 km × 100 m region of the fluvial-deltaic Frio formation using transition probability geostatistics. Permeability varies by nearly six orders of magnitude in the model, making preferential flow a significant effect.

We define capacity as the volume fraction of the subsurface within a defined stratigraphic interval available for CO_2 sequestration and consider it as the product of four factors: (1) the intrinsic capacity, controlled by multiphase flow and transport phenomena; (2) a geometric capacity factor, controlled by formation geometry; (3) a heterogeneity capacity factor, controlled by geologic variability; and (4) the formation porosity, the fraction of void space within the formation.

ACCOMPLISHMENTS

Numerical simulation results illustrate how CO_2 sequestration capacity depends on a combination of factors, including multiphase flow processes, formation and injection well configuration, geologic heterogeneity, and formation porosity. Capacity also depends on the time in the sequestration process at which it is measured: the capacity obtained when the storage-volume spill point is first reached can be much smaller than the capacity obtained for quasi-steady flow conditions.

SIGNIFICANCE OF FINDINGS

Based on the simulation results, the following factors are favorable for sequestration capacity:

- High intrinsic capacity, which depends on the relative permeability to CO_2 and the viscosity ratio between brine and CO_2
- A high geometric-capacity factor, which depends on the shape of the structure, permeability anisotropy, and the density ratio between brine and CO_2
- A high heterogeneity-capacity factor, noteworthy because preliminary indications suggest that layered-type heterogeneities enhance sequestration capacity by counteracting gravitational forces
- High porosity, which signifies that large pore volume is available for sequestration

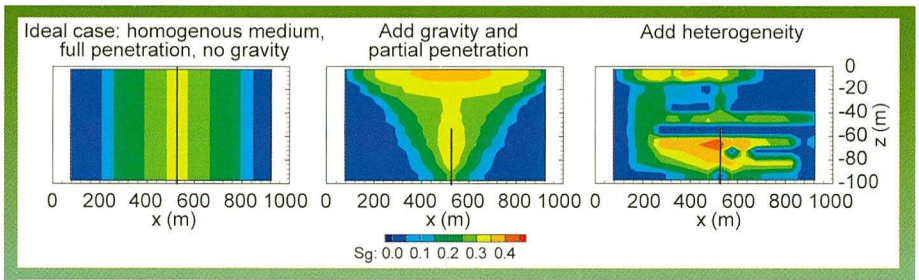

Figure 1. Modeled gas saturation distribution after two years of injection of supercritical CO_2 into a brine-saturated formation for increasingly complex model assumptions. Each frame shows a vertical cross section through the center of the three-dimensional model; the injection well is shown as a black line.

RELATED PUBLICATIONS

Doughty, C., K. Pruess, S.M. Benson, S.D. Hovorka, P.R. Knox, and C.T. Green, Capacity investigation of brine-bearing sands of the Frio Formation for geologic sequestration of CO_2, First National Conference on Carbon Sequestration, May 14–17, Washington DC, National Energy Technology Laboratory, 2001.

Hovorka, S.D., C. Doughty, P.R. Knox, C.T. Green, K. Pruess, and S.M. Benson, Evaluation of brine-bearing sands of the Frio Formation, upper Texas Gulf Coast, for geological sequestration of CO_2, First National Conference on Carbon Sequestration, May 14–17, Washington DC, National Energy Technology Laboratory, 2001.

ACKNOWLEDGMENTS

This work is supported by the Assistant Secretary for Fossil Energy, Office of Coal and Power Systems and Office of Natural Gas and Petroleum Technology, of the U.S. Department of Energy under Contract No. DE-AC03-76SF00098.

CROSSWELL IMAGING AT THE WEYBURN FIELD FOR CO_2 TRACKING

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RESEARCH OBJECTIVES

This work is an integral part of a comprehensive time-lapse seismic-monitoring program for monitoring a massive CO_2 flood in a thin, fractured carbonate reservoir in PanCanadian's Weyburn field, located at Williston Basin in southeast Saskatchewan, Canada. The goals of the project are to deploy technology that could track the detailed changes in CO_2 content as a function of time and to validate the monitoring capability of the surface seismic data (3-C and 9-C 3D) and 3D vertical seismic profiling (VSP), which were collected at the same time.

APPROACH

In September 2000, Pan Canadian started the first phase of an extensive long-term CO_2-miscible injection at its Weyburn field, located at Williston Basin. The flooding project is expected to expand over the field area for many years. To determine the applicability as well as refine the borehole methods, we carried out a comprehensive plan for using geophysical methods for mapping fluid migration and dynamics. In addition to the baseline 3-C 3D VSP and surface-seismic surveys acquired by PanCanadian, Colorado School of Mines Reservoir Characterization Project's (CSM/RCP) on-going efforts in 9-C 3D surface seismic and VSP are being augmented with Berkeley Lab's high- resolution crosswell and Schlumberger's single-well efforts. The higher-resolution borehole data will be integrated with the surface seismic to provide an overall understanding of reservoir definition and the dynamics of fluid migration. The crosswell seismic is intended to provide tomographic images of changes in reservoir properties at a meter scale, or less. When integrated with the surface seismic and VSP, these data will provide the proper scaling relationships for understanding overall flow behavior of the CO_2 fluid at reservoir dimensions. Addressed will be the trade-off between the spatial resolution and the spatial coverage of surface methods and borehole methods, respectively.

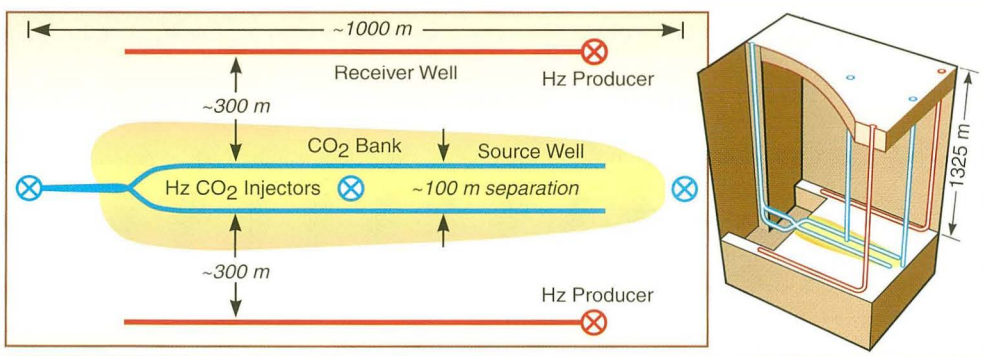

Figure 1. Plan and perspective views of the horizontal wells used in the Weyburn CO_2 monitoring experiment. One producer well was used as the receiver well, and one injector well was used as the sound well.

ACCOMPLISHMENTS

A baseline horizontal crosswell-seismic survey was successfully acquired in August 2000 prior to the injection. To accomplish the goals in a cost-effective manner and within a production-constrained time window, we combined coiled-tubing deployment of a piezoelectric source with a 48-level hydrophone string in two parallel horizontal wells. The raw data recorded exhibit a wave field rich in many useful wave modes, including compressional, shear, and guided waves. A schematic of the geometry is displayed in Figure 1. The acquisition was performed as follows: The source was activated with a sweep of 200 to 2000 Hz every 3 m. After the source was dragged along the horizontal section of the hole, it was pushed back to its starting position for another run. The receiver string was then pulled three meters and the source sweep was repeated. This was done five times, so that a complete crosswell survey at three-meter spacing was accomplished. Overall, we have demonstrated that crosswell tomography is feasible between horizontal wells. With careful repeat acquisition to accommodate potential positioning errors, CO_2 monitoring using velocity differencing should be feasible. Crosswell data will be processed for P- and S-wave images as well as dispersion and amplitude effects. This will be done on a time-lapse basis during the course of the project as the data are collected. To interpret the results, correlations will be made with the injection data to derive migration-path relationships.

ACKNOWLEDGMENTS

The authors gratefully acknowledge OYO Geospace, Tomoseis, TriCan, and PanCanadian for assistance in the acquisition of these data. We wish to thank the IEA Weyburn CO_2 Sequestration Monitoring Research Project, in association with the Petroleum Technology Research Centre, Regina, Saskatchewan, for its financial support.

PILOT STUDY INVESTIGATIONS OF CSEGR

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RESEARCH OBJECTIVES

Carbon sequestration with enhanced gas recovery (CSEGR) is the process whereby CO_2 is separated from fossil-fuel power-plant or industrial-process waste gases, pressurized for transport by pipeline to a depleted gas reservoir, and injected into the depleted gas reservoir to pressurize the reservoir (and sweep CH_4 toward production wells) for enhanced CH_4 recovery. Although enhanced oil recovery by CO_2 injection is an established technology, enhanced gas recovery by CO_2 injection has never been attempted. We are carrying out numerical simulations of injecting CO_2 into depleted natural gas reservoirs for CSEGR as scoping calculations that will guide selection of a gas reservoir suitable for a pilot study of the injection and gas recovery part of CSEGR.

APPROACH

We are using a new TOUGH2 module for simulating gas and water flow and transport in gas reservoirs. The simulator handles five components (water, brine, CO_2, tracer, and CH_4) along with heat and uses the Peng-Robinson equation-of-state model for gas-mixture densities. By Henry's Law, gas species partition between the gas and liquid phases according to their temperature- and pressure-dependent solubilities. We have applied the simulator to investigate pressure response and CO_2 transport in a prototypical depleted gas reservoir of area 3.2 km^2 (800 acres), thickness 20 m, porosity 0.20, and permeability 1 darcy.

ACCOMPLISHMENTS

Figure 1 shows the two-dimensional numerical grid and color contours of CO_2 mass fraction in the gas phase after one year of CO_2 injection, at a total rate of 2 kg s^{-1} (5,740 ton mo^{-1}), into two wells (A1 and ME2). This injection corresponds to a relatively high rate if delivery is by tanker trucks (capacity approximately 50 tons, corresponding to nearly 5 truckloads per day per well). As CO_2 is being injected, CH_4 is being produced equally from wells HJ1, HJ2, and W1 at a total rate of 0.3 kg s^{-1} (41,000 Mcf mo^{-1}). The inset of Figure 1 shows the pressure response in bars and mass fraction CO_2 in ppm in the observation well (ME1). As shown, the injection rate of CO_2 is small relative to the size of the reservoir. Pressure increases, while small, are measurable despite the fact that CH_4 is being produced.

SIGNIFICANCE OF FINDINGS

Simulations of CO_2 injection into a depleted natural gas reservoir, carried out with TOUGH2, demonstrate that reservoir pressure maintenance or pressure increases can be produced by CO_2 injection with minimal contamination on the time scale of one year. This investigation suggests that larger sources of CO_2 (e.g., from an existing pipeline with CO_2 intended for enhanced oil recovery) may be a better prospect for the pilot study than CO_2 supplied by truck on a smaller scale.

RELATED PUBLICATION

Oldenburg, C.M., K. Pruess, and S.M. Benson, Process modeling of CO_2 injection into natural gas reservoirs for carbon sequestration and enhanced gas recovery, Energy & Fuels 15(2), 293–298, Berkeley Lab Report LBNL-45820, 2001.

ACKNOWLEDGMENTS

This work was supported by the Assistant Secretary for Fossil Energy, Office of Coal and Power Systems through the National Energy Technology Laboratory, and by Laboratory Directed Research and Development funds at Berkeley Lab provided by the Director, Office of Science, of the U.S. Department of Energy under Contract No. DE-AC03-76SF00098.

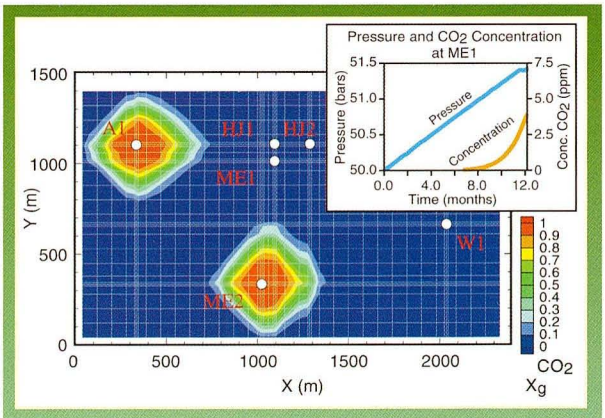

Figure 1. Contours of mass fraction of CO_2 in the gas phase after one year of CO_2 injection with inset showing pressure and concentration increases over time at the observation well ME1. ([CH_4 production is from HJ1, HJ2, and W1]. CH_4 Prod. = 0.3 kg/s = 41,000 Mcf/mo. CO_2 Inj. = 2 kg/s = 5,740 ton/mo.)

AN INTERCOMPARISON STUDY OF SIMULATION MODELS FOR GEOLOGIC SEQUESTRATION OF CO_2

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RESEARCH OBJECTIVES

Mathematical models and numerical simulation tools will play an important role in evaluating the feasibility of CO_2 storage in subsurface reservoirs, such as brine aquifers, producing or depleted oil and gas reservoirs, and coalbeds. We have proposed and initiated a code intercomparison study that aims to explore the capabilities of numerical simulators to accurately and reliably model the important physical and chemical processes that would be taking place in CO_2 disposal systems. The overall objective of the study is to advance and document the state of the art for modeling CO_2 injection into subsurface reservoirs, and to establish credibility for modeling approaches.

APPROACH

Code intercomparison is viewed as an iterative process, progressing from relatively simple and uncoupled test cases to problems that feature comprehensive process descriptions in settings approaching realistic geologic complexity. Key issues that need to be addressed include (1) thermodynamics of sub- and supercritical CO_2 and pressure-volume-temperature properties of mixtures of CO_2 with other fluids, including (saline) water, oil, and natural gas; (2) fluid mechanics of single and multiphase flow when CO_2 is injected into aquifers, oil reservoirs, and natural gas reservoirs; (3) coupled hydro-chemical effects resulting from interactions between CO_2, reservoir fluids, and primary mineral assemblages; (4) coupled hydromechanical effects, such as porosity and permeability change resulting from increased fluid pressures from CO_2 injection; and (5) space and time discretization effects.

We propose to organize and manage the model intercomparison study; facilitate the development and selection of appropriate test problems; distribute them to interested groups of scientists and engineers; and solicit, collect, reconcile, and document solutions. The Internet will be used as a convenient vehicle for organizing this effort. Workshops will be held to discuss results, refine problem definitions, develop new test problems, and agree on future plans and schedules. Participants are expected to use numerical simulation codes available to them and obtain their own funding.

ACCOMPLISHMENTS

A standard format for specification of test problems was developed. A first set of eight test problems has been assembled to initiate the study. The first two problems address issues arising in CO_2-enhanced gas recovery. Problems 3 and 4 deal with CO_2 disposal in saline aquifers. Problem 5 involves a batch chemical-speciation calculation, while Problem 6 explores a coupled hydromechanical process. Problem 7 involves a 2D field-scale aquifer disposal problem, and Problem 8 addresses CO_2 injection into an oil reservoir. Simulation capabilities for CO_2 injection into coalbeds are still in an early stage of development; no coalbed-related test problems are proposed at the present time, but they may be included in future problem sets.

Full problem specifications were mailed to an address list numbering approximately 150 and were also posted on the Web (http://esd.lbl.gov/GEOSEQ/) to be accessible to groups worldwide with relevant expertise and access to simulation tools for geologic sequestration of greenhouse gases.

As of this writing, the following ten groups from six countries have committed to participating: (1) Berkeley Lab (U.S.A.), (2) Stanford University (U.S.A.), (3) Lawrence Livermore National Laboratory (U.S.A.), (4) Los Alamos National Laboratory (U.S.A.), (5) Alberta Research Council (Canada), (6) Industrial Research Ltd. (New Zealand), (7) CSIRO Petroleum (Australia), (8) University of Stuttgart (Germany), (9) Institut Français de Petrol (France), (10) BRGM (Geological Survey of France).

RELATED PUBLICATIONS

Pruess, K, C.F. Tsang, D. H.-S. Law, and C.M. Oldenburg, An intercomparison study of simulation models for geologic sequestration of CO_2, First National Conference on Carbon Sequestration, Washington, DC, May 14–17, 2001.

Pruess, K., C.F. Tsang, D. H.-S. Law, and C.M. Oldenburg, Intercomparison of simulation models for CO_2 disposal in underground storage reservoirs, Berkeley Lab Report LBNL-47353, 2000.

ACKNOWLEDGMENTS

We thank Tianfu Xu, Jonny Rutqvist, Carl Steefel, and Tony Kovscek for contributing test problems. This work was supported by the Assistant Secretary for Fossil Energy, Office of Coal and Power Systems and Office of Gas and Petroleum Technology, through the National Energy Technology Laboratory (NETL) of the U.S. Department of Energy under Contract No. DE-AC03-76SF00098.

THE CALIFORNIA WATER RESOURCES RESEARCH AND APPLICATIONS CENTER

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RESEARCH OBJECTIVES

The California Water Resources Research and Applications Center is designed around a set of integrated activities that focus on issues related to California water resources. Its primary objectives are to advance understanding of California climate and hydrologic variability and change. Core projects include building research partnerships that focus on analysis of (and educational outreach related to) hydroclimate impact on natural systems, society, and infrastructure. The following highlights our approach and results.

APPROACH

The California Water Resources Research and Applications Center uses dynamic and statistical downscaling schemes within our Regional Climate System Model framework. We produce hydroclimate simulations at short-term, seasonal, and long-term time scales for weather and river-flow forecasts, climate change analyses, uncertainty estimates, landslide modeling, water-quality monitoring and forecasting; and climate-change assessments of water resources, agriculture, rural economy, and hazards (see Figure 1).

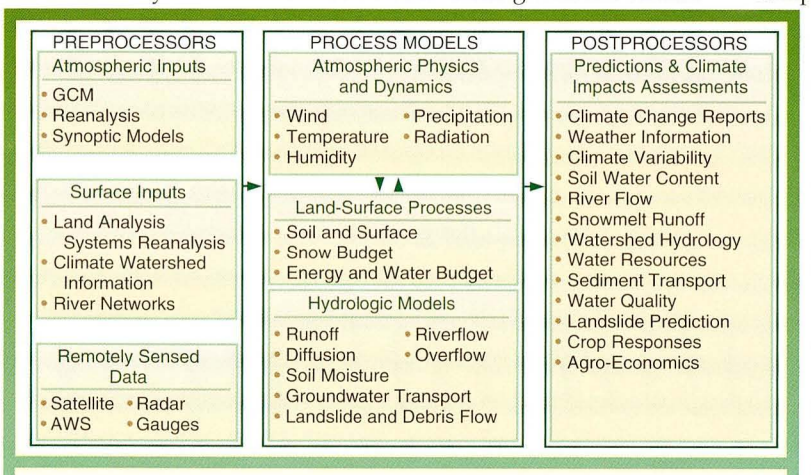

Figure 1. The Regional Climate System Model is composed of process models nested between preprocessed and postprocessed output data. The models are physically based and represent hydroclimate and impacts at a range of scales.

Our applications projects include:

- Runoff contaminant monitoring and real-time management in the San Joaquin Basin with the U.S. Bureau of Reclamation
- Contaminant identification and monitoring from Sierra Foothills mine sites with the University of California Space Sciences Laboratory
- Development of a dynamic sediment-transport and landslide-hazards prediction system with the University of California Earth and Planetary Science Department
- Snow cover area and water equivalent maps for California with University of Arizona
- Geostatistical uncertainty analysis of precipitation and streamflow simulations
- Contributions to impact-assessment reports

ACCOMPLISHMENTS

Our center became a member of the Earth Science Information Partnership, providing value-added climate, weather, streamflow and impact information to the broad user community and the 2000 U.S. National Assessment and the Intergovernmental Panel on climate change reports. We have completed a series of seasonal and multiyear regional climate and streamflow simulations, developed a new statistical downscaling technique for estimating the limits of uncertainty (Kyriakidis et al., 2001), and have used our results as input to the above applications. Recent analysis of 2040 to 2049 projected climate and streamflow analysis has been submitted (Kim et al., 2001, Miller et al., 2001) and received national media coverage.

SIGNIFICANCE OF FINDINGS

The climate change and streamflow analyses indicate that the likelihood of extreme weather events will increase and that nighttime temperature will increase at a faster rate than daytime temperature. The simulated shift in stream peakflow implies an increase in winter and spring high flow (flooding) and a decrease in summer and fall streamflow. We received new support from the California Energy Commission, CALFED, and DOE based on our accomplishments. The California Water Resources Research and Applications Center has become a voice in California climate change assessments, increasing the awareness of potential water resource problems in California and the United States.

RELATED PUBLICATIONS

Kyriakidis, P.C., N.L. Miller, and J. Kim, Uncertainty propagation of regional climate model precipitation forecasts to hydrologic impact assessment, J. Hydrometeorology 2, 140–160, Berkeley Lab Report LBNL-45852, 2001.

Miller, N.L., W.J. Gutowski, J. Kim, and E. Strem, Assessing California streamflow for present day and 2040 to 2049 scenarios, J. Hydrometeorology (submitted), Berkeley Lab Report LBNL-47987, 2001.

ACKNOWLEDGMENTS

Support is provided by the NASA Office of Earth Science/Earth Science Applications Research Program (OES/ESARP) under grant No. NS-2791.

MODELING THE WATER RESOURCE AND ENVIRONMENTAL IMPACTS OF CLIMATE VARIABILITY ON THE SAN JOAQUIN BASIN

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RESEARCH OBJECTIVES

Water-resource planners need to develop contingency plans to deal with the potential effects of global warming and its related impacts on the San Joaquin Basin. The literature suggests that precipitation may be warmer and runoff earlier in the season, reducing the reservoir capture of snowmelt and rainfall runoff under current reservoir operational policy. Research also suggests an increase in the variability of future weather and the incidence of extreme weather events under a global-warming scenario. Mathematical models most useful to analyze the impacts of climate change scenarios on water resources and the environment do not lend themselves to a system-wide impact analysis. Hence, the objective of this research is to develop an integrated modeling system that simulates a broad array of water resource and environmental impacts resulting from a range of future climate scenarios. The goals of this project are to produce a public-domain toolbox, available on CD, that can be readily used by agencies such as the Bureau of Reclamation and the Department of Water Resources; and to analyze the impacts of climate change on water resources and the environment.

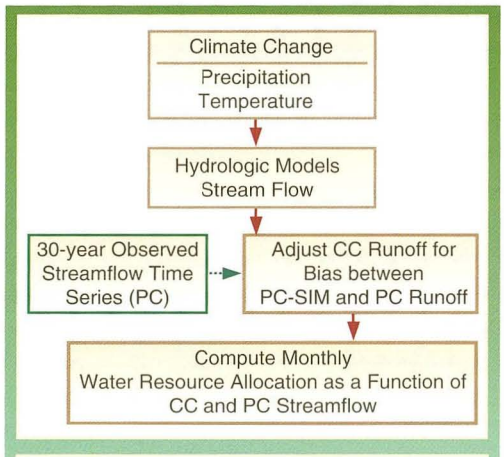

Figure 1. Water-resource allocation is being modeled as a linked set of models within our Regional Climate System Model.

APPROACH

State-of-the-art simulation models have been acquired from the U.S. Bureau of Reclamation, Department of Water Resources, the U.S. Geological Survey, and the University of California. The first phase of the study has involved becoming familiar with the various models and making preliminary runs to validate model codes. The second phase, begun in June 2000, will customize the Modular Modeling System (MMS), a software platform developed by the U.S. Geological Survey, and link the models as a single toolbox postprocess of our Regional Climate System Model (see Figure 1). We are building sets of subroutines for streamflow, water quality, water demand, sediment transport, agro-economics, and related ecosystem response. Once the subroutines are implemented within the MMS toolbox, the thirc phase of the project will be to complete a series of impact analysis runs for the San Joaquin Basin. We will compare climat change scenarios with historic time series to determine th potential impact on the San Joaquin basin.

ACCOMPLISHMENTS

The MMS has been imported and i running on our local workstations, and a training session with U.S. Geologica Survey personnel took place on Jun 19–20, 2000, at Berkeley Lab. A paper ha been prepared on the initial phase of ou research and was presented at th International Society of Environmenta Systems Software conference on June 2 2000, in Austria.

SIGNIFICANCE OF FINDINGS

Model integration has become a topi of great importance to land and water resource agencies, owing to the increasing complexity of water-resource and environ mental-management problems. Berkeley Lab is uniquely qualified to assist in this area of applie research.

RELATED PUBLICATION

Quinn, N.W.T, N.L. Miller, J.A. Dracup, L. Brekke, an L.F.Grober, An integrated modeling system for environ mental impact analysis of climate variability and extrem weather events in the San Joaquin Basin, California Environmental Software Systems, Environmenta Information and Decision Support, IFIP TC5 WG5.11, 3r International Workshop on Environmental Software System (ISESS 2000), Zell Am See, Austria, May 28–June 4, 2000.

ACKNOWLEDGMENTS

This research is supported by the NASA Office of Earth Science/Interdisciplinary Studies (OES)/IDS) Grant No. NS729 and the EPA STAR Grant No. 99-NCERQA-GI.

APPLICATIONS OF REMOTELY SENSED DATA FOR SEASONAL CLIMATE PREDICTIONS IN EAST ASIA AND SOUTHWEST UNITED STATES

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RESEARCH OBJECTIVES

The objectives of this study are to improve seasonal-to-interannual climate prediction by incorporating remotely sensed land-surface data into more realistic starting values for land-surface models. The improved climate predictions will provide input forcing to water resources, river flow, and agricultural productivity models, with climate variability represented. The modeling framework, methodology, and data obtained in this study will be applied toward advancing seasonal and interannual regional climate predictions and climate impact assessments for East Asia and Southwest United States.

APPROACH

We have generated improved land-surface data for snow-cover, soil moisture content, and vegetation by combining satellite-observed and station data in collaboration with the University of Arizona, NASA Data Centers, and East Asia institutions. Satellite data to be used includes NASA's Earth Observing System/Moderate Resolution Imaging Spectroradiometer, the National Oceanic and Atmospheric Administration's (NOAA) Advanced Very High Resolution Radiometer for snow cover and vegetation characteristics, and the Advanced Microwave Scanning Radiometer for soil moisture. Improved land-surface data is then used to initialize the Soil-Plant-Snow (SPS) model as coupled with the Mesoscale Atmospheric Simulation (MAS) model for dynamic downscaling. The SPS will be modified to examine the effects of different interpretations of satellite-observed surface data. The coupled MAS-SPS will be used to investigate the effects of improved land-surface data on regional simulations for seasonal and interannual time scales (see Figure 1). Predicted atmospheric data will be used to predict streamflow and agricultural production.

ACCOMPLISHMENTS

This new NASA IDS (Interdisciplinary Studies) project began in March 2000 and is a follow-on from our previous NASA IDS precipitation and streamflow hindcast project. Our preliminary investigation is focused on an evaluation of our Regional Climate System Model and the generation of data sets for this study. We have investigated the accuracy of the system and the large-scale forcing data. Simulations for the 1998 and 1999 East Asia monsoon season have been completed, using the large-scale analysis data sets from NOAA and the Korean Meteorological Agency. Additionally, an eight-year simulation for the western U.S has been completed and is being studied for the effects of vertically varying root density on warm-season regional climate. Fine-scale global vegetation data sets are being analyzed and processed to generate surface-vegetation-characteristic data for the SPS. We are also obtaining hydrologic data for several basins in China and Korea for streamflow research.

SIGNIFICANCE OF FINDINGS

We found a significant difference in the location and intensity of East Asian monsoon rain bands simulated with the two different large-scale data sets. We have completed a multiyear simulation of basin-scale precipitation and streamflow resulting in fair to good predictability of the mean monthly streamflow (Miller et al. 2001). These results imply a potential for dynamic downscaling applications related to water resources and agriculture in this region.

RELATED PUBLICATION

Miller, N., J. Kim, and J. Zhang, Coupled precipitation and streamflow simulations at the GAME/HUBEX site: Xixian Basin, J. Japan. Meteorol. Soc., 2001 (in press).

ACKNOWLEDGMENTS

This work is supported by the NASA Office of Earth Science/Interdisciplinary Studies (OES/IDS) under Grant No. MDAR-0171-0368.

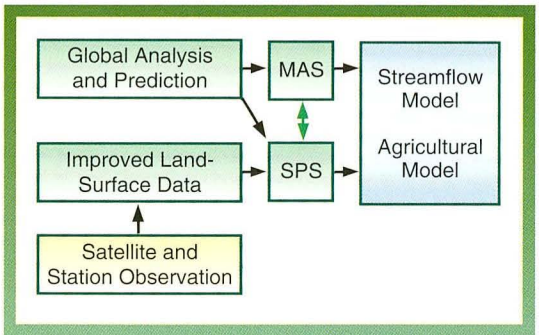

Figure 1. An outline of the regional-climate-prediction experiment in this study. Black arrows indicate one-way data flow; the green arrows indicate interactive coupling.

THE DOE WATER CYCLE INITIATIVE PILOT: MODELING AND ANALYSIS OF SEASONAL AND EVENT VARIABILITY AT THE WALNUT RIVER WATERSHED

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RESEARCH OBJECTIVES

The DOE Water Cycle Initiative pilot is designed to use isotopic measurements of water (deuterium and $\delta^{18}O$) to constrain hydroclimate models, assimilate remotely sensed data into hydroclimate models, and test process descriptions and sensitivities at multiple scales-to better understand water cycle variability. The primary research objectives are to (1) evaluate predictions of Walnut River water-budget components, using a set of nested models having different spatial resolutions with archived and new field data; (2) evaluate water-isotope modeling as a means of tracing sources and sinks; and (3) identify water-budget-model improvements and data needs.

APPROACH

Our approach consists of three main tasks: database development, model advancements, and simulations/evaluation. The first task, Berkeley Lab's primary database activity, involves building a comprehensive set of isotopic data for all components of the water cycle. The second task is the advancement of our Regional Climate System Model (RCSM) to include water-isotope mass-conservation equations and introduce data assimilation to the land-surface and hydrology model (see Figure 1). A generic isotope cloud-physics and diffusion scheme is being developed. This will be upgraded as available measurements provide more realistic rate values that take into account in-cloud evaporation, condensation, autoconversion, and accretion, and are implemented into the RCSM. An initial set of deuterium and $\delta^{18}O$ parameterizations for surface and subsurface water transport will be implemented to our hydrology model. Isotopic validation will be based on precipitation and stream-sampling data. Data assimilation will focus on testing a nudging scheme for forcing prognostic equations related to soil moisture and snow cover area, using remotely sensed data products.

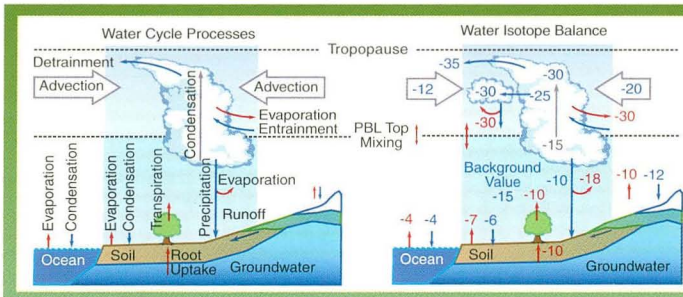

Figure 1. Understanding the water cycle processes at Walnut River Watershed requires atmospheric-land surface-hydrologic models that adequately simulate moisture advection, evapotranspiration, precipitation, runoff, groundwater transport, etc. To trace the water cycle, we are including water-isotope mass-conservation estimates and measurements of hydrologic processes.

The third task is a synthesis of the first two tasks combined with model simulations and evaluation. Berkeley Lab will be responsible for isotopic analysis of all water samples collected during the pilot study. We will use the resulting water-isotope data for model parameterization and prediction studies. Satellite-derived data will be evaluated independently, with surface observations and model simulations. Multiscale Berkeley Lab RCSM simulations at 36 km, 12 km, and 4 km will determine the spatial scales for realistic precipitation and soil moisture distributions. Tests of the RCSM, which including land-surface hydrology models with water isotopes, will yield information toward reducing uncertainties in predictability.

ACCOMPLISHMENTS

During the start-up period, we have accessed most of the land-surface characterization data and some historical time series of weather variables. We have completed an initial water-budget simulation for a single station in the Whitewater Watershed (using our land-surface and streamflow water- and energy-budget model) and performed dynamic atmospheric downscaling over the United States, nested to 12 km using the MM5 model. Water-isotope collection is being prepared for this year's wet season at the Walnut Watershed. Finally, based on literature studies (Gedzelman and Arnold, 1994; Hendricks et al., 2000) and communication with Global Climate Model (GCM) water-isotope modelers (D. Noone, personal communication), we have begun to evaluate the procedure for simulating water isotopes in mesoscale atmospheric models forced by GCMs.

SIGNIFICANCE OF FINDINGS

The significant aspect of this work, in addition to simulating hydrologic closure, is the generation of a mesoscale water-isotope map for the continental United States. These resulting atmospheric deuterium and $\delta^{18}O$ distributions will help to answer a number of paleoclimate questions. The DOE Water Cycle Initiative pilot is the precursor to the DOE Water Cycle Dynamics and Prediction Program that was initiated in January 2001 by a team primarily composed of hydrologists and meteorologists. Now under review, it may become the 2003 phase of this water cycle initiative pilot.

RELATED PUBLICATIONS

Gedzelman, S.D., and R. Arnold, Modeling the isotope composition of precipitation, JGR 99, 10455–10471, 1994.

Hendricks, M.B., D.J. DePaolo, and R.C. Cohen, Space and time variation of delta O-18 and delta D in precipitation: Can paleotemperature be estimated from ice cores? Global Biogeochemical Cycles, 14, 851–861, 2000.

ACKNOWLEDGMENTS

This work is supported by the Director, Office of Science, Office of Biological and Environmental Research, the Water Cycle Initiative Pilot, under U.S. Department of Energy Contract No. DE-AC03-76SF00098.

CARBON MONITORING AT THE ARM SOUTHERN GREAT PLAINS SITE

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RESEARCH OBJECTIVES

Current challenges in carbon cycle research include bridging plot-scale measurements with regional- and global-scale models, and linking the fluxes of carbon, water, and energy from heterogeneous natural and managed ecosystems. To address these challenges, we are developing a carbon-monitoring program at DOE's Southern Great Plains (SGP) Atmospheric Radiation Measurement (ARM) Cloud and Radiation Testbed (CART) site. This site is ideal for carbon cycle research because of ARM's comprehensive atmospheric measurements, simple topography, and the region's mixture of land uses.

APPROACH

We are performing the bulk of our work near the ARM Central Facility (CF) located in north-central Oklahoma. The land use in the region consists of crops (dominated by wheat), pasture, and native tallgrass prairie. To better understand the complex land-surface carbon exchange, we are building and deploying (1) three portable eddy covariance towers for CO_2 and energy fluxes, (2) a precise CO_2 measurement system at the CF 60 m tower, (3) an eddy covariance system at the CF 60 m tower, and (4) an isotope sample collection system for the CF and portable towers. Simultaneous measurements from the three 4.5 m portable towers will be used to characterize the heterogeneous ecosystem sources impacting concentrations and fluxes at the CF tower. We are also applying established models (SiB2 and LSM1.0) to simulate CO_2 and energy fluxes, and developing new methodologies to simulate $H_2{}^{18}O$, $C^{18}OO$, and $^{13}CO_2$ fluxes. Improved understanding of ^{13}C and ^{18}O fluxes from ecosystems will allow us to more accurately partition net ecosystem exchange into respiration and photosynthetic uptake, thereby improving our ability to predict ecosystem behavior under changing environmental conditions.

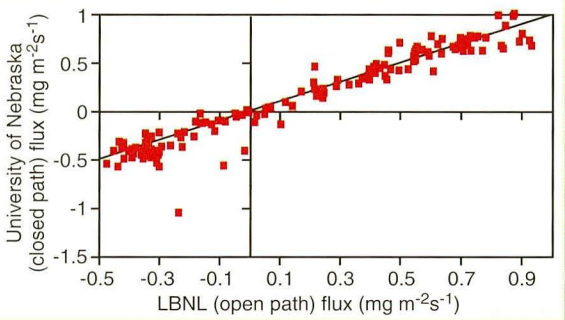

Figure 1. Cross calibration of Berkeley Lab-ARM system at the Ameriflux tallgrass prairie site in Oklahoma.

ACCOMPLISHMENTS

The portable eddy covariance system compared well in a cross-calibration test with a permanent Ameriflux site in Oklahoma (Figure 1). The permanent eddy covariance system was installed on the 60 m tower at the CF and is now continuously measuring fluxes over spatial scales that cover a mixture of land uses. We have tested the high-precision CO_2 system in the laboratory and installed it on the CF tower; in the tests, the system matched the NOAA standard to within 0.05 ppm. The land-surface model is accurately capturing the dynamics and magnitude of ecosystem carbon and energy exchanges at the tallgrass prairie site. We have also completed integration of submodels into LSM1.0 to simulate canopy vapor, leaf water, and vertically resolved soil water $H_2{}^{18}O$ content; leaf photosynthetic and retro-diffusive fluxes of $C^{18}OO$; root and microbial production of CO_2; and soil CO_2 and $C^{18}OO$ diffusive fluxes and equilibration with soil water.

SIGNIFICANCE OF FINDINGS

The good performance of the portable eddy covariance tower implies that we can effectively test the ecosystem model predictions over various land uses and meteorological conditions. During this year's summer field season, we intend to characterize the various ecosystems in the CF footprint and test the integrated flux measured at the 60 m tower against the measured and modeled distributed source. This approach will allow us to integrate ecosystem sources and sinks from the heterogeneous landscape and predict regional-scale carbon fluxes.

ACKNOWLEDGMENTS

This work was supported by the Director, Office of Science, Offfice of Biological and Environmental Research, Atmospheric Radiation Measurement Program, under U.S. Department of Energy Contract No. DE-AC03-76SF00098.

ISOTOPIC ANALYSIS OF CARBON CYCLING AND SEQUESTRATION IN A CALIFORNIA GRASSLAND

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RESEARCH OBJECTIVES

Anthropogenic activities are altering atmospheric CO_2 and climate as well as increasing nitrogen fixation and deposition globally. We are investigating the impacts of global change on carbon cycling in an annual grassland at Jasper Ridge Biological Preserve, Stanford, California (Figure 1). Here we report the treatment effects on decomposition of soil organic matter (SOM) and the relative contribution of "Recent" versus "Old" SOM to soil respiration losses from the ecosystem.

APPROACH

The Jasper Ridge experiment has grassland plots exposed to elevated CO_2, warming, increased precipitation, and nitrogen (N) fertilization, singly and in combination, since the fall of 1998. The fossil source of elevated CO_2 is depleted in ^{13}C relative to the ambient atmosphere. This creates an isotopic label in plant inputs to the elevated CO_2 plots that we can use to trace carbon cycling through plant inputs, soil organic mater, and soil respiration. We are using the isotopic signature to partition soil respiration into recently (i.e., since the experiment began) photosynthesized carbon (Recent) and carbon fixed in previous years (Old). The ecosystem is dominated by annual plants that begin growing after the first rains in fall and die in late spring the following year.

Figure 1. Jasper Ridge Global Change Experiment, March 2000

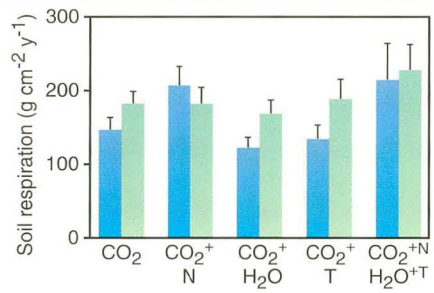

Figure 2. Soil respiration over growing season 1999–2000 by treatment. The blue bars are Old C (pre-1998 growing season) and the green bars are Recent C (1998 growing season and later). The error bars are standard error of cumulative season total.

RESULTS

We measured soil respiration six times over the second growing season (1999–2000) of the experiment. By interpolating between the sampling points, we can estimate the cumulative respiration from the whole growing season by treatment (Figure 2). There was no treatment effect on the amount of Recent C respired. In contrast, the treatments had a pronounced effect on the decomposition rate of Old soil organic matter. The warming or watering treatments had the lowest rates of old C respiration, despite most models having decomposition rates increasing with soil moisture and temperature. The two nitrogen-addition treatments stimulated the most decomposition. One hypothesized mechanism for N stimulation of decomposition is that, under N limitation, an increase in plant growth (e.g., resulting from elevated CO_2) leads to a decrease in microbial activity, and fertilization at Jasper Ridge released soil microbes from this constraint.

SIGNIFICANCE OF FINDINGS

In many studies, elevated CO_2 causes an increase in plant photosynthesis. However, sustained plant growth, and thus continued C sequestration, is N-limited in most temperate ecosystems. As a result, scientists have hypothesized that the combination of CO_2 and N fertilization will cause net sequestration in many ecosystems. This is the first study we are aware of showing that N fertilization or increased N deposition can increase decomposition of stable soil organic matter and thus result in loss of C stored in soils.

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Front Cover	Top left: Numerical simulation of effect of shear stress on the anisotropic wave propagation within a medium containing parallel fractures. Top right: Mammoth Mountain, Long Valley Caldera in eastern California, *Roy Kaltschmidt, Berkeley Lab.* Bottom left: Drill bit of the Tunnel Boring Machine (TBM) used to drill the Exploratory Studies Facility (ESF) at Yucca Mountain, Nevada, *Roy Kaltschmidt, Berkeley Lab.* Bottom right: Contours of mass fraction of CO_2 in the gas phase after one year, *Curt Oldenburg, Berkeley Lab.*
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