Earth Sciences Division

Annual Report
1998 - 1999

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# Earth Sciences Division

## A Perspective from the Division Director

## Resource Departments

- **Ecology**
- **Geophysics and Geomechanics**
- **Geochemistry**
- **Hydrology and Reservoir Dynamics**
- **Center for Environmental Biotechnology**

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As we approach the millennium, the importance of the earth sciences in shaping our future grows larger than ever. Not only must we continue to address the issues that were so pressing during the past century—energy and water resources, ground water and surface water pollution and natural hazards—we must face the challenges of the coming century. The potential for global climate change and the need for safe and secure nuclear waste management have emerged at the forefront of the concerns faced by our nation and others around the world. As one of the U.S. Department of Energy's national laboratories, our mission is to provide a robust scientific foundation to better understand and identify solutions to these pressing issues.

This year has been an exciting one. We have launched several new initiatives to prepare ourselves for the future, and we have made great strides in our ongoing research programs. In this report we present examples of both new and continuing research. While it is not a complete accounting, it is representative of the nature and breadth of our research effort.

New programs in regional climate modeling, carbon cycling in the oceans and terrestrial biosphere, methane hydrates and carbon sequestration are the cornerstones of a major new research thrust related to global environmental change. Significant progress has already been made in each of the following areas:

- The Regional Climate System Model (RCSM) has been used to predict California stream flow in a double CO2 environment.
- We have been selected, in partnership with Lawrence Livermore National Laboratory, to create the new DOE Center for Research in Ocean Carbon Sequestration.
- A reservoir simulator for predicting production from methane hydrate reservoirs has been developed.
- ESD researchers have played a leading role in defining the national research agenda for sequestration of CO2 in geologic formations.

This has also been an exciting year for many of our ongoing research programs. Our core fundamental research program in flow and transport, geochemistry and subsurface imaging continues to push the state of the art and provide the foundation for new insights, approaches and technologies that are relevant to all of our mission-focused programs. Furthering our understanding and quantification of vadose zone flow in fractured and heterogeneous rocks continues to be a central goal of our fundamental research program. This year's highlights include new insights about the episodic and chaotic nature of vadose zone flow in fracture media, better models of colloid transport and a greater understanding of the range of conditions over which film flow on fracture faces may occur.

Our fundamental research program in geochemistry, with primary emphasis on isotopes and reactive transport modeling, has broadened to include experimental and theoretical research in molecular geochemistry. Development of TOUGHREACT, a version of the TOUGH2 family of codes that simulates reactive subsurface transport, represents a major new research capability for our group. Our subsurface imaging program focuses on de...
opining higher resolution imaging methods for geologic structures, transport properties and fluid composition. This year an award-winning project to construct permeability maps from high resolution cross-borehole seismic tomography was completed, providing the launching point for a new initiative in joint inversion of hydrologic and geophysical imaging data.

Scientists working in our Nuclear Waste Program continue to provide leadership in identifying and addressing key research questions related to flow and transport in the unsaturated zone at Yucca Mountain—a site in Nevada that is being investigated as a potential repository for spent nuclear fuel from commercial power plants. As our understanding of the natural flow system improves, we are focusing on the interaction between the waste package and the natural environment. One key question is: How much water will actually seep into the drift and contact the metal canisters that enclose the spent nuclear fuel rods? We have conducted a set of field experiments and theoretical studies which show that only a small fraction of the water percolating through the mountain will seep into the drifts. Some experiments even suggest that there may be a threshold below which no water will seep into the drifts. If this is true, canister corrosion rates and radionuclide fluxes will be lower than currently expected. Over the next several years researchers will address these and other issues about the interaction between the engineered and natural systems.

Scientists and engineers in our Energy Resources Program work closely with the fossil fuel and geothermal industries to develop more effective methods for locating and producing energy resources. This year we have made a major step toward development of new seismic methods for characterizing fractured reservoirs, a problem of utmost importance to the oil, gas and geothermal industries. At the Conoco Oil Company Test Site in Oklahoma, we completed the first successful field demonstration of high resolution single-well seismic imaging of fluid-filled fractures. These same tests provided field validation of new theoretical models for the seismic response of fractures developed as part of our core fundamental research program.

Looking closer to home, researchers in the Environmental Remediation Technology Program continue to lead the soil and groundwater cleanup activities taking place at our own site. Since the inception of Lawrence Berkeley Laboratory in the mid-1930s, the site has been used as a major research facility. With that comes the pollution typically associated with light industrial operations. Several plumes of mixed solvents, hydrocarbon fuels, freon and tritium are located across the site. The complexity of the geologic environment here makes locating the source of these plumes, tracking their migration and designing effective remediation schemes a major challenge. Persistence, a good deal of hydrogeologic sleuthing and a pragmatic approach to remediation have resulted in significant progress towards resolving site cleanup issues. From this and many related experiences we have come to believe that detailed source characterization is the necessary foundation for all successful and cost-effective groundwater remediation activities. Circumventing this time-consuming and often costly step will be paid for many times over.

Finally, one of the major highlights of the year was an International Symposium on the Dynamics of Flow in Fractured Rocks held in honor of Dr. Paul Witherspoon’s 80th birthday. Dr. Witherspoon, the founding director of the Earth Sciences Division, continues to play an active role in many of our activities. In honor of his birthday, at which he gave a keynote speech on “Thirty Years of Fracture Flow Research at Berkeley,” more than 250 participants from around the world joined us for an outstanding technical workshop.

Organization of this Report

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

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

These programs draw from the each our disciplinary departments: Ecology, Geophysics and Geomechanics, Geochemistry, Hydrogeology and Reservoir Dynamics, and the Center for Environmental Biotechnology. Short descriptions of these departments, along with a listing of our personnel are provided as introductory material. A list of publications for the period June 1997 to June 1999 are provided in Appendix A.

Acknowledgments

The Earth Sciences Division consists of 199 scientists and engineers. We gratefully acknowledge the support of our many sponsors in the Department of Energy. We also appreciate the support we receive from other federal agencies: the U.S. Bureau of Reclamation, the U.S. Department of Defense and the U.S. Environmental Protection Agency. These activities support and enrich our programs by broadening the range of applications of our research. We also appreciate support from our industrial collaborators and colleagues, both financial and through partnerships that bring ideas, data and experience to the division.
Ecology

Geophysics and Geomechanics

Geochemistry

Hydrology and Reservoir Dynamics

Center for Environmental Bioremediation

Departments
The current expertise of the Ecology Department (ED) is focused on bioremediation, ecosystem engineering, microbial ecology and environmental risk assessment. Department scientists support research in the Environmental Remediation Technology Program, Center for Environmental Biotechnology, Energy Resources Program, Nuclear Waste Program and Climate Change and Carbon Management Program.

Bioremediation

Ecology Department staff are internationally known for their research in bioremediation. This work has included both in-situ, ex-situ and end-of-pipe treatments and natural attenuation (intrinsic bioremediation). The department has published papers on bioremediation of chlorinated solvents, polycyclic aromatic hydrocarbons, poly-chlorinated biphenyls, fuels, BTEX, MTBE, actinides, selenium, uranium and chromium. In addition to Department of Energy and Department of Defense waste sites, ED researchers have also studied municipal landfills, agricultural drainage areas, sewage treatment systems, groundwater treatment systems, pulp mills, oil refineries, oil production areas, explosives-contaminated soil, nuclear waste storage areas, solvent-contaminated sites, canneries, creosote treatment areas and nitrogen fertilizer factories. Researchers have several patents on bioremediation technologies, many of which have been licensed and are being used at sites around the world. A fascinating new area has developed over the last two years using the unique capabilities at LBNL’s Advanced Light Source (ALS). Ecology Department researchers have shown that by using infrared analyses they can detect the juxtaposition of bacteria, toxic metals and solvents on basalt rocks from DOE waste sites. Indeed, they have shown that naturally occurring bacteria can detoxify Cr$^6$ to Cr$^3$, which is very stable. This promises to be a rapidly developing area for basic research in bioremediation.

Ecosystem Engineering

The Ecology Department has researched selenium transport in the Grassland Water District 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 San Luis Drain. Microbial studies have shown that selenium in-transit losses occur and that the fate of this selenium is bed sediments. 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.

Microbial Ecology

The Ecology Department has considerable expertise in monitoring and characterizing microbes in all types of soil, groundwater, food, freshwater, marine, animal and human environments. Researchers have developed a large number of state-of-the-science techniques to detect and identify microorganisms in the environment using nucleic acid probes, polymerase chain reaction (PCR), polar lipid fatty acids, fatty acid methyl esters, signature enzymes, fluorescent antibodies and direct fluorochrome staining. Ecology department researchers have been actively characterizing microbes from the Chernobyl nuclear site and from...
Lake Baikal in Siberia. The department has also developed expertise using the ALS to visualize individual microbes on mineral surfaces and identify their juxtaposition with minerals and organic compounds in-situ.

Environmental Risk Assessment

Using the ALS and various new techniques for enzyme assays, ED researchers have developed unique methods for a physiologically based protocol to estimate bioavailability and health hazards of petroleum products from soils to humans. This research is providing practical and realistic tools for evaluating various remedial technologies that cost-effectively protect humans—especially children—from exposure to residual petroleum hydrocarbons in surface soils of petroleum-contaminated sites.

Funding

Ecology Department research is funded by several DOE programs: (1) Office of Science, Office of Biological and Environmental Research; (2) Office of Environmental Management, Offices of Science and Technology and Environmental Restoration; (3) Office of Fossil Energy, Office of Gas and Petroleum Technologies; and (4) Office of Non-proliferation and National Security, Office of Research and Development. Support is also received from the Department of Defense, U.S. Army Corps of Engineers; Department of the Interior, Bureau of Land Management; and from the State of California, Department of Water Resources and Department of the Interior, Bureau of Reclamation under the CALFED program. Finally, funding is received through LBNL's Laboratory Directed Research and Development Program.
The Geophysics and Geomechanics Department performs a wide variety of work ranging from fundamental to applied research.

**Scientific Thrusts**

The department is organized into four different groups:
- Center for Computational and Applied Seismology
- Potential Methods
- Geosciences Measurement Center
- Rock and Soil Physics

These groups work closely together to address issues in subsurface imaging. The scientific thrusts have been in joint inversion, wave propagation in complex media (seismic and electromagnetic), coupled-process definition and heterogeneity definition. Much of the work focuses on developing and applying high-resolution geophysical methods to derive physical 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 the bacterial injection work. Another primary thrust is using geophysical methods for fracture quantification. This is evident in fundamental to very applied studies 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 for not only characterizing static properties of the subsurface, but for estimating the 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. We have found that to address complex issues such as site remediation, flow and transport in fracture systems, vadose zone transport, CO₂ sequestration and reservoir stimulation and definition we must use an integrated approach to geophysics and geomechanics.

**Funding**

The work of the Geophysics/Geomechanics Department is derived from a variety of DOE and Work-for-Others sources. The primary funding is received from DOE’s Office of Science (Basic Energy Sciences/Geosciences and Office of Health and Remediation), Fossil Energy, Geothermal Technology, Environmental Remediation and Nuclear Waste Isolation. 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 companies, including Chevron, Conoco, Texaco, Exxon and Shell Oil.
The Earth Sciences Division's Geochemistry Department combines expertise in chemical and isotopic analysis, molecular environmental science and mineralogy, along with data-gathering methodology over the full range of earth environments to enable characterization of geochemical systems from the macroscopic to the molecular. The department comprises four groups with complementary interests and capabilities, as described below.

**Aqueous Geochemistry**

Studies in this group address issues of environmental contaminant sequestration, migration, dissolution and oxidation-reduction via a variety of natural and anthropogenic operants. Recent work has included characterization of the selenium speciation, transport and reaction rates within soil horizons at the Kesterson Reservoir, where national attention has focused on the selenium poisoning of wildlife from buildup of agricultural runoff. Other work has determined inorganic chemical processes that reduce the dangerous selenite species to elemental selenium. Related investigations have examined 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, with the aim to provide improved modeling capability for contaminant migration and other surface processes, such as weathering, sediment transfer, ion exchange and the biogeochemistry of nutrient cycles. Current work includes: state-of-the-art molecular dynamics modeling of the interlayer solvated cations in clays; studies of the solvation environment of contaminant and nutrient molecular units in aqueous solution; determination of the molecular identity of initial iron oxide precipitates on quartz surfaces; and characterization of the "acid-mine-drainage" mineral schwertmannite 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, noble gas and cosmogenic isotope laboratories; a soil carbon laboratory; an analytical chemistry laboratory; and a thermal ionization mass spectrometry laboratory located on the UC Berkeley campus. 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 the geometry and spacing of fractures in rock matrices; (2) the analysis of rock samples from the San Andreas fault zone to determine the source of fluids that produce the lubrication and hence reduce the friction on this fault; (3) the implementation and analysis of large-scale experiments simulating the effects of nuclear waste heat generation within the nuclear repository in Yucca Mountain; (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; and (5) the use of general atmospheric circulation modeling in concert with wildfire historical analysis to study the effect of climate on wildfire severity in California.

**Atmosphere and Oceans**

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 hydrologic data to explain and predict climatic change. The group operates the Regional Climate Center (RCC), where large-scale simulations using the Regional Climate System Model (RCSM) are used for weather forecasts, climate prediction and basic research. The RCC's numerous ongoing collaborations include: streamflow simulations with the US Geological Survey; runoff contaminant monitoring and management with the US 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 DOE/ACPI (Accelerated Climate Prediction Initiative) collaborators. Researchers in the group are currently working with the National Energy Research and Scientific Computing Center (NERSC) at LBNL to develop a new high-performance version of the RCSM.

The U.S. Department of Energy has also recently funded LBNL as co-host (with Lawrence Livermore National Laboratory) for the development of a new center for global climate change. The Center for Research on Ocean Carbon Sequestration will be headed at LBNL by ESD's Jim Bishop, and will include collaborators from Massachusetts Institute of Technology, Rutgers University, Scripps Institute of Oceanography, Moss Landing Marine Laboratories and the Pacific International Center for High Technology Research. At Lawrence Livermore the leader will be Ken Caldeira. The goal of the center will be to research the feasibility, effectiveness and environmental acceptability of ocean carbon sequestration. The other new DOE center will concentrate on carbon sequestration in terrestrial ecosystems.

**Geochemical Transport**

A major effort of this group is the simulation and study of coupled mineral-water-gas reactive transport in unsaturated multiphase systems, in particular fractured rock and nonisothermal systems. This allows the prediction of processes accompanying the emplacement of high-level nuclear waste at Yucca Mountain, Nevada, and can be utilized to study several types of natural geochemical systems. The simulation has been implemented by introducing chemical reactivity into the existing multiphase flow code TOUGH2, developed at LBNL, resulting in a general reactive chemical transport code called TOUGHREACT.

TOUGHREACT was first developed on a PC, and after testing on other platforms, has been ported to the Cray T3E supercomputer at NERSC, where a parallelized version has been implemented. TOUGHREACT has been applied to several different reactive transport scenarios: (1) supergene copper enrichment processes deriving from the oxidative weathering of pyrite (FeS2) and chalcopryte (CuFeS2). Here the associated acid generation activates metal ion transfer into the unsaturated zone where ore deposits of chalcocite (CuS) and covellite (Cu2S) can form; (2) prediction of the hydrothermal and chemical processes introduced by a strong heat source in unsaturated fractured rock such as at Yucca Mountain, which also complements work by the isotope geochemistry group in identifying transport paths and mechanisms at that site; (3) refinement of kinetic models of dissolution and precipitation of silica and calcite at low (10-100°C) temperatures. The natural evolution of groundwater chemistry at Yucca Mountain is also being interpreted using extant chemical analyses of pore and ground waters. This work will be coordinated with ongoing TEM studies of devitrified tuff at Los Alamos National Laboratory, New Mexico, that will identify the mineral phases and their relation to rock texture and void geometry.

**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; DOE Office of Energy Efficiency and Renewable Energy, Office of Utility Technologies, Office of Geothermal Technologies; 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; and the Laboratory Directed Research and Development Program at LBNL.
The Hydrogeology and Reservoir Dynamics Department (HRD) is one of the most active groups in the world doing research in different fields of hydrogeology and reservoir engineering. HRD conducts research for various projects of the Department of Energy in the areas of nuclear waste geological disposal, environmental management, fossil fuel development, geothermal engineering and basic energy sciences. The department is also involved in projects with the U.S. Environmental Protection Agency and U.S. Department of the Interior, and participates in various international collaborative projects with Japan, Sweden, Russia and others.

HRD research covers several areas, briefly described below.

**Contaminant Hydrology**

Work conducted in this area covers various theoretical and experimental studies, including a major evaluation of contamination at LBNL. In this multi-year evaluation, details of the hydrogeologic structure of the site were explored, measured and modeled, then the contaminant plumes (which are relatively minor) were characterized, monitored and studied. Finally, a control and remediation strategy was developed in collaboration with local and federal regulatory agencies. The work involves the multi-disciplinary effort of geologists, hydrologists, geophysicists and hydrogeochemists, characterizing many of HRD's research projects.

Another major effort is the development and study of in-situ barriers and their emplacement for control and containment of contaminant plumes. This includes the choice of gelling barrier materials, their characterization in laboratory studies, development and optimization of emplacement methodology through modeling studies and pilot studies in the field. Besides these two efforts, advanced well-test methods are also being designed for characterization of the subsurface hydrology, and various analysis and modeling techniques are being developed.

**Vadose Zone Hydrology**

The study of the soil and geologic layer between the ground surface and the water table is a very active area of HRD's research, with applications in both the nuclear waste disposal and environmental remediation programs of DOE. A number of basic studies were made on fast paths in the vadose zone, such as the development of flow channeling in the unsaturated medium and on the chaotic model of flow in such systems. Various field-testing techniques have been developed, including new geophysical methods of measuring soil tension and new designs for studying water percolation in unsaturated fracture-porous media in the field. The latter are especially noteworthy, as they are being applied a series of experiments in the underground "exploratory shaft" at Yucca Mountain, Nevada. There, the effects of fractures, a major fault and a porous matrix on the flow through the system and the threshold for seepage into the tunnel are being studied.

Another major set of experiments was conducted at Idaho National Engineering and Environmental Laboratory, where a multi-scale study was made to study the characteristics of unsaturated flow through complex structures that strongly vary with scale, ranging from centimeters to tens of meters. Extensive modeling efforts accompany these field activities both for the experimental design and for data evaluation.
Heterogeneous/Fracture Flow Systems

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 the annealing model 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 data evaluation of heterogeneous porous-fracture systems and studies with the stochastic continuum and double-permeability models. A hierarchical model has also been developed for the study of multi-level fracture systems. Furthermore, new field measurement techniques are being developed to measure strongly varying permeabilities in the borehole. General considerations of predictive evaluation have been developed with recommendations for an approach to iterative site characterization and performance modeling for such heterogeneous systems.

Integrated Site Characterization

The need for a well-designed and optimal site characterization program at a site is well recognized for many geosciences-related problems of national concern. HRD research emphasizes field measurement using hydrologic, geophysical, chemical and geomethodical methods and integrates the analyses of these different types of data to obtain the best conceptualization of the site. A large-scale example is the characterization of the fracture tuff formation at Yucca Mountain, where DOE is conducting an eight-year heater test over a block of the order of 100 m with temperatures of up to 200°C. To understand the flow of fluids, including evaporation and condensation, in the complex unsaturated fractured porous rocks, measurements of air permeability, water sampling with isotope chemistry analysis and ground penetrating radar, are conducted in the same area. Integrated analysis of the data helps provide a good understanding and characterization of the system. In addition to such major field studies, basic studies related to integrated data analysis techniques are also performed.

Flow and Transport Modeling

HRD has a long history in numerical modeling of flow and transport in geological media. A suite of numerical models using finite difference finite element 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 multi-phase, multi-component fluids in complex fracture-porous media. A number of equation-of-state packages were 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 the inverse calculations of parameter estimation for such complex systems. Current development involves the implementation of 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.

Coupled Processes in Fractured Rocks

The coupling of mechanical stress and temperature effects on permeability of fractured rocks is important in injection testing, stimulation of oil and gas reservoirs and nuclear waste repository performance. HRD's work involves the development of a coupled thermo-hydro-mechanical (THM) simulator, with fully coupled HM processes and thermal convection and temperature-dependent property parameters. Recent improvement of the code to handle processes in unsaturated systems has been motivated by nuclear waste storage in unsaturated media and isolation of waste canisters in bentonite near-field barriers. The developed model has been tested against a number of laboratory measurements and applied to a study of a major THM experiment in the Kamaishi Mines in Japan. The capability of the coupled THM code has also been applied to the understanding of HM effects occurring in pressure injection tests of a borehole intersecting fractures in hard rocks. A number of field tests in Sweden and Iceland are being analyzed to understand injection-induced fracture opening and propagation.

Production Optimization and Testing

HRD is also very active in the study of oil and gas reservoirs. This includes optimization and control theory to maximize oil production with the hydrofracturing process, using injection wells. Advanced and unconventional well-test methods to determine and characterize production zones have been developed. Pore network models are being developed to understand drainage and imbibition processes in reservoir rocks during flooding operations. An interesting application being studied is the diatomic 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. Research into hydrofracturing with flooding is being conducted to explore optimal production strategies.

Funding

Funding for the Hydrology and Reservoir Dynamics Department comes primarily from the U.S. Department of Energy, including: Office of Science, Office of Basic Energy Sciences, Division of Engineering and Geosciences; Office of Biological and Environmental Research; Assistant Secretary for Energy Efficiency and Renewable Energy; Office of Geothermal Technologies; Office of Civilian Waste Management; and Assistant Secretary for Environmental Management. Other funding is provided through the Laboratory Directed Research and Development Program at LBNL.
The Center for Environmental Biotechnology (CEB) is a virtual center for integrated multi-disciplinary research in three main focus areas: biogeochemical transformations, environmental diagnostics and environmental health risk assessment based on bioavailability. The Center's core staff members represent four major LBNL divisions: Earth Sciences, Life Sciences, Environmental Energy Technologies and Engineering. In addition, the Center has collaborating scientists from Information and Computing Sciences, Accelerator and Fusion Research, Nuclear Physics, Materials Sciences and the Advanced Light Source.

CEB’s responsibilities are to coordinate, integrate and provide multi-disciplinary research teams to address specific environmental problems at Department of Energy sites (mixed wastes) and Department of Defense sites (explosives, polycyclic aromatic hydrocarbons, polychlorinated biphenyl and heavy metals) and within the State of California (mining, forestry, water quality and agricultural). CEB also manages the U.S. Army Core of Engineers’ BEST (Bioremediation, Education, Science and Technology) Program and houses the Cal/EPA Bioremediation Validation and Certification Program. In addition, CEB coordinates LBNL’s efforts in non-proliferation detection reagents, antibiotic discovery and enzyme screening.

**Biogeochemical Transformations**

Volatile organic compounds (VOCs) are the most common organic contaminants detected in polluted subsurface soils and fractured rock vadose zones. We are examining this microbial biodegradation in fractured rocks by investigating the use of intrinsic endolithic (rock-inhabiting) bacteria to transform VOCs, with respect to the range of critical environmental factors. In addition, stable isotopes are used to monitor the biotransformation processes. Comparative analysis of results from the agar printing-off experiment suggest that at the mesoscale level, there is a significant heterogeneity in the distribution and diversity of cultivable microbial consortia inside the vesicular basalt. It appears that many of the endolithic microorganisms live in pore space with or without direct connection with the surface.

**Infrared Microspectroscopy**

Pollution of subsurface geologic zones and the possibility of using the intrinsic endolithic (rock/mineral-inhabiting) bacteria to either detoxify or immobilize the pollutants have stimulated new interest in the exploration of endolithic bacteria and their long-term survival in the geologic environment. We have developed and demonstrated the applicability of surface-enhanced infrared absorption-reflection (SEIRA) microspectroscopy to study—quickly and with minimum sample preparation—in-situ relationships between the microbial localization and the microscopic physiochemical structures of geologic materials such as rocks. Unlike traditional microscopy approaches, SEIRA microspectroscopy can provide researchers simultaneously the biological, geochemical and physical characteristics of the intact environmental samples. This study has demonstrated that surface-enhanced infrared absorption-reflection (SEIRA) microspectroscopy using a metal-overlayer is a promising tool for studying the in-situ localization of bacteria within geologic materials.
Biodegradation of Fuels

Another focus area in biogeochemical transformations is our work on the biodegradation of methyl tert-butyl ether, MTBE, an additive in gasoline that is a potential carcinogen. By designing a bioreactor that simulates the actual "process reactor," we have isolated indigenous microorganisms attached to the carbon material that have the capability of biodegrading. These microorganisms are currently being identified and optimized for use in an ex-situ bioreactor. A pilot plant has been constructed in Southern California for treatability studies with Kinder Morgan Energy Partners, U.S. Filter/Envirex and North Carolina State University.

Biodegradation of Mixed Wastes

We are working on the biosorption of actinides in the presence of organics and chelating agents and assessing the fate and transport of actinides. This combination of actinides and organics represents a truer picture of the actual mixtures found at the Hanford Site near Richland, Wash. Results indicate that the fate and transport of actinides is very different in a mixture versus pure actinides and that certain bacteria are capable of absorbing actinides at high levels. We have also begun a collaboration with the Seaborg Center for Actinide Chemistry to better understand environmental parameters affecting the interaction of actinides and microorganisms.

Algal-Bacterial Selenium Treatment

A selenium and nitrate treatment system has been operated on agricultural land within the Panoche Water District for the past three years. Two side-by-side systems consisting of a shallow, high-rate algal pond, a deep reduction pond, a sedimentation unit and filter bed were constructed close to the tile sump draining a 1,000-acre field. Removal rates vary from 40 to 80% depending on the configuration of the system. Ongoing research is focused on increasing the removal efficiency and throughput of these systems under a variety of environmental conditions. The ultimate objective is to develop a low-cost, easy-to-implement technology to help farmers reduce selenium loads exported to the San Joaquin River and San Francisco Bay-Delta.

Environmental Diagnostics

CEB, in collaboration with Earth Sciences Division's Center for Isotope Geochemistry, has been employing stable isotope monitoring to validate bioremediation activities in field sites. The isotopic ratios of soil, gas and groundwater compounds are monitored to distinguish byproducts of biodegradation of petroleum hydrocarbons (e.g., CO\textsubscript{2}, CH\textsubscript{4}) from other potential sources. Furthermore, distinctive shifts in the isotopic compositions of the contaminants and metabolic byproducts have been used to differentiate between specific metabolic path-ways used by the microorganisms to degrade the contaminants. More recently, we have concentrated on using isotopic measurements to detect in-situ biodegradation of more recalcitrant contaminants, such as chlorinated solvents and gasoline oxygenates.

Mass Spectometric DNA Diagnostics

Biological activity has often been attributed to changes in pollutant profiles found in contaminated soils when abiotic processes actually caused pollutant removal. LBNL engineers are working with CEB molecular biologists to evaluate a monitoring strategy that relies on the combined use of DNA diagnostic procedures and mass spectrometry as the detection scheme. The intent is to track bioremediation by measuring the occurrence of genes in soil samples that are known to code for enzymes capable of degrading specific pollutants. This type of test is commonly performed with PCR and gel electrophoresis, but matrix-assisted-laser-desorption ionization mass spectrometry offers the possibility for automation and high throughput as needed to track the course of bioremediation over large polluted areas. We are currently working with the naf gene from Psedomonas stuterzi.

Environmental Risk Assessment

Assessing environmental risk based on bioavailability, i.e., what is actually being taken up by human, animal and plant cells, is a challenge for CEB. There is much data in the literature on high-dose exposure rates or single-dose, single-compound exposure rates to animals. CEB has taken the approach of examining the weathered material as it exists in nature and exposing human cell lines to this material over time. In many instances our cell-line models consist of co-culturing two different types of cell lines on thin membranes. We are assessing the effects of ingested weathered PAH mixtures, organochlorines and dioxin by simulating the human digestion system. One team is examining the digestion of the material by human enzymes, uptake by intestinal cell lines (KACO\textsubscript{2}) and conversion by metabolic cell lines such as liver, kidney and breast cell lines. Using a combination of molecular biomarkers and the synchrotron, we can measure what material is left behind in the intestinal cell lines, what the compounds may be metabolized to and any DNA damage and repair using specific molecular biomarker assays developed by our cell biologists.

Partners and Funding

CEB research is funded by the U.S. Department of Energy and Department of Defense. Industrial collaborators are Kinder Morgan Geokinetics and the Petroleum Environmental Research Forum. Academic partners include the University of California at Davis, California Polytechnic Institute, University of Utah and the BEST Program partners: Jackson State University, Ana G. Mendez University System, Southern University of Mississippi, University of Texas at El Paso and University of California at Berkeley.
Fundamental and Exploratory Research

Nuclear Waste

Energy Resources

Environmental Remediation Technology

Climate Variability and Carbon Management

Programs
The Fundamental and Exploratory Research Program (FERP) area covers fundamental earth sciences research conducted in support of the Department of Energy’s science mission, which 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 use. This part of the Earth Sciences Division’s program 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, described below.

- Fundamental studies of chemical and mass transport in geologic media with special reference to predictive modeling of multiphase, multicomponent, non-isothermal fluid flow in saturated and unsaturated fractured rocks.
- 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 global climate variations.
- Fundamental studies in the propagation of waves through geologic media with emphasis on new computational techniques for analyzing seismic/acoustic and broadband electromagnetic signals for high-resolution imaging of near-surface 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 major impacts on applied energy, environmental and radioactive waste management programs. Current research projects are briefly described in the following sections.

Fluid-Chemical Transport Investigations

Building on their previous findings that film flow is an important mechanism for fast fluid transport along fractures in the unsaturated zone, researchers can now demonstrate that even in rocks with low matrix permeability (<10^-15 m²) but containing fracture apertures larger than 50 microns, fast paths for fluid flow will occur in the vadose zone, and these films will transport colloids. This work verifies that contaminants sorbed onto colloids smaller than the film thickness may be transported effectively from the vadose zone to the ground water.

Efforts continue to accurately model subsurface multiphase fluid and heat flow, along with solute transport and chemical reactions. By incorporating reactive chemistry into the framework of the exiting TOUGH2 code, ESD researchers have been able to model ore-forming processes such as supergene copper enrichment and to predict the thermal, hydrological and chemical processes that are likely to occur around a thermal source that simulates conditions in a high-level nuclear waste repository.

Molecular modeling of cesium cation (137Cs⁺) - smectite clay interlayer systems has confirmed the previous findings from bulk diffusion experiments that clay liners will impede the mobility of radioactive 137Cs⁺, a fact important to the design of nuclear waste containment facilities. Prior to this study, detailed experi-
ment characterization of this system proved difficult due to the high degree of disorder within these clays.

**Isotope Geochemistry**

The Center for Isotope Geochemistry (CIG) is a state-of-the-art analytical facility established in 1988 for the measurement of 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 the way mantle-derived or deep crustal fluids move through the crust.

In a effort to reconstruct global climate and climate changes during the past 20,000 years, CIG researchers measured the oxygen and hydrogen isotope ratios ($\delta^{18}O$ and $\delta D$) in Antarctic ice cores from three locations to develop a model that relates isotopic compositions to water available in the ancient atmosphere and past surface temperatures. They have found clear evidence in the ice cores for the temperature transition from the last glacial maximum to the warmer and wetter Holocene, and found evidence that temperatures during the last glacial maximum were substantially lower than previously estimated on the basis of $\delta^{18}O$ data and the modern spatial relationships.

The presence of He, C, and O isotopes in approximately 250 samples of fault gouge, breccia and host rocks collected along the San Andreas and adjacent faults confirms that a significant fraction of He is of mantle origin and is accompanied by deep crustal water and CO$_2$. These findings support earlier results suggesting that deep crustal and mantle fluids enter and lubricate the fault zone, thus causing the low-friction conditions observed from seismological and deformation data.

In their continuing study of a present-day volcanic system, researchers have found that co-variations between He and Nd isotopes in olivines from continental basalts can be used to differentiate between separate magma chambers and to assess the rates for heat and magma recharge into the crust.

**Advanced Computation for Earth Imaging**

The Center for Computational Seismology (CCS) serves as the LBNL 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, some of which are reported here.

Researchers have successfully demonstrated the use of joint geophysical-hydrological data sets for estimating stochastic hydrologic parameters of a test site. Using data collected at the Oyster, Va., bacterial transport test site, they have been able to integrate hydraulic conductivity information from flowmeters and radar cross-hole tomograms to obtain improved images of permeability.

Researchers have completed a major study of wave propagation along the San Andreas fault zone as part of the Parkfield Prediction Program. On the basis of more than 6,000 natural earthquakes and 720 source-receiver paths obtained from a controlled-source program, they have developed a detailed elastic model confirming that there are temporal velocity changes occurring in a region suspected to be the nucleation area for past and future magnitude-6 earthquakes. These velocity variations are strongly believed to be related to changing fluid conditions in the shallow section of the fault zone.

Researchers have also developed and tested advanced techniques for modeling elastic and electromagnetic wave propagation through media heterogeneous in two and three dimensions. In one study they treated elastic wave propagation as a series of forward scattering problems, where the medium is described as a random distribution of scatterers of various sizes and physical parameters. Analytical results based on simple models compare well with numerical simulations for a wave propagating through a medium containing a random distribution of spherical scatterers.

In another study, researchers developed a new coupled integral equation-differential equation approach for the nonlinear inversion of electromagnetic, seismic velocity and hydrologic conductivity data sets. New GILD and SGILD methods provide a high-resolution, robust and stable algorithm suitable for high-performance parallel machines.

**Funding**

Funding for research in the Fundamental and Exploratory Research Program comes from a variety of sources, including primarily the Office of Basic Energy Sciences, Department of Engineering and Geosciences, and Office of Biological and Environmental Research, both in the Office of Science of the U.S. Department of Energy, and the Laboratory Directed Research and Development Program at LBNL. Additional support comes from DOE’s Office of Environmental Management, Environmental Management Science Program.
Identifying Limits of Film Flow
In Unsaturated Fractures

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Research Objectives

In an earlier study (Tokunaga and Wan, 1997), we identified film flow as a mechanism that can contribute to fast flow along unsaturated fractures. The combination of low-permeability rock, large fracture aperture and near-zero matric potential was qualitatively identified as necessary for development of fast film flow. However, more quantitative determinations of the ranges of matrix permeabilities, fracture apertures and matric potentials that permit development of thick, transmissive films along fracture surfaces remained unspecified. This study is directed at identifying the approximate region of stability for thick films, within the parameter space defined by rock matrix permeability, local fracture aperture and matric potential.

Approach

Our initial studies on flow in unsaturated fractures identified film flow as a mechanism capable of permitting fast flow and transport. That study revealed limitations of earlier conceptual models for unsaturated flow in fractured rock, introduced the film flow hypothesis and provided experimental results supportive of the hypothesis. The water “films” investigated in the previous study as well as the present one develop on rough surfaces typical of rock fractures, range in average thickness from about 1 to 50 μm and flow in the laminar regime. The initial study showed that film flow becomes important when matric potentials along rock surfaces are high enough (less negative) to effectively saturate the surficial rock matrix. Here, more specific constraints are identified for parameter ranges within which film flow can occur.

The first step in this study consisted of identifying a single parameter to represent each of the primary system components, the rock matrix, fracture and water. In this simplification, the selected parameters were the rock matrix permeability, fracture aperture and matric potential, respectively. Since the matrix permeability and local fracture aperture are essentially fixed at any given location along a fracture surface, one can then consider the range of matric potentials over which stable thick films exist. The lower energy limit will then be associated with the matric potential at which the local rock matrix is effectively saturated (satiated), and the upper limit associated with local saturation of the fracture aperture.

The critical matric potential at which the rock matrix is effectively saturated and above which water films can begin to emerge on fracture surfaces is approximately equal to the air-entry matric potential. Because of hysteresis in the potential-saturation relation, and also because of generally unknown wetting history, the actual critical matric potential will typically have a magnitude between about 50% and 100% of the air-entry value. The lower range of matric potentials, at which thick films begin to emerge from fracture surfaces, was estimated through correlations between matrix permeabilities and air-entry matric potentials of a wide range of porous media, including soils, glass bead packs, rocks and ceramics (Figure 1). We seek only rough correlations since the range of permeability spans nearly 10 orders of magnitude. This correlation was shown to predict the air-entry matric potential within one order of magnitude, for 92% of the data (N = 76). The correlation was also fairly consistent with predictions based on Miller-Miller geometric similitude, even though the highly varied sample set does not rigorously conform to prerequisites for geometric similitude. The exponent in the regression fit is -0.425, whereas Miller-Miller similitude predicts a value of -0.5.

Upon effectively saturating the rock matrix, local topographic minima on the fracture surface become progressively water-filled as the matric potential is brought closer to zero. Filling of local topographic minima on fracture surfaces progresses from finer roughness features to coarser ones, as the matric potential is brought closer to zero, in accordance with continuously increasing the radius of curvature characteristic of the air-water interface. Thus, the average film thickness on rough fracture surfaces increases as the matric potential approaches zero, primarily because of surface capillary relations. In this progression to thicker average films, the transmissivity and hydraulic diffusivity also increase, as shown in earlier work.

In typical rock fractures, film thickening has a finite limit imposed by the fracture aperture. The upper range of matric potentials, at which films give way to locally saturated fracture apertures, is
Identifying Limits of Film Flow in Unsaturated Fractures

estimated from parallel plate capillary considerations used in previous models for partially saturated fractures. These two limiting matric potentials, one for rock matrix saturation (satiation), and the other for local aperture saturation are plotted as surfaces with respect to their dependence on matrix permeability and aperture size in Figure 2. The combination of local material properties for a given segment of fracture, the local matrix permeability and fracture aperture, specifies a given vertical line intercepting the base of this parameter space. The energy status of water at this location on the fracture surface specifies a particular point along this vertical line. Thus, at lower (more negative) matric potentials, characterized by unsaturated matrix flow, systems occupy the region below the lower surface shown in Figure 2. At higher (closer to zero) matric potentials, the local rock matrix becomes effectively saturated, permitting stable thick films along fracture surfaces. This condition lies between the two surfaces. At still higher matric potentials, the local aperture becomes water-saturated, thereby locally eliminating water films. This last state of local aperture saturation occupies the upper region of the parameter space shown in Figure 2.

**Significance of Findings**

The result summarized in Figure 2 identifies the approximate stability region for thick water films in unsaturated fractures. This finding is of interest because earlier conceptual models did not recognize the existence of thick water films in unsaturated fractures (i.e., the middle region in Figure 2), and because a significant volume of the fracture flow parameter space is associated with thick films. Note that low permeability rock (with permeability \(<10^{-15}\) m²), with apertures larger than about 50 µm have a significant near-zero matric potential range over which film flow can occur. This combination of permeabilities and apertures is quite common, indicating that film flow may be important in many fractured vadose environments.

**Related Publication**


**Funding**

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

Bubble suspensions, also known as colloid gas aphrons (CGAs), have been used for scouring organics from contaminated aquifers and for delivering oxygen for bioremediation. CGAs have typical bubble size ranging from 30 to 100 μm. Therefore, bubbles have a short lifetime (a few hours) and can only flow through large pores and preferential flow paths. The objective of this research is to generate small size and long-lasting microbubbles (0.7-15 μm) that present suitable physico-chemical conditions at the gas-water interface for preferential sorption of contaminants and to provide a steady flow of microbubbles upward through contaminated zones, including those advectively inaccessible zones, for in-situ remediation.

Approach

The microbubble suspension was generated by mixing surfactant solutions at high speeds. The generator, built in-house, comprises a 5-cm disk mounted at the end of a shaft, two vertical baffles and a 4.5-L mixing beaker. The disk, when rotating at high speeds, entrains air into the solution; upon hitting the baffles, the entrained air breaks into microscopic bubbles. The microbubble generator was located in a stainless steel chamber to generate microbubbles under pressure. This design would also allow the use of oxygen or other gases as opposed to air. Concentration, size distribution and stability of microbubbles generated with several surfactants and surfactant mixtures were measured to determine the optimal “microbubble formulation.”

Microbubble transport experiments were conducted in vertical sand columns under steady flow conditions. Three grain sizes were used: 415-500 μm (coarse sand), 150-212 μm (medium sand), and 53-106 μm (fine sand). One pore volume of microbubble suspension was injected into the bottom end of the water-saturated columns. Microbubbles were generated either under atmospheric pressure or under pressure (30 psig). For the microbubbles generated under ambient conditions, the suspension was injected using a syringe pump. Injection of microbubbles generated at 30 psig was controlled with an in-line differential pressure flowmeter. Microbubble concentration and size distribution were measured using a Coulter Multisizer II.

Results

Microbubble Generation and Characteristics: Coalescence between bubbles and gas diffusion from the bubbles toward water is responsible for the lack of stability of gas bubbles in pure aqueous solutions. The presence of surface-active compounds such as surfactants greatly improves the stability of the bubbles by forming a film at the gas-water interface. Formation of stable microbubbles is accomplished by mixing surfactant solutions at high speed. Stable microbubbles were only formed with mixtures of water-soluble surfactants and solid non-soluble surfactants. The best formulation is a combination of sodium dodecyl sulfate, SDS, and sorbitan monostearate, Span 60. The number of microbubbles greatly depends on the concentration and size of Span 60 particles. It was found best to grind Span 60 to a fine powder before mixing with SDS. The optimum SDS concentration is 1 g/L. Figure 1a is a photograph of a SDS/Span 60 microbubble suspension taken seven days after generation. Two size fractions are shown: <1 μm and 2-5 μm. The microbubble concentration is 1.5 x 10⁹ bubbles/mL and the size ranged from 0.7 to 7 μm, with 75% of the microbubbles <2 μm (Figure 1b).

The specific volume of this sample is 12 x 10⁹ μm³/mL, which corresponds to an air volume of 1.2% (assuming the contribution

Figure 1a. Photograph of a microbubble suspension. Objective = 40x.

Figure 1b. Microbubble size distribution on a number and volume basis. Concentration = 1.5x10⁹ microbubble/mL and 12.2x10⁹ μm³/mL.
Microbubble Generation, Stability and Transport: A Potential Subsurface Remediation Technique

of the surfactant coating to the size of the microbubbles is negligible). Concentrations as high as 2.5-3.0x10^9/mL have been achieved with air content of 4 to 7%, as determined by the multizer or by direct gravimetric measurements. Stability experiments have revealed that microbubbles, as well as diluted microbubble suspensions, 1/10 and 1/100 in deionized water and salt solution, are stable for several weeks.

The effect of pressure on concentration and stability of the microbubble suspension was also investigated. For example, microbubble concentration (specific volume) increased from 1.1 (24.3) to 1.6 (37.0) to 1.8 x 10^9/mL (38.8 x 10^9 μm^3/mL) when the pressure under which they were generated increased from 5 to 18 to 30 psig, respectively. Conversely, microbubbles are significantly altered when subjected to static pressures slightly above ambient pressure (6 to 10 psi): microbubble concentration (specific volume) was reduced from 1.6 (45.3) to 1.2 (4.0) to 0.76 x 10^9/mL (0.79 x 10^9 μm^3/mL) when the applied pressure increased by 10 and 20 psi, respectively. These numbers also indicate that the larger microbubbles (4 to 15 μm) are most sensitive to pressure increase.

**Microbubble Transport in Porous Media:** Low-concentration and small-size (<3 μm) microbubbles, generated under atmospheric pressure, were injected with the syringe-pump into coarse sand. Figure 2 shows essentially conservative transport with some retardation. Approximately 100% recovery was obtained. Flow experiments through fine sand were inconclusive as the backpressure caused microbubbles to break/dissolve in the syringe-pump. To circumvent this problem and to increase the amount of air delivered, microbubbles were generated under pressure and then directly injected from the pressure chamber into medium and fine sand columns. In these experiments, microbubble size ranged from 0.7 to 10 μm and concentration (specific volume) was 1.3 x 10^9 microbubble/mL (ca. 9 x 10^9 μm^3/mL). As shown in Figure 2, microbubbles exhibited early breakthrough in the medium sand (size exclusion effect) and recovery was ~67%. Flow through the fine sand was significantly retarded and recovery was <35%, suggesting significant losses of microbubbles in the porous media. Microbubble losses could be attributed to microbubble breakage (large air bubbles were observed in the column effluent) and/or irreversible sorption phenomena.

**Significance of Findings**

Generation of long-lasting and stable microbubble suspensions is accomplished using a mixture of surfactants (SDS and Span 60). These microbubble suspensions are characterized by very large specific volumes and concentrations. Good microbubble recovery is achieved in coarse- and medium-size sand columns, suggesting that microbubbles can effectively be transported in such porous media. These results indicate that microbubble suspensions could be used to deliver in-situ significant amounts of air (or oxygen) for bioremediation of contaminated soils and groundwaters. Furthermore, the large specific surface area of the microbubbles, up to 50 cm^2/mL, suggests that microbubble suspensions could potentially be used as a sorptive phase to remove contaminants from the subsurface.

**Related Publication**


**Funding**

This work has been supported by the Assistant Secretary of Environmental Management, Environmental Management Science Program, of the U.S. Department of Energy under Contract No. DE-AC03-76SF00098.
Particle Motion in Film Flow

Research Objectives

Srinivas Veerapaneni, Jiamin Wan and Tetsu K. Tokunaga

Transport of colloids through unsaturated subsurface environments has significant environmental implications. For instance, movement of contaminants from vadose zone to the groundwater table may be facilitated by their sorption onto the colloids. Despite its importance, the effect of flowing thin liquid films on colloid transport in partially saturated rock fractures and porous media is poorly understood. In a recent study, Wan and Tokunaga presented a film-staining model to predict the effect of thin water films on colloid transport in partially saturated porous media. Experimental results confirmed model predictions that the movement of colloids is inhibited if the particle sizes are larger than the film thickness. However, the mechanistic understanding of the effect of the characteristics of films, particles and medium surfaces on particle motion is still lacking. The objective of this research is to provide the fundamental understanding of particle movement in thin water films, upon which the predictive models of unsaturated colloid transport will be based. To address this issue, a study is undertaken to examine the effect of particle size \( \frac{d_p}{h_0} \) or film thickness \( h_0 \) on the motion of a sphere in a liquid film flowing down an inclined flat surface.

Approach

Theoretical considerations: The dominant forces and torques acting on a particle completely submerged in a flowing liquid film and moving in contact with a smooth plane surface are fluid drag, friction, lift, buoyancy and gravity. For a partially submerged sphere, additional forces, such as surface tension acting along the three-phase contact line between the film surface, particle and air, and pressure force also act on the particle (Figure 1). The translational and rotational velocities of the particle can be obtained by balancing all the forces (in the direction parallel to the solid plane) and torques (about z-axis) acting on a particle (Equations 1 and 2)

\[
F_{\text{drag}} + F_{\text{grav}} + F_{\text{fric}} + F_{\text{surf.ten.}} + F_{\text{pressure}} = 0
\]

\[
T_{\text{drag}} + T_{\text{fric}} = 0
\]

The drag forces acting on the particle are corrected for the presence of the solid boundary beneath the particle. The effect of free interface above the particle is neglected, limiting the validity of the model when the free surface influence on particle motion is significant. Particle roughness, expressed as a percentage of particle size, and friction coefficient between particle and glass plate are used as the adjustable fitting parameters in the model. The estimation of surface tension and pressure force for a particle partially submerged in a film requires knowledge of capillary rise \( h_c \) and angle \( \alpha \) (Figure 1). Although these two parameters can be estimated by calculating capillary rise profile using the Young-Laplace (YL) equation, we believe that the interface profiles for the physical parameters of this study may have significantly larger radius of curvature than predicted by YL equation. Model predictions are therefore limited to particles smaller than film thickness (i.e., \( \frac{d_p}{h_c} < 1 \)).

![Diagram of forces and torques acting on a particle in a flowing liquid film](image)
**Experiments:** A liquid film is generated on an inclined smooth glass plate with film thicknesses ranging from 140 to 700 μm under steady-state flow. Motions of spherical hydrophilic particles in the range of 20 to 800 μm in diameter were recorded by a CCD camera attached to a long working distance microscope. Film velocity and thickness and particle size were directly measured. A schematic of the experimental setup is shown in Figure 2.

**Results**

Results from a typical experiment are shown in Figure 3. The velocities of the particles, normalized with maximum fluid velocity at the undisturbed air-water interface, are plotted as a function of particle size, normalized with the film thickness ($d_p/b_0$). Model predictions for particles smaller than film thickness are also shown in the figure as a solid line. Four regions can be identified in the figure as discussed below.

1. When particle diameters are smaller than 50% of the film thickness, particle velocity increases nearly linearly with particle size, reflecting the motion of the particle in a flow field characterized by constant fluid shear (linear velocity profile) that is prevalent at these depths.

2. When the particle size is in the range of 50-100% of film thickness, the increase in the velocity of the particle with its size is relatively low, compared to Region I. This is due to the decrease in the fluid shear rate, as the velocity profile in this region is nonlinear. The velocity of the particle peaks when its diameter is close to the film thickness. The measured velocities of the particles in regions I and II (i.e., $d_p/b_0 \leq 1$) agree well with model predictions, as indicated in Figure 3.

3. When particle size is comparable to or slightly greater than the film thickness, it is observed that there is a significant drop in the velocity of the particle. This may be attributed to the surface tension acting on the particle along the three-phase contact line. The proximity of the free interface to the particle surface is also likely to influence the motion of the particle. It is interesting to note that there appears to be a critical range of $d_p/b_0$ ratio when gravity begins to negate the decrease in particle velocity caused by surface tension.

4. When the particles are larger than the film thickness, the influence of gravity force increases with particle size, resulting in increased particle velocities with size.

**Significance of Findings**

Results from this study indicate that particle motion in film flow is strongly dependent on the particle size/film thickness ratio. When particles are smaller than film thickness, significant transport of particles occurs with flow, aided by fluid drag. When particles are comparable to film thickness, surface tension may retard particle motion considerably. Motion of particles larger than film thickness may be aided by gravity.

**Related Publications**


**Funding**

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

Laboratory flow experiments on transparent fracture replicas permit direct visual investigation of flow processes and identification of controlling mechanisms of larger-scale phenomena that are critical in many areas. These include flow and transport around repositories for high-level nuclear wastes, contaminant migration and remediation and enhanced petroleum recovery. Fracture flow visualization experiments have been conducted in parallel rough surface glass plates and fracture casts made with epoxy resin. Rough glass plates do not represent actual natural fractures, but can provide water-wetting characteristics similar to many rock surfaces. On the other hand, epoxy fracture casts can provide reasonably accurate reproductions of natural fracture aperture fields, but have hydrophobic surfaces. For some purposes it is desirable to combine the wetting characteristics of glass with the fracture surface topography reproduction obtained through casting. Glass casts have the combined advantages of closely reproducing natural fracture surface roughness and of being treatable to provide the wide range of wettabilities found for natural rock surfaces. Here we present a new method for replicating natural rock surfaces using molten glass.

Approach

The glass fracture pairs reported in this paper were cast from two different original rock fractures. The larger (120 x 160 mm) glass fracture cast replicated a Swedish granite. The smaller (70 x 70 mm) cast replicated a fractured gabbro (Dixie Valley, Nev.). The casting procedure involves five steps. In the first step, silicone rubber molds (negatives) are made of each rock slab. In step two, wax patterns (positives) are made from the silicone rubber molds. In step three, investment molds (negatives) are made from the investment molds. The final step entails finishing the glass fracture casts. Five sides (4 edges and back) of each half cast are ground and polished as a pair.

The topography of a glass cast surface was compared with that of the original rock fracture using laser profilers and an atomic force microscope (AFM). For coarse-scale measurements, surfaces were profiled with an LK-081 CCD laser displacement sensor (Keyence Corp., Woodcliff Lake, N.J.) mounted on a View Precis 3000 coordinate measuring machine (View Engineering Division, General Scanning, Inc., Simi Valley, Calif.). For higher resolution measurements over smaller areas and narrower topographic ranges on rock and glass casts, a UBM laser (UBM, Sunnyvale, Calif.) was used. The UBM laser has a spot size of 1 μm, a z measurement range of 100 μm, and a z resolution of 0.06 μm. This system was also used to obtain surface profiles on the roughened quartz glass samples. For higher resolution topography, small areas of glass casts were scanned with an AFM (Autoprobe M5, Park Scientific Instruments, Sunnyvale, Calif.). We used this AFM in the standard contact scanning mode to obtain information on finer-scale topography and also to obtain values of surface roughness for comparison with laser profilometry results.

Results

One set of casts will be discussed with respect to each characterization of the finished products. The simplest characterization is that of visual comparisons between an original rock fracture surface and its corresponding glass cast. A photograph of one side of the granite fracture (Figure 1a) and its corresponding finished glass cast (Figure 1b) qualitatively shows reproduction of fracture surface texture and roughness. Reflected light was used for photographing the rock,
while only transmitted light photography was suitable for the glass cast (because of strong reflections and glare under reflected light). Due to differences in lighting, these photographs do not provide a good comparison of the detailed surface textures. Differences between casts and original rock surfaces were quantified through surface profile measurements. In Figure 2a, typical coarse-scale (100-mm line scans, 50-μm in-line steps, at 60-mm lateral line separation) laser profiles of a rock surface and glass cast are compared. The root mean-squared roughness (rmsr) values of the cast along these two profiles (2.22 and 1.14 mm) are very similar to that of the rock original (2.25 and 1.04 mm). However, since the rmsr is strongly influenced by larger amplitude features encountered at larger distances, comparisons over shorter intervals are needed to obtain more direct information on replication of finer-scale features. Example profiles of the fracture and cast surface over shorter distances (10-mm lengths) are shown in Figure 2b. Note that the rmsr values are substantially lower than in the longer profile scans, and that rock and glass casts still yield similar rmsr values, ranging from 0.63 to 0.84 mm.

Although fair reproduction of individual surface topography is achieved in glass casts, mated pairs can still exhibit fairly wide ranges in average aperture and saturated transmissivity. The average aperture and transmissivity of the granite fracture pair under 5.7 kPa average stress were 122 μm and 6.1 x 10⁻⁷ m² s⁻¹, respectively. Three glass casts of this granite fracture pair were molded. The average apertures of these three different glass cast pairs were 75, 173 and 255 μm under the same average normal stress. Transmissivities of these three glass cast pairs were 2.1 x 10⁻⁷, 1.0 x 10⁻⁶, and 1.9 x 10⁻⁶ m² s⁻¹, respectively. All average apertures and transmissivities were determined with a relative uncertainty of ±5%.

The artifact of slight bowing of one surface relative to its opposing surface tends to increase the cast transmissivity, and this effect will be more problematic with larger area casts. For purposes of observing flow and transport under a given cast aperture field, this is not problematic. When transparent fracture replicas are used in studies of multiphase fluid statics and flow, accurate reproduction of surface wettability is a very important factor. Epoxy cast surfaces are quite hydrophobic. Water “wets” dry epoxy surfaces with contact angles of about 90° (Figure 3a). In contrast, clean glass cast surfaces provide excellent water-wettability, with near zero contact angle (Figure 3b). Previously mentioned techniques can be used to alter glass surface wettabilities.

**Significance of Findings**

A method for casting transparent glass replicas of rock fractures was developed. The glass casts obtained using this method provided close reproduction of major features of natural fracture topography. The glass casts are generally more water-wettable than epoxy casts, and can also be treated to exhibit specific desired wettabilities. Thus, for visualization studies of multiphase fluid environments in fractures, glass casts are suitable to use for a wide range of natural fracture surface wettabilities. They can be used to study mechanisms controlling multiphase fluid flow and contaminant transport (including solutes, colloids, microorganisms and NAPLs), to examine remediation techniques at small scale and to conduct laboratory studies for enhancing petroleum recovery redistribution seen by the active testing data.

**Related Publication**


**Funding**

This work has been supported by the Office of Science, Office of Basic Energy Sciences, Division of Engineering and Geosciences, of the U.S. Department of Energy under Contract No. DE-AC03-76SF00098. The authors thank Dr. Peter Persoff (LBNL) for providing the Dixie Valley rock fractures and epoxy casts and for helpful internal review comments.
Research Objectives

Coupled modeling of subsurface multiphase fluid and heat flow, solute transport and chemical reactions can be used for the assessment of acid mine drainage remediation, waste disposal sites, hydrothermal convection, contaminant transport and groundwater quality. We have developed a comprehensive numerical simulation model, TOUGHREACT, which considers nonisothermal multi-component chemical transport in both liquid and gas phases. A wide range of subsurface thermo-physical-chemical processes is considered. The model can be applied to one-, two- or three-dimensional porous and fractured media with physical and chemical heterogeneity. The model can accommodate any number of chemical species present in liquid, gas and solid phases. A variety of equilibrium chemical reactions is considered, such as aqueous complexation, gas dissolution/exsolution, cation exchange and surface complexation. Mineral dissolution/precipitation can proceed either subject to local equilibrium or kinetic conditions.

Approach

The coupled model is implemented by introducing reactive chemistry into the framework of the existing nonisothermal multiphase flow code TOUGH2 (Pruess, 1991), resulting in the general reactive chemical transport code TOUGHREACT. Our model uses a sequential iteration approach, which solves the transport and reaction equations separately. Flow and transport in geologic media are based on space discretization by means of integral finite differences. An implicit time-weighting scheme is used for flow, transport and geochemical reaction. The chemical transport equations are solved independently for each component, whereas the reaction equations are solved on a gridblock basis using a Newton-Raphson iteration. An improved equilibrium-kinetics speciation model for simulating water-rock-gas interaction is used. Quasi-stationary approximation and an automatic time stepping scheme are implemented in TOUGHREACT. The code was first developed on a PC and then tested on VAX and UNIX systems. Later, the simulator was ported to the Cray T3E at the National Energy Research Scientific Computing Center (NERSC) at Berkeley Lab, and a parallelized version was developed, resulting in significant improvement of computing efficiency.

Results

The model was extensively verified and validated for a wide range of subsurface physical and chemical processes. Four applications were carried out using TOUGHREACT. Here we report two applications. The first is supergene copper enrichment, which involves oxidative weathering of pyrite (FeS2) and chalcopyrite (CuFeS2) and associated acidification, which causes mobilization of metals in the unsaturated zone, with subsequent formation of enriched ore deposits chalcocite (CuS) and covellite (Cu2S) in the reducing conditions below the water table (Figure 1). A total of 52 aqueous species, 10 primary minerals and six secondary minerals are considered. The aqueous complexation and gas dissolution are assumed at equilibrium. Mineral dissolution and precipitation are subject to kinetics. The alteration of primary minerals and the development of secondary minerals predicted by our model are consistent with observations in supergene copper deposits in the Atacama Desert, Northern Chile.

The second application con-
A Model for Non-Isothermal Multiphase Multi-Species Reactive Chemical Transport in Porous and Fracture Media

<table>
<thead>
<tr>
<th>Primary Species</th>
<th>Secondary Species</th>
<th>Minerals and Gas</th>
</tr>
</thead>
<tbody>
<tr>
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<td>CO₂(aq)</td>
<td>anhydrite</td>
</tr>
<tr>
<td>H⁺</td>
<td>CO₂⁻</td>
<td>calcite</td>
</tr>
<tr>
<td>Ca²⁺</td>
<td>OH⁻</td>
<td>quartz</td>
</tr>
<tr>
<td>Mg²⁺</td>
<td>Al³⁺</td>
<td>cristobalite</td>
</tr>
<tr>
<td>Na⁺</td>
<td>Al(OH)₂⁺</td>
<td>amor. Silica</td>
</tr>
<tr>
<td>K⁺</td>
<td>H₂O₂</td>
<td>microcline</td>
</tr>
<tr>
<td>SiO₂(aq)</td>
<td>Cl⁻</td>
<td>albite</td>
</tr>
<tr>
<td>HCO₃⁻</td>
<td>CaCl⁺</td>
<td>kaolinite</td>
</tr>
<tr>
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<td>CaCO₃(aq)</td>
<td>sepiolite</td>
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<td></td>
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<td>CO₂(g)</td>
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</tbody>
</table>

Table 1 Aqueous species, minerals and gas considered in the simulation.

consists of predicting thermal, hydrological and chemical processes induced by emplacement of a strong heat source in unsaturated fractured rocks to simulate a high-level nuclear waste repository. A dual permeability model was used. Aqueous species, minerals and gas considered in the simulation are shown in Table 1. Mineral dissolution and precipitation reactions proceed according to kinetics. Preliminary modeling results (Figure 2) indicate the importance of considering hydrochemical interactions between fracture and matrix for this type of system. The simulations are useful to investigate mineral dissolution and precipitation under boiling conditions in fractured unsaturated rock.

**Significance of Findings**

The model is well suited for flow and reactive transport in variably saturated porous and fractured media. Major features of the model include heat driven fluid flow and effects on chemical reactions, and gaseous species transport and interaction with the aqueous phase. The capabilities of the model have been illustrated with a few examples. The full potential is yet to be explored.

**Related Publications**


Sonenthal, E., N. Spycher, J. Apps and A. Simmons, Thermo-hydrochemical predictive analysis for the drift-scale heater test, Yucca Mountain Project Level 4 Milestone

**Funding**

This work was supported by the LBNL Laboratory Directed Research and Development Program and by the Director, Office of Civilian Radioactive Waste Management, through Memorandum Purchase Order EA9013MC5X between TRW Environmental Systems, Inc., and the Ernest Orlando Lawrence Berkeley National Laboratory under U.S. Department of Energy Contract No. DE-AC03-76SF00098.
The Center for Isotope Geochemistry (CIG) was established in 1988 with three major goals. The first is to maintain a state-of-the-art analytical facility for the measurement of the concentrations and isotopic compositions of elements in rocks, minerals, fluids and gases in the earth’s crust, oceans and atmosphere. The second is to develop new ways of using isotopic ratio measurements to study earth processes. This involves improvements in analytical techniques, as well as exploration of the natural isotopic variations of key elements and development of conceptual models relating isotopic variations to earth processes. The third objective is to apply well-known isotopic and chemical approaches to specific energy and environmental problems, such as groundwater contamination and remediation, geothermal resource development, nuclear waste isolation and global climate change.

The Center’s lab facilities include laboratory and field equipment for oceanographic studies, a stable isotope laboratory, a noble gas laboratory, a cosmogenic isotope laboratory, a soil carbon laboratory and an analytical chemistry laboratory. There is a thermal ionization mass spectrometry laboratory on the University of California’s Berkeley campus. In the coming year the Center will obtain a multiple-collector, magnetic sector mass spectrometer with a plasma ion source, which will greatly expand its analytical capabilities. ESD researchers have established the Regional Climate Center (RCC) and are associated with the Center for Isotope Geochemistry to take advantage of the overlap in research interests. The RCC specializes in a Regional Climate System Model (RCSM) that down scales global model information to provide research information, climate predictions and impact assessments on a regional scale. The model can be applied to weather forecasting, soil water content, river flow, hydrology at a watershed scale, climatic trends, water resources, crop responses and ecological and environmental impacts.

A pressing question in climatology is what the impact of future climate change will be on regional and local scales. Climate researchers, using a regional climate hindcast, are evaluating the effectiveness of the Regional Climate System Model and its various components, such as the Mesoscale Atmospheric Simulation and Soil-Plant-Snow models, to reproduce western U.S. climate. Agreement between observed and simulated climate features suggests that the RCSM is capable of long-term regional climate simulation. Another project couples general circulation models, which simulate global climate change scenarios, with California Department of Forestry wildfire models to predict the impact of future climate change on the occurrence and magnitude of wildfires at a local scale. The average insured cost of wildfires in the United States is about $300 million dollars per year. Insurers and climatologists have long known that fire danger is intimately linked to climate. For instance, local and regional droughts linked to the recent El Niño led to devastating fires in Florida, Indonesia and elsewhere. In most cases, climate change driven by a two-fold increase in atmospheric carbon dioxide would lead to dramatic increases in both the area of land burned by California wildfires and the number of potentially catastrophic fires.

In many natural systems, fracture permeability exerts a dominant influence on fluid flow. A simple model is under development to test the feasibility of using the isotopic compositions of element pairs in fluids to constrain fracture-matrix geometry and spacing. Fluids acquire heat from matrix blocks by conduction and solubility and ionic diffusivity limits the exchange of chemical and isotopic constituents. Therefore, the thermal, chemical and isotopic evolution of fluids flowing through fractured rock depends strongly on fracture geometry and spacing. Reservoir modeling relies on geometric information from rock outcrops and core, but the geometry of the reservoir fractures carrying the bulk of the fluid is generally not known. The sensitivity of isotopic ratios to matrix block size (or average fracture spacing) is related to the differing solubility and diffusivity of the elements. The degree to which a matrix block is isolated from a fracture fluid decreases with increasing solubility and diffusivity.

Researchers measured helium, carbon and oxygen isotopes in samples from fault zone gouge, breccia and host rock of the San Andreas Fault. Their study confirms that a significant fraction of the helium in the fault zone fluids has come from the mantle and is accompanied by deep crustal or metamorphic water and carbon dioxide. This supports their earlier work that suggested fluids are entering the fault from the mantle and acting to lubricate the fault, which would explain the well-known dearth of friction on the San Andreas Fault. In a

Figure 1. Mono Lake, California. Photo by Roy Kalschmidt, LBNL.
project with researchers from the U.S. Geological Survey and Oxbow Geothermal, it is shown that noble gas concentrations, water isotopes and chloride concentrations in geothermal production streams provide a quantitative measure for tracing the return of injectate to geothermal reservoirs. The rate at which cooler injectate fluids invade a production reservoir is extremely important for establishing injection programs and constraining future reservoir models. Other research has shown that co-variations between helium and neodymium isotopes in continental basalts can be used to differentiate between magma sources or chambers and to assess the present rate of magma chamber recharge with new mantle material. This provides valuable information for assessing volcano hazards and the potential of a region for geothermal energy development.

The drift-scale heater test at Yucca Mountain, Nevada, the proposed nuclear waste repository site, is being conducted to test the effect of heat generated by the stored nuclear waste. Researchers are monitoring the time evolution of the CO\textsubscript{2} carbon isotopic composition in gas released during the heating test. The changing isotopic composition will help quantify factors such as the degree of porewater degassing and identify zones of calcite deposition within the thermally disturbed region which bear directly on fluid movement and changing permeability of the system.

The Environmental Measurements Laboratory (EML) consolidates the inorganic and organic chemical analytical facilities of the Earth Sciences Division. The EML provides chemical characterization of soil, rock, mineral and fluid samples for many researchers and projects within the division and the UC campus. The EML is equipped with state-of-the-art instrumentation, including ICP-MS with laser ablation capabilities, atomic adsorption spectrometry, GC/MS, HPLC, and facilities for standard wet chemical analysis.

**Funding**

The research of the Center for Isotope Geochemistry has been supported by the Office of Science, Office of Basic Energy Sciences, Materials Sciences and Engineering and Geosciences divisions; the Environmental Science Management Program; the Office of Energy Efficiency and Renewable Energy, Office of Geothermal Technologies; the U.S. Environmental Protection Agency, via Energy Efficiency and Renewable Energy, Office of Building Technologies and State Community Programs of the U.S. Department of Energy. Research has also been supported by the U.S. Navy; the Office of Space Science of the National Aeronautics and Space Administration; the Office of Polar Programs of the National Science Foundation; and the LBNL Laboratory Directed Research and Development Program.
Molecular Modeling of Clay Mineral Surface Geochemistry: Hydrated Cesium-Smectites

Rebecca Sutton, Garrison Sposito, Sung-Ho Park and Jeffery A. Greathouse

Contact: Rebecca Sutton (510) 643-9951, sutton@nature.berkeley.edu

Results

An iterative MC method was used to determine the number of water molecules present in stable Cs-smectite systems with layer spacings of ~12 Å. Previous experimental work indicated that a water content of 0.3-0.7 monolayers, or 0.03-0.07 kg water/kg clay, would suffice. Once we had established the water content of a stable Cs-smectite system, we were able to collect thermodynamic information such as layer spacing, total potential energy, density profiles and atom-atom radial distribution functions.

We then performed 800 ps MD calculations on the MC-equilibrated clay systems in order to collect trajectory information and learn about the motions of cations and water in the interlayer. Comparison of Cs-smectite systems with the same water content but different clay minerals revealed the dramatic effect of clay charge sites on Cs" mobility. The tetrahedrally-charged beidellite system and the octahedrally-charged hectorite system both held Cs" in a nearly fixed location. The tetrahedrally-charged beidellite system and the octahedrally-charged hectorite system both held Cs" in a nearly fixed location (Figure 1). The specific cation locations varied with the type of clay charge site, with the near-surface tetrahedral charges drawing the Cs" closer to the surrounding clay layers, while the more distant octahedral charge held all of the Cs" at the midplane of the interlayer. However, when these two types of charge sites were combined in montmorillonite, we did not observe intermediate behavior in the location of the cations. Instead, the Cs" within montmorillonite was much less tightly bound to a particular location, showing a much greater ease of movement.

A closer examination of the motions exhibited by Cs" within smectite systems reveals very lit-
Figure 2. X-Y trajectories of Cs+ cations and a selected water molecule over 400 ps of MD simulation. The x-axis is the same as the crystallographic a-axis of the clay mineral and the y-axis is the same as the b-axis. Two systems are shown. Cs-hectorite with 0.3 monolayer of water and Cs-hectorite with 0.7 monolayers of water. In the latter system, a Cs+ cation (in brown) hovers at the edge of the simulation cell, jumping from one side to the next, creating two trajectory clusters. Black points represent the surface oxygens of one of the clay mineral surfaces. Below the trajectory data are visualizations of the clay system, with the simulation cell outlined in black. Green spheres represent Cs+ ions, while blue spheres are water O and red spheres are clay surface O. Small white spheres represent water H and small grey spheres represent clay mineral Si.

**Significance of Findings**

The results from these experiments confirm the findings of bulk diffusion experiments, which predict a low mobility of Cs+ in clays due to their retention near clay charge sites. Such agreement indicates that the potential functions used to describe the Cs-smectite system may be reasonably accurate, and provides further evidence supporting the use of clay liners within nuclear waste containment facilities in order to retard the movement of $^{137}$Cs+. Cs-smectite molecular simulations can also aid an understanding of basic geochemistry, through comparison of these simulations with those of other alkali metal-smectite systems in order to identify trends exhibited by alkali metal cations.

**Related Publications**


Sposito, G., S.-H. Park and R. Sutton, Monte Carlo simulation of the total radial distribution function for interlayer water in sodium and potassium montmorillonites, Clays Clay Miner., 47, in press.

**Funding**

This work has been supported by the Office of Science, Office of Basic Energy Sciences, Division of Engineering and Geosciences of the U.S. Department of Energy under Contract No. DE-AC03-76SF00098.
Isotopic Effects in Dual-Porosity Fluid-Rock Systems

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Research Objectives

The thermal and chemical behavior of fractured rock systems depends to a substantial degree on the average spacing between fractures. Fluid moving through a system of fractures interacts thermally and chemically with the matrix blocks between them mainly by heat conduction and diffusion of chemical constituents dissolved in the pore fluid or vapor phase. The spacing of fractures can be estimated in some cases from rock outcrops and cores, but the spacing of the fractures actually carrying the bulk of the fluid is not usually known directly.

Isotopic ratios of certain pairs of elements dissolved in fluids can be used in theory to measure the effective matrix block size (or average fracture spacing) in some fractured rock systems. The research described here was aimed at producing a simple theory that relates isotopic ratios in fluids and rocks to fracture spacing, and at using available data to assess whether the expected effects are present in natural systems.

Approach

The sensitivity of isotopic ratios to matrix block size stems from the differing solubilities of the elements, which can be expressed in terms of a rock/fluid concentration ratio ($K_{rf}$), and differing fluid-phase ionic diffusivities. For example, $K_{eff}$ for oxygen is about 0.8, whereas $K_{eff}$ for Sr and C is typically ~10 to 1000. The degree to which the cores of matrix blocks are chemically isolated from the fracture fluid is less for high solubility elements (large $K_{rf}$) than for low solubility elements.

The degree of isolation of matrix blocks can be determined from the diffusive reaction length ($L_d$), which depends on the fluid-rock reaction rate (=$R$) and the effective diffusivity for a dissolved element in matrix pore fluid. If this reaction length is smaller than the average block dimension ($L_b$), then the interiors of the blocks are not in equilibrium with the fracture fluid. The reaction length for element “$i$” that is applicable to the matrix blocks is given by:

$$L_{e,i} = \left( \frac{D_i \phi_m \rho_f}{R(1 - \phi_m) \rho_3 K_{rf}} \right)^{1/2}$$

where $\phi$ is matrix porosity, $\rho$ is density, and $D_i$ is the ionic diffusivity. For two elements of differing solubility, the ratio of the reaction lengths is:

$$\frac{L_{e,i}}{L_{e,j}} = \left( \frac{D_i K_{rf} / (1 + \phi)}{D_j K_{rf} / (1 + \phi)} \right)^{1/2}$$

For oxygen versus strontium, for example, this ratio is typically about 10 to 100. If the average block size falls between $L_{e, Sr}$ and $L_{e, O}$, then the isotopic effects in the fracture fluids provide information on the matrix block size.

In cases where the reaction length is very large relative to the matrix block size, a steady-state system behaves chemically as if it had a single-porosity, and reaction effects on the fluid are determined mainly by the reaction rate, $R$, which describes the solution-precipitation rate averaged over the minerals in the rocks. The advective reaction length, which can be measured in the field, in this case is:

$$L_{e\text{ (single)}} = \frac{\gamma_f \rho_p}{R_{\text{eff}}(1 - \phi) \rho_3 K_{rf}}$$

In general, the effective reaction rate as inferred from the effects of water-rock interaction on the fluid moving through the fractures in a dual porosity system can be shown to be related to the actual reaction rate $\dot{R}$ in the matrix (with some simplifying assumptions) by:

$$R_{\text{eff}} = 8 R \frac{R}{L_b^2} \sum_{n \text{ odd}} (1 + n^2 \pi^2 \frac{L_{e,i}^2}{L_b^2})^{-1}$$

For $L_e < L_b$, then $R_{\text{eff}} = R(L_e/L_b)$. As long as the block dimension is larger than the reaction length, diffusion in the matrix blocks retards chemical and isotopic exchange between the rocks and the fluids by the factor $L_e/L_b$.

Results

The model was applied to published data from mid-ocean ridge hydrothermal systems, where Sr and O isotopes have been measured (although they were not reported on the same samples). These systems involve

Figure 1. Calculated dual porosity effect for fluids moving in fractures and communicating with matrix blocks by fluid-phase diffusion. $R$ is the solution-precipitation time constant in the matrix blocks, and $R_{\text{eff}}$ is the apparent reaction time constant that is sensed by fluid moving in the fractures under steady-state conditions.
circulation of seawater through the basaltic rocks of the oceanic crust. Reaction is believed to take place mostly at a temperature of about 350°C, so these systems are similar to some commercial geothermal systems. Fluids exit the vents with somewhat lower temperatures. A number of assumptions need to be made, but several important parameters are well known for this example — the isotopic compositions of the initial and final fluid, the isotopic composition of the rocks, and the concentrations of the elements in both rocks and fluids. The reaction rate is less well constrained; it is assumed to be $10^{-3}$ yr$^{-1}$.

The model calculations suggest that fracture spacings in the MOR hydrothermal systems are in the range of 2 to 8 times the reaction length for Sr. The latter is estimated to be about 10 cm, so the fracture spacings are estimated to be 20 to 80 cm. The estimated fracture spacing is proportional to the estimated reaction rate, so if the reaction rate is lower, the fracture spacings could be larger.

**Significance of Findings**

It is normally assumed that fluid-rock systems behave as single-porosity systems, or that dual-porosity effects are the same for all elements. If the model results above are applicable, then instead it may be possible to use isotopes of multiple elements to infer important aspects of the structure of geothermal and groundwater systems. Other elements that have variable natural isotopic abundances and could be used in a like manner include hydrogen, helium, boron, carbon, sulfur, lead, uranium, neodymium, thorium and radon.

In non-steady systems, for example those with time-varying flow, the response time for re-establishment of a new steady state between the fracture fluids and the matrix blocks will also vary element by element. This effect could also be used to estimate the effective matrix block size or porosity. It is theoretically possible to constrain all of the parameters if isotope ratios of three or four elements are measured concurrently.

**Related Publications**


**Funding**

This research was supported by the Office of Science, Office of Basic Energy Sciences, Division of Engineering and Geosciences of the U.S. Department of Energy under Contract No. DE-AC03-76SF00098.
Research Objectives

Various geophysical and geochemical observations in the Long Valley, California, area suggest that magma may be present at relatively shallow crustal levels beneath the region. Evidence includes inflation of a resurgence lava dome within the Long Valley caldera; recent (1989-present) and numerous shallow (6-2 km) earthquake swarms beneath Mammoth Mountain, thought to be related to magma injection; increased emissions of cold CO$_2$ from the flanks and summit of Mammoth Mountain, responsible for significant tree kill zones; and a significant increase in magmatic helium and CO$_2$ in gases from a fumarole near the Mammoth Mountain summit that coincided with the earthquake swarms. Understanding the relationship of these observations to one another, and their relationship to the geologic history of Long Valley, is important both for evaluation of volcano hazards and to understand the potential of the region for geothermal energy development (a small geothermal plant already exists in the area).

Approach

Magmas have higher helium abundances and $^3$He/$^4$He ratios than the crust into which they intrude, and depending on the region of mantle which has melted, the helium isotopic ratios of the magma will be different. Although most of the helium in the magma is lost upon eruption, enough remains trapped in olivine crystals to be measured. We have measured helium isotope ratios in olivines from basalts erupted over the past 3.2 million years to better understand the relationship between helium isotopic ratios currently measured at the Mammoth Mountain Fumarole (MMF) and those found in the magma during periods of eruption and recorded in the rocks.

Samples were collected from more than a dozen olivine-bearing basalt flows. From approximately 1-2 kg of rock 0.5 to 1.5 grams of the freshest, largest olivine grains were selected for analysis. The olivine grains were crushed under vacuum to release gases from fluid inclusions, which contain a representative sample of the magma chamber atmosphere during crystal
growth. The chemically purified and cryogenically separated helium was admitted into a mass spectrometer for determination of the isotopic composition.

**Results**

A spatial pattern in the helium isotopic composition of the different basalt flows is evident (Figure 1). Basalts along the edges of the caldera, ranging in age from 3.2 million years to less than 100,000 years, have relatively uniform helium isotopic ratios of 5.8 to 6.2 times that of air. However, the three westernmost basalts in the area, which are outside the Long Valley caldera —June Lake (IL), Devils Postpile (DP) and Black Point (BP) — have much lower helium isotope ratios, from 4.6 to 5.2 times that of air. Since the ages of these basalts overlap with those of the caldera basalts, it appears that these two groups of basalts are derived from two different magmatic systems, isolated from each other in the crust.

Figure 2 illustrates that the caldera basalts are isotopically similar to others found in the eastern Sierra; they are primarily melts of mantle lithosphere with a small contribution from the convecting asthenospheric mantle. Their helium and neodymium isotopic ratios lie along a mixing line between these two types of mantle. The western basalts, on the other hand, have lower helium isotopic ratios than either the MMF today or other eastern Sierra basalts. Their neodymium isotopic ratios are similar to those of Mono and Inyo Craters rhyolites, suggesting that they may be related to these rocks. Unfortunately, the mineralogy of the rhyolites is not suitable for helium analysis.

During the recent period of earthquake swarms beneath Mammoth Mountain, the helium isotopic composition in gases from the Mammoth Mountain fumarole increased significantly, to about six to seven times the air ratio. The similarity between this ratio and those of the caldera-rim basalts indicates that the magmatic system sampled at the MMF is probably the one responsible for generation of these small-scale basalt flows. (SM) basalts, for instance, were erupted from source vents along the western edge of the caldera and flowed eastward into the caldera moat. Recent drilling into the resurgent dome found no noticeable heat anomalies or evidence for magma at depth, supporting this interpretation.

The fact that the MMF helium ratios are similar to those of the caldera-rim basalts, and are probably not the same as those of the Mono and Inyo Craters rocks, has important implications for volcanic hazard evaluation. The Mono and Inyo Craters magmas have undergone significant residence at depth prior to eruption, as demonstrated by their silicic nature. This type of volcanic system requires significant recharge of basaltic magma to provide heat to the magma chamber, and therefore such systems can be quite large and produce large, violent volcanic eruptions.

In contrast, the caldera-rim volcanic system appears to be a relatively small one in which basaltic magmas frequently rise through the crust and erupt as small basaltic lava flows. While this may provide some comfort, the fact that the helium isotopic ratios in the MMF fluids are similar to those exhibited by the system during eruptive periods suggests that the potential for such an eruption is significant.

**Related Publications**


**Significance of Findings**

Our data suggests that magma may be located to the west of the resurgent dome, rather than beneath the dome itself. The North Moat (NM) and South Moat (SM) basaltic magmas have undergone significant residence at depth prior to eruption, as demonstrated by their silicic nature. This type of volcanic system requires significant recharge of basaltic magma to provide heat to the magma chamber, and therefore such systems can be quite large and produce large, violent volcanic eruptions.

In contrast, the caldera-rim volcanic system appears to be a relatively small one in which basaltic magmas frequently rise through the crust and erupt as small basaltic lava flows. While this may provide some comfort, the fact that the helium isotopic ratios in the MMF fluids are similar to those exhibited by the system during eruptive periods suggests that the potential for such an eruption is significant.

**Funding**

This project has been supported by the Office of Science, Office of Basic Energy Sciences, Division of Engineering and Geosciences of the U.S. Department of Energy under Contract No. DEAC03-76SF00098.
Research Objectives

Fluids are suspected to play a major role in earthquake mechanics, especially in the case of the weak San Andreas Fault (SAF). Models developed to explain the weakness of the fault include either low-friction fault zone materials or super-hydrostatic fluid pressures within the fault zone. Models invoking high fluid pressures are similar but rely on different fluid sources. During the earthquake cycle, fault-zone fluid pressure increases to near lithostatic values and induces rupture. Dilation accompanies rupture, locally lowering the fault zone fluid pressures, and the cycle begins again. Potential fluid sources include meteoric, crustal, and mantle. A recent study of groundwaters associated with the SAF found elevated \( ^{3} \text{He}/^{4} \text{He} \) ratios, providing evidence for a geopressured mantle fluid source (Kennedy et al., 1997). Because mantle fluids must pass through the lower plastic crust, they enter the base of the fault zone in the brittle upper crust at or near lithostatic pressures. In transit, the \( ^{3} \text{He}/^{4} \text{He} \) ratios are diluted with radiogenic \( ^{4} \text{He} \) that is produced locally in the crust, generating a vertical gradient in the fault-zone helium isotopic composition that depends on the vertical rate of fluid flow. Calculated flow rates vary from \(-1 \text{ to } -10 \text{ mm yr}^{-1}\), sufficient to maintain near lithostatic fluid pressures at the shallower depths of the seismogenic zone of the fault.

One can assume that the mantle \( ^{3} \text{He} \) is associated with other more abundant mantle volatiles, certainly \( \text{CO}_2 \) and perhaps water. However, using the mantle \( \text{CO}_2/^{3} \text{He} \) ratio, the \( \text{CO}_2 \) flux \((-3 \times 10^4 \text{ kg km}^{-2} \text{ sec}^{-1}) \) inferred from the helium isotopic data is inadequate, by at least an order of magnitude, to re-establish fault-weakening fluid pressures on a time scale relevant to earthquake cycles (Figure 1). This project is an isotopic study designed to (a) compare deformation zones and vein fillings with their hosts and the fluids associated with these materials to confirm the presence of mantle helium in San Andreas fault zone fluids, and (b) identify and characterize the various potential fluid sources.

Approach

Approximately 250 samples from more than 20 localities were collected along the San Andreas and adjacent faults (the San Gabriel Fault, a deeper equivalent of the SAF and the Santa Ynez Fault, a former strand of the SAF) from South San Francisco to East Los Angeles. The samples consisted of gouge, fault breccia, slickenslide, cataclasite material from deformation zones, vein fillings, and their undeformed host rocks. The samples are being analyzed for helium isotopic composition in fluid inclusions and the isotopic composition of carbon and oxygen in the bulk samples.

Results

The helium isotopic composition of noble gases in fluid inclusions from the various fault zone samples are in the range \(-0.1 \text{ to } -2.5 \text{ Ra} \) (Ra is the \( ^{3} \text{He}/^{4} \text{He} \) ratio in air). This indicates that past fluids percolating through the SAF system contain mantle helium contributions of \(-1 \text{ to } -32\% \), similar to that measured in present-day groundwaters associated with the fault (Kennedy et al., 1997). This confirms the involvement of mantle fluids and shows, from structural relationships observed in the field and in thin sections, that these fluids are directly associated with the process of faulting.

Calcite is the dominant vein material and repeatedly occurs as an accessory mineral in deformation zones. The C- and O-isotope compositions of carbonates from veins, deformation zones and their hosts are summarized in Figure 2. By comparing relative depletions in the \( ^{13} \text{C} \) and \( ^{18} \text{O} \) isotopic compositions of the deformation zone or vein carbonates with host rocks at various scales, fluid infiltration can be identified.

At each sampling site, several trends in the C- and O-isotope depletion are observed:

1. The deformation zone and vein material are the most depleted compared to their host rocks.
2. Veins that cut through deformation zones are even more isotopically depleted.
3. With increasing distance from what can be structurally defined as the core of fault zones, host rocks are less isotopically affected and the density of veins and deformation zones decreases.
Host-rock carbonates display progressive evolution towards greater depletion in the order limestone, marble, gneiss, granite and basalt, mirroring the increase in metamorphic grade or deep crustal origin of the host-rocks.

We infer the following from these trends and the isotopic compositions:

1. the fault zones have been infiltrated by fluids of deeper origin during deformation; and
2. the fluids are dominated by crustal or connate water ± CO₂. Meteoric water does not appear to represent a significant contribution and the CO₂ is inferred to have a metamorphic or mantle origin.

### Significance of Findings

The infiltrated deformation zones, veins and host rocks show that fault zones in the San Andreas system maintain a higher permeability than that of adjacent regions. The noble gas and stable isotope compositions both provide evidence that mantle-derived fluids are involved in faulting and that the mantle helium is accompanied by deep crustal or metamorphic water ± CO₂. Some or all of the CO₂ may be of deep crustal origin. This supports the model invoking a deep source of fluids at or near lithostatic pressure weakening the fault zone (Rice, 1992).

### Related Publications


### Funding

This project has been supported by the Office of Science, Office of Basic Energy Sciences, Division of Engineering and Geosciences of the U.S. Department of Energy under Contract No. DE-AC03-76SF00098.
The Center for Computational Seismology

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Research Objectives

The Center for Computational Seismology (CCS) serves as the core data processing, computation and visualization facility for seismology-related research at LBNL. Pursuing an objective of providing modern tools for seismological research, the Center is designed and operated to provide a focused environment for research in modern computational seismology by scientists whose efforts at any time may be distributed among diverse research projects. A large number of varied, separately funded research projects from many different sponsors rely upon this resource for intellectual exchange as well as computational needs. Users include LBNL scientists, along with collaborating UC professors, postdoctoral fellows, visiting scientists, graduate and undergraduate students. Doctoral theses and journal publications reveal a spectrum of effort from the most fundamental theoretical studies to field applications at all scales.

Approach

CCS provides a specially equipped and staffed computational facility to support and advance a wide-ranging program of seismological research. Beyond computers, work stations, seismic processing packages and visualization capabilities, it is a physical facility in which scientists pursuing individual research interact with other scientists and technical support staff in a multidisciplinary intellectual environment. The data management and processing techniques at CCS are integrated with the data acquisition instrumentation in LBNL's Geophysical Measurements Facility (GMF) within which field projects are designed and managed.

A wide range of research projects relies upon CCS resources for development and application of methods for characterization, process definition and process monitoring in the rock-fluid-thermochemical subsurface environment. Consequently, CCS research reaches from the most fundamental investigations to those driven by the most applied technologies. CCS supports research in the general areas of wave propagation, geophysical inverse methods, earthquake and explosion source theory, seismic imaging, borehole geophysics, four-dimensional process monitoring and visualization technology.

Results

Results from the diverse seismological program at CCS are best demonstrated in the CCS research output. Major accomplishments flow largely from the breadth of research support provided by CCS and the cross-fertilization between applications and fundamental studies. The list of publications, produced with CCS support to varying degrees, displays the range of research accomplishments. For example, at the time this report is being prepared (March, 1999), there are more than 20 articles either published, in press or submitted to major peer-reviewed journals for 1999. The list of doctoral thesis topics developed with some CCS resource support over the years is a good measure of results and major accomplishments. On average, two or three Ph.Ds per year are produced (six in 1998) spanning a wide spectrum of research interests.

Significance of Findings

Findings for a facility and scientific environment such as that provided by CCS must be defined in the context of the multidisciplined research base that is supported there, rather than project-specific accomplishments (those appear in other sections of this report). Significance lies in the enhanced productivity and innovation that are produced by the rich mix of intellectual pursuits that come together in CCS. It is fair to attribute a large part of the scientific reputation in seismology at LBNL to the CCS environment.

Related Publications

Recent Ph.D. theses:
Kaelin, B., Seismic imaging of the shallow subsurface with high frequency seismic measurements, 1998.
Nakagawa, S., Acoustic resonance characteristics of rock and concrete containing fractures, 1998.

Selected 1999 journal publications:
Keers, H., L. Johnson and D. Vasco, Crosswell imaging using asymptotic waveforms, Geophysics, submitted.
Hubbard, S., Y. Rubin and E. Majer, Spatial correlation structure estimation using geophysical and hydrogeological data, Water Resources Research, in press.
Rubin, Y., K. Grote and S. Hubbard, Precision moisture content estimation using radar data; Applications to transportation studies, Geophysical Research Letters, submitted.


Nihei, K.T., S. Nakagawa and D.L. Hopkins, Defect detection in bonded structures using the reverberant wavefield, Rev. of Prog. in Quant. Nondestr. Eval., 18, in press.

Mars, J., J.W. Rector and S. Lazaratos, Filter formulation and wavefield separation of crosswell seismic data, Geophysical Prospecting, in press.


Herman, G.C., P. Milligan, R. Huggins and J.W. Rector, Imaging shallow objects with scattered guided waves, Geophysics, in press.


**Funding**

This work has been supported by the Office of Science, Office of Basic Energy Sciences, Division of Engineering and Geosciences, of the Department of Energy under Contract No. DE-AC03-76SF00098.
Log-Permeability Estimation Using Multiple Geophysical Data Sets Within a Bayesian Framework

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Research Objectives

Subsurface investigations often require characterization of hydraulic parameters. Conventional sampling or borehole techniques for estimating these parameters are costly, time-consuming and invasive. The difficulty of collecting representative and sufficient hydraulic property measurements using conventional sampling techniques, the large spatial variability of hydraulic properties in natural geologic systems over a wide range of scales and the dependence on the measurement support scale render measurement of hydraulic properties difficult. The purpose of this study is to explore the use of joint geophysical-hydrogeological data for estimation of hydrological parameters. As the ability to detect changes in physical and hydrological properties using geophysical data varies with the method selected, it is becoming more common for site characterizations to use multiple geophysical methods. In this study, we focus on the improvement to the log-permeability estimate offered by systematic incorporation of multiple, co-located tomographic data sets with limited hydrological data. Our estimation is performed in a stochastic framework using a Bayesian approach. Here we present the methodology followed by a case study using co-located hydrological and geophysical data from the NABIR (Natural and Accelerated Bioremediation Research Program) Oyster Bacterial Transport Site at Oyster, Virginia.

Approach

Mathematical Statement of the Bayesian Approach: The goal of the estimation procedure is to estimate \( Y(x) \) over the entire synthetic aquifer, where \( Y(x)=\ln(k(x)) \) is log-permeability and \( x \) is a vector of coordinates along a vertical plane. The data assumed available for this procedure include a limited number of permeability measurements, as well as complete sets of co-located geophysical data \( g(x) \), such as seismic velocity, seismic attenuation, electrical resistivity, dielectric constant or radar tomography data. Log-permeability is treated as a spatial random function; the available measurements are assumed to be realizations of this random function and the distribution of log-permeability at each location within the aquifer is described by its probability distribution function (pdf). The geophysical data are used to produce log-permeability estimates using a linear relationship between coincident log-permeability and geophysical measurements; thus the geophysical data are assumed to be fixed for this study. All attributes are modeled as second-order stationary random fields whose pdfs are assumed to be normally distributed. The log-permeability pdf is expressed as:

\[
f_Y(y) = \frac{1}{\sqrt{2\pi}\sigma_y} \exp \left[ -\frac{1}{2} \frac{(y-\mu_y)^2}{\sigma_y^2} \right] \tag{1}
\]

where \( y \) is a realization of the log-permeability and \( \mu_y \) and \( \sigma_y \) are the mean and standard deviation of \( Y \) that completely describe the distribution.

A log-permeability pdf can be obtained from borehole permeability measurements using a variety of estimation or inversion techniques; the result is considered to be a prior pdf, and is annotated by \( f_{Y0}(y) \). Log-permeability estimates, obtained from geophysical tomographic data together with petrophysical relationships, can be used to update this prior pdf in a Bayesian sense. The updated log-permeability pdf is referred to as a posterior pdf, and is denoted by \( f_{Y(X)}(y) \). The posterior pdf of \( Y \) at a single location in space, \( X_0 \), given additional geophysical information at that location, \( g_0(x) \), is given by:

\[
f_{Y(X_0)}(y) = f_{Y(X_0)}(y|g_0(x)) = f_{Y(X_0)}(y|\hat{y}(g_0(X_0))) \tag{2}
\]

where \( \hat{y}(g_0(X_0)) \) is the prediction of permeability based on geophysical data, henceforth abbreviated as \( \hat{y}(X_0) \). This implies that the conditional distribution of log-permeability given geophysical measurements is just a function of the predicted log-permeability based on those geophysical methods. Using Bayes’ Theorem (Ang and Tang, 1975), the posterior pdf \( f_{Y(X_0)}(y) \) can be written as:

\[
f_{Y(X_0)}(y) = \frac{f_{Y(X_0)}(\hat{y}(X_0) | y(X_0) = y) f_{y(X_0)}(y)}{\int f_{Y(X_0)}(\hat{y}(X_0) | y(X_0) = y) f_{y(X_0)}(y) dy} \tag{3}
\]

Equation (3) shows that the posterior pdf, \( f_Y(y|X_0) \), can be expressed as the product of two pdfs (the numerator) divided by a normalizing constant.

An iterative Bayesian methodology is used for log-permeability estimation. A prior pdf at each location within the aquifer, \( f_{y(X)}(y) \), is defined initially using solely hydrological measurements. This prior is then updated using information from one tomographic data set and a petrophysical relationship. For example, if estimates of log-permeability, obtained from one tomographic data set \( g_1(x) \), are available at a particular location \( x_0 \), the “first posterior” obtained using this conditional information can be expressed as:

\[
f_{Y(X_0)}(y) = f_{y(X_0)}(y|\hat{y}(g_1(x_0))) \tag{4}
\]

Equation (4) can in turn be updated using information available from another co-located tomographic data set \( g_2(x) \):

\[
f_{Y(X_0)}(y) = f_{y(X_0)}(y|\hat{y}(g_2(x_0))) \tag{5}
\]
Equation (5) yields a log-permeability field, which has been updated using two geophysical data sets, it is referred to as the "second posterior." The second posterior field can in turn be updated by information from another co-located data set, and so on. Using the assumption of Gaussianity, Baye's procedure (Eq. 3) can be implemented using a simple analytical expression. Numerical simulations show that including multiple, co-located geophysical data in the log-permeability estimation procedure using the iterative Bayesian technique presented in Equations (4) and (5) decreases the error, variance and entropy associated with the log-permeability estimate (Hubbard, 1998).

**Case Study:** The Oyster bacterial transport site is located on the southern Delmarva Peninsula, situated on the eastern coast of the United States between the Chesapeake Bay and the Atlantic Ocean. A field-scale bacterial transport study within a sandy Pleistocene aquifer is being undertaken at the Oyster Site by a multidisciplinary NABIR research team funded by the Department of Energy Subsurface Science Program. The purpose of the study was to evaluate the relative importance of physical, chemical and hydrological heterogeneities in controlling bacterial transport. This in-situ bacterial transport investigation was the first of its kind, and extensive characterization using hydrological, geological, geochemical and geophysical methods is required to build an accurate numerical flow model necessary to predict bacterial transport.

Here we integrate hydraulic conductivity information available from electromagnetic flowmeters and radar tomography data using the Bayesian approach outlined above. For this study, a single tomographic radar profile, collected using a PulseEKKO 100 system with 200 MHz central frequency borehole antennas, was analyzed. This profile begins at the bacterial injection well where flowmeter data were collected, and extends 4.7 m down-gradient in the expected injectate flowpath, which traverses the locations of three other flowmeters. The flowmeter data are reported in hydraulic conductivity ratios, or \( K_i/K_{ave} \), where \( i \) refers to the measurement interval and \( ave \) refers to the average value over the entire measured interval. The flowmeter and tomographic data were used to estimate a spatial covariance structure following a method developed by Hubbard et al. (accepted). This correlation structure was then used in an ordinary kriging routine, conditional to the flowmeter data, to obtain prior hydraulic conductivity estimates along the expected injectate flow centerline.

The prior field was subsequently updated using the Bayesian methodology (Eq. 4) with hydraulic conductivity ratio information obtained from radar dielectric constant data. This field was in turn updated using Equation (5) with hydraulic conductivity ratio information obtained from radar attenuation tomographic data. This second posterior field, obtained using flowmeter, dielectric constant, and attenuation data, is shown in Figure 1. The flowmeter data are superimposed on top of the estimated hydraulic conductivity profile. Analysis of these estimates revealed that mean error and variance associated with the estimates, calculated from the estimated fields and values from flowmeter data that were not used in the estimation procedure, were reduced when geophysical data were included in the estimation procedure at the Oyster Site.

**Significance of Findings**

The results presented here suggest that updating prior hydrological measurement estimates with successive geophysical information improves the log-permeability estimation. Numerical studies revealed that the offered improvement is more substantial far from the wellbore, where the prior estimates are more likely to be diffuse. This approach offers a practical and efficient method of incorporating multiple, co-located tomographic data sets to improve the hydraulic parameter estimation and retain the spatial structure.

**Related Publications**


**Funding**

This study has been supported by National Science Foundation Grant EAR 9628306 and by the Office of Science, Office of Biological and Environmental Research, Subsurface Science Program of the U.S. Department of Energy under Contract No. DE-AC03-76SF00098. All computations were carried out at the LBNL Center for Computational Seismology.
Research Objectives

A unique data set for the study of wave propagation in the San Andreas, California, fault zone has been acquired in the Parkfield Prediction Experiment (PPE) underway in central California. Data have been collected with a 10-station borehole network in a search for evidence of changes associated with the nucleation process of the anticipated magnitude-6 earthquake at Parkfield. More than 6,000 earthquakes have been recorded since 1987 in the magnitude range -1<\(M<5\). In addition, seismograms for 720 source-receiver paths have been obtained for repeated illumination of the network using a large shear-wave vibration (using the Vibroseis machine), from June 1987 until November 1996, when the program ended. That investigation reported significant travel-time changes in the coda of \(S\) for paths crossing the fault zone southeast from the epicenter of the 1966 \(M_6\) earthquake. Progressively decreasing travel times in the anomalous region reached 50 msecs or more by the end of the study. Changes in frequency content and polarization were also found and those effects, too, could be localized to the zone of common nucleation and rupture onset for the previous \(M_6\) earthquakes, and, possibly, the region of slip initiation for the great earthquake of 1857. The temporal pattern in these variations appears to be synchronous with changes in deformation and seismicity measured independently. Because similar variations are not seen in the waveforms recorded from microearthquakes in the same part of the fault, in previous studies we concluded that changing fluid conditions in the uppermost section of the fault zone in response to deeper, tectonic stress perturbations are the likely cause of the temporal variations. Exploring that possibility further for plausible velocity perturbations in the shallow fault zone, in this study we model the observed waveform changes numerically.

Approach

At Parkfield, the San Andreas fault zone is a striking nearvertical low-velocity zone which very clearly acts as a waveguide for seismic energy from earthquakes on the fault and from surface sources. Velocity models there show a high \(V_p/V_s\) ratio along the fault near the surface and at depth within the fault zone, and a pronounced vertical velocity gradient in the upper 2 km of the section. The geometry of the Vibroseis source and receiver network, the approximate two-dimensionality of the fault zone in the region of the travel-time anomaly and the existence of detailed \(P\) and \(S\)-wave velocity models for the area all combine to provide well-determined constraints in modeling the observations. In this study we consider only data recorded at stations VCA and JCN from vibrator site VP2. At VP2 we have the routine Vibroseis monitoring data from the repeated point source as well as a cross array of sources with 17 VPs on each leg. We confined our modeling exercise to the VP2 data for VCA and JCN for several reasons. Both source-receiver paths are in the anomalous region and reveal substantial travel-time variations. The two paths are approximately co-linear and orthogonal to the San Andreas fault, permitting the use of a 2-D formulation in simulating wave propagation. The paths sample segments of similar length on the two sides of the fault zone. Finally, the data profile from the closely-spaced source array at VP2 defines the spatial coherency of the wavefield that is helpful in phase identification and interpretation of the recorded wavefield. The velocity model used in numerical simulation incorporates the known properties of the region, where tomographic 3-D velocity models have already been determined. A major factor controlling the character of wave propagation at short range from a surface source is the severity of the shallow vertical velocity gradient. We found a velocity gradient model by matching the observed and computed direct arrivals in the early part of seismograms. For the NE side of the fault, the direct arrivals at JCN could be matched with a velocity profile reduced to 0.76 of that for VCA, and to 0.5 for the narrow fault zone, modeled as a vertical layer with a thickness of 200 m, bounded by interfaces \(F_1\) and \(F_2\). Computations were performed using a 2-D elastic finite-difference formulation with a staggered grid. The model was digitized on a 2200 x 500 grid with 5 m spacing, which yields a model space of 11 km horizontal and 2.5 km vertical extent, as depicted in Figure 1.

Results

A snapshot of elastic field development is shown in Figure 1. Two features dominate the process: energy trapping near the surface by the shallow gradient and wavefield scattering from the fault zone. Most of the energy is confined to the upper part of the section in multiple reflections at the free surface, producing a complex train of surface-guided waves made up of many arriving phases.

Synthetic seismograms (horizontal component) are shown in Figure 2. Initial direct \(P\) and \(S\) waves arrive at VCA at around 1 and 2 seconds, respectively. At JCN they are seen at 2.2 and 4.4 s.

![Figure 1. A snapshot of wavefield propagation from VP2 source at 2 seconds.](image)
The magnitude of the calculated travel-time variations match with the initial P-wave and increases throughout the seismogram. The latter are especially strong for P-waves, e.g., PS, PPS, etc. Strong reflections are also produced by the fault-zone boundaries, F1 and F2. PF1E, the first F1 reflection at VCA, is small and masked by the large direct S-wave just before it. F2 reflections at VCA have passed twice through the fault zone, and these late phases, such as PF2PP (3.5 s) and SF2S (4.7 s), are quite strong, arriving well after the direct waves have passed. At JCN the internal fault-zone reflections produce sequences of strong, distinct arrivals following the direct P- and S-waves. The times in the synthetic seismograms where large travel-time changes were observed in the monitoring project at VCA and JCN contain significant energy that has been scattered from the fault zone. This result suggests a ready explanation for the cause of the observed progressively decreasing travel-times. For the path VP2-VCA the changes were seen at arrival times after 3.5 s, i.e., for our model seismograms, after the direct waves have passed and the fault-zone reflected waves are arriving. On the other hand, the travel-time changes for the VP2-JCN fault-crossing path begin with the arrival of the direct P-wave and occur through the entire seismogram. We take these results to be strong evidence that the observed variations are most likely caused by changes within the fault zone itself. To test the fault-zone hypothesis we modeled travel-time variations that would be produced by a small velocity change at the fault. To compare with seismograms for the reference model described above, we computed new seismograms at VCA and JCN for a velocity increase of 6% localized in the narrow fault zone. These seismograms are shown in Figure 2 along with their differences from the reference traces. As expected, the changes at VCA appear only after the fault-zone F2 reflections reach the station, while at JCN the travel-time advance begins with the initial P-wave and increases throughout the seismogram. The magnitude of the calculated travel-time variations match the observed data quite closely. In Figure 3 we make a direct comparison with the Vibroseis data, where the synthetic-derived variations are plotted with the observed travel-time shifts at both stations. The match is quite good in character, magnitude and timing. The first unstable waveform at VCA corresponds well to the PFZPP reflection from the fault zone. At JCN the pattern of steady increase in the travel-time shift due to progressive involvement of slower S-waves is quite clear.

Significance of Findings

Previous studies clearly detected real changes in travel-times in the eight-year controlled-source monitoring program at Parkfield, and localized the anomalous changes to a region southeastward from Middle Mountain, roughly in the presumed nucleation zone for the past and future M6 Parkfield earthquakes. Their best hypothesis for the phenomenon called for changing fluid conditions in the shallow section above the fault zone. Our study supports that hypothesis and offers a more quantitative model for the actual wave propagation involved. The final link in the puzzle lies in the responsible mechanism for the velocity change in the fault zone. We are inclined to accept the idea of a deeper tectonic deformation that somehow changes the fluid environment in the shallow fault zone. The striking importance of the shallow vertical velocity gradient cannot be overstated. It is clear from this study that surface sources employed in highly heterogeneous environments such as the San Andreas fault zone can be expected to generate an overwhelming near-surface wave field that must be dealt with in looking for deeper images. If the individual phases can be identified, however, they may provide an important tool for studying near-surface details of the fault structure.

Related Publication


Funding

This work has been supported by the U.S. Geological Survey through NEHRP award 1434-95-G-2540 and through the Office of Science, Office of Basic Energy Sciences, of the U.S. Department of Energy under Contract No. DE-AC03-76SF00098. Data processing was done LBNL's Center for Computational Seismology.
Research Objectives

A computationally efficient overlap domain decomposition (ODD) technique based on Huygens' Principle has been developed for modeling wave propagation. The ODD technique divides a large domain into several smaller overlapping subdomains and allows the exchange of waves between subdomains through the overlapping regions without the need for any internal interface connecting conditions. Calculations are performed independently in each subdomain, and the wavefield in the whole domain is then obtained from the local solutions in the subdomains. The ODD technique is not restricted to a specific numerical method for solving the wave equation and different methods can be used in each subdomain. This flexibility is particularly advantageous because it enables very accurate but computationally expensive methods to be used in selected subdomains to achieve a desired level of accuracy and computing speed. In addition, calculations can be "turned-off" in subdomains that do not have appreciable wave activity, resulting in savings in computing time and memory use.

Approach

A detailed description of the overlap domain decomposition (ODD) technique is given in Fan (1998). Here, we present a specific application of the ODD technique to the finite difference method.

To apply the ODD technique to the finite difference (FD) method, we must first determine the appropriate size for the overlap areas. Starting with the 1-D wave equation for a medium with a constant density \( \rho \)

\[
\frac{1}{c^2} \frac{\partial^2 p(x,t)}{\partial t^2} = \frac{\partial^2 p(x,t)}{\partial x^2},
\]  

where \( p \) is the pressure and \( c \) is the velocity. The explicit finite difference scheme for fourth-order space and second-order time

\[
p(x_{m+1}, t_{n+1}) = 2p(x_m, t_n) - p(x_{m-1}, t_n) + \frac{c^2\Delta t^2}{12\Delta x^2} \left[ -30p(x_m, t_n) + 16p(x_{m-1}, t_n) - p(x_{m-2}, t_n) \right]
\]

accuracy is

To apply the ODD technique to Equation (2), we divide the domain \( \Omega \) into two subdomains \( \Omega_1 \) (dark shaded area) and \( \Omega_2 \) (light shaded area) shown in Figure 1, where grid points 1, ..., \( m-2, m-1, m \) belong to \( \Omega_1 \) and grid points \( m+1, m+2, ..., M \) belong to \( \Omega_2 \). Grid point \( m \) is the last point in \( \Omega_1 \) where the spatial derivative must be computed. Point \( m+1 \) is the first point in \( \Omega_2 \). The amount of overlap required between these two subdomains can be determined as follows. According to Equation (2), in order to compute \( p(x_{m+1}, t_{n+1}) \) in \( \Omega_1 \), the values of two previous time steps are needed from the grid points \( m-2 \) through \( m+2 \). Assume that the pressures \( p(x_i, t_n) \) and \( p(x_i, t_{n-1}) \) for \( i = 1, 2, ..., M \) at time step \( n \) and \( n-1 \) are known values. If \( \Omega_1 \) is overlapped to cover the grid points \( m+1 \) and \( m+2 \), then \( p(x_{m+1}, t_{n+1}) \) can be solved within \( \Omega_1 \).

The grid points \( m+1 \) and \( m+2 \) that originally only belonged to \( \Omega_2 \) now also belong to \( \Omega_1 \). Thus, these points form the overlap region. The pressure \( p(x_{m+1}, t_{n+1}) \) can be computed from \( \Omega_1 \) just as in the conventional finite difference method. Similarly, for the grid point \( m+1 \) in \( \Omega_2 \), the addition of two grid points \( m-1 \) and \( m \) to \( \Omega_2 \) allows the calculation of \( p(x_{m+1}, t_{n+1}) \) at the grid point \( m+1 \) in \( \Omega_2 \) using the values of \( p \) from grid points \( m-1 \) and \( m+3 \). The total overlap region now spans the grid points from \( m-1 \) through \( m+2 \). As can be seen from this analysis, the overlap region only requires four grid points.

\[
\begin{align*}
\Omega_1 & : m-2, m-1, m, m+1, m+2, m+3, \ldots \ M \\
\Omega_2 & : 1, 2, \ldots, m-1, m, m+1, m+2, \ldots, M \\
\end{align*}
\]

Calculate at grid point \( m \) in subdomain \( \Omega_1 \)

Combine two subdomains together to get \( p \) at all grid points

\[
\begin{align*}
\Omega & : 1, 2, \ldots, m-2, m-1, m, m+1, m+2, m+3, \ldots \ M \\
\end{align*}
\]
Overlap Domain Decomposition Technique for Modeling Wave Propagation

Results

Several advantages of the ODD technique can be illustrated with the following example of two-dimensional elastic wave propagation in a low velocity layer. The computational domain is divided into nine subdomains with overlap areas that are shared between neighboring subdomains. These overlap areas allow transfer of the wave from one subdomain to the next, as described in the previous section.

During the course of the calculation, the wavefield may not have spread over the entire domain, particularly at early time steps. The calculations in these inactive subdomains are not necessary and can be "turned off." Figure 2 shows snapshots of the wavefield for the nine-subdomain model. At the earlier time step, the wavefield is present only in subdomain $\Omega_6$. Thus, computation of the wavefield need only be performed in this subdomain. Similarly, at the later time step, computations in all the subdomains except $\Omega_7$, $\Omega_4$ and $\Omega_7$ can be turned off. This simple procedure can save a significant amount of computing time.

Significance of Findings

The ODD technique is a flexible framework that allows a large computational wave propagation problem to be divided into many smaller problems. The technique can incorporate different numerical methods for solving the wave equation (e.g., finite difference, pseudo-spectral, staggered grid methods) in each subdomain to achieve a desired level of accuracy, computing speed and memory usage. In addition, the ODD technique has the ability to "turn off" subdomains that contain little or no wave activity. This feature can be used to save computation requirements in problems with localized wavefields. Finally, the ODD framework is ideal for parallel computing because of the modular nature of the algorithm. Future work will explore the application of the ODD technique to 3-D wave propagation problems using parallel computers.

Related Publications


Funding

This work has been supported by the Office of Science, Office of Basic Energy Sciences under U.S. Department of Energy Contract No. DE-AC03-76SF00098.
Research Objectives

When subjected to compressive stresses, a granular rock is reduced in volume by the deformation of the compliant grain contacts and solid grains and by compaction due to frictional slip between grains. While the first two processes have been studied extensively in the context of linear elasticity, fewer studies have examined the role of nonlinear grain contact deformation and frictional intergranular slip on the volumetric strain of granular rocks. An understanding of these processes and their contributions to the deformation of rock is important in many areas of the geosciences, including reservoir production and stimulation. The objective of this work is to investigate the basic character and effects of grain contact nonlinearity and frictional slip on the volumetric strain of sandstone using a Hertz-Mindlin sphere pack model and stress-strain measurements on Berea sandstone. Here, we summarize several of the findings from the analysis of the sphere pack model.

Approach

There are a number of closed-form analytic solutions for the stress-strain behaviors of regular packings of identical spheres (e.g., simple cubic, face-centered cubic, hexagonal close-packed) that were developed by Mindlin and others. These models have the disadvantage of lacking grain packing disorder, grain angularity and intergranular cementation that are prevalent in most sandstones. However, because these models do include the contributions of grain contact nonlinearity and frictional slip to the volumetric strain, they represent a logical starting point for the investigation of the effects of friction on the nonlinear, hysteretic deformation of sandstones.

To examine the contribution of friction to the volumetric strain of granular rock, we use the face-centered cubic packing (fcc) model of spheres of identical size and properties (Figure 1). This model is one of the densest regular arrays of elastic spheres with a porosity of 25.95% and a coordination number of 12. Both the effects of Hertzian grain contact deformation and Mindlin-type intergranular slip are included in the model. The primary advantage of using an idealized model of rock is that closed-form stress-strain relations can be derived for loading, unloading and reloading paths.

Results

Analysis of the fcc packing stress-strain relations for uniaxial strain consolidation along the z-axis revealed that the elastic modulus that describes P-wave velocities are path-independent functions of the axial strain

\[ \sigma_{zz}^{\text{nonlin}} = \left[ \frac{\mu (4 - 3v)}{(1-v)(2-v)} \right] \varepsilon_{zz} \left( 1 + \frac{3}{2(1-v)(2-v)} \right) \varepsilon_{zz}^{3/2} \]  

where \( \mu \) and \( v \) are the shear modulus and Poisson’s ratio of the grains, respectively. By integrating this modulus, it is possible to construct a new stress-strain curve that is identical for loading and unloading paths:

\[ \sigma_{zz}^{\text{locked}} = \int_{0}^{\sigma_{zz}} \frac{\mu (4 - 3v)}{(1-v)(2-v)} \varepsilon_{zz} \left( 1 + \frac{3}{2(1-v)(2-v)} \right) \varepsilon_{zz}^{3/2} \]

Figure 1. Face-centered cubic packing of identical spheres.

Figure 2. Comparison of the volumetric strain resulting from nonlinear grain contact deformation and frictional slip compaction for the fcc sphere packing.
Simple inversion of this stress-strain relation yields an expression for the volumetric strain resulting from nonlinear deformation of the grain contacts that is path-independent (i.e., it depends only on the final stresses and not on the historical sequence of stresses to which packing was subjected):

\[
\varepsilon_{zz}^{\text{nonlin}} = \left[ \frac{3(1-v)(2-v)}{2\mu(4-3v)} \right]^{2/3} \sigma_{zz}^{2/3} .
\]  

(3)

Using this expression, the total volumetric strain for uniaxial strain consolidation along the z-axis can be decomposed into contributions due to (path-independent) nonlinear grain contact deformation and (path-dependent) frictional slip compaction:

\[
\varepsilon_{total} = \varepsilon_{nonlin} + \varepsilon_{friction} .
\]  

(4)

It is of interest to determine the relative magnitudes of the nonlinear and frictional contributions to the total volumetric strain. Figure 2 shows the volumetric strain of the fcc packing for a range of friction coefficients. The frictional slip contribution (for the loading path) approaches zero for large friction coefficients and a maximum (54% of the nonlinear contribution) as the friction coefficient approaches zero. While the nonlinear contribution dominates, the frictional component can be significant when the friction coefficient is low.

**Significance of Findings**

The results of this study highlight the importance of considering frictional effects when attempting to evaluate the volumetric strain of sandstone. For the specific conditions of this study (i.e., uniaxial strain loading, unloading and reloading paths), frictional slip between grains was shown to result in a path-dependent volumetric strain. However, for these conditions, the nonfrictional part of the volumetric strain can be extracted by integration of the path-independent, small-strain elastic moduli obtained from seismic velocity measurements made at different static loads. Additional work is needed to determine both the magnitude and character of the path-dependence of the volumetric strain and the anisotropic elastic moduli of sandstones, and to determine if the analysis presented here can be extended to general three-dimensional loading.

**Related Publication**


**Funding**

This work has been supported by the Office of Science, Office of Basic Energy Sciences under U.S. Department of Energy Contract No. DEAC03-76SF00098.
Research Objectives

Seismic, electromagnetic and hydrological modeling and inversion are important to the field of oil exploration, environmental sciences, CO2 sequestration and atmospheric sciences. Many imaging approaches in geophysical research areas are based on deterministic and traditional nonlinear inversion. Because the data are often incomplete and contaminated by random noise, the deterministic approach does not provide accurate or stable solutions. During the iteration of the traditional nonlinear inversion, inexact reflections of the artificial boundary condition enter the inversion domain; these degrade resolution and even cause divergence. The discretization of the volume integral equation is ill posed and its full matrix needs very large storage and lengthy computational time. The conjugate gradient (CG) method requires a long computation time and often terminates in local minima, thus producing a wrong result. Our objective is to develop a new parallel stochastic Global Integral and Local Differential (SGILD) electromagnetic (EM), seismic and hydrological modeling and coupled inversion. This method can overcome the shortcomings of traditional deterministic nonlinear inversion. We have derived new integral equations for magnetic, acoustic and flow field in the frequency domain (Xie and Li, 1995 and 1997) and time domain (Xie et al., 1999). We couple the integral equation on the boundary and differential equation in the interior of the domain to develop SGILD modeling. We couple the Jacobian volume integral equation on a small selected sub-domain and variation differential equation on the remaining large sub-domain to develop SGILD inversion for updating the electric conductivity/permittivity, seismic velocity and hydrological conductivity. We use a new hybrid direct-iteration algorithm and a regularizing method associated with the constitutive law to solve the equation.

Approach

**Stochastic GILD modeling and inversion:** The outline of the SGILD method is as follows: (1) we decompose the domain into the two subdomains; (2) we use a new stochastic moment integral equation on the boundary and moment differential equation in the interior of the domain to calculate the moments of the wave field in the modeling; (3) we use new Jacobian volume moment integral equations in the small selected subdomain and variation differential equations in the remainder large subdomain for the joint inversion. Supposing that the parameters and data are random variables, we derive the new integral and differential equation system for the statistical moments of the mean, covariance, and standard deviation. We use our parallel SGILD algorithm to solve the moment integral and differential equations and obtain the high resolution imaging of the mean impedance, covariance standard deviations and confidence interval for the acoustic velocity, electric conductivity and flow conductivity, etc. The advantages of our SGILD method are that: (1) we use the global integral equation and local differential equations to compensate each other to improve the ill-posed property and obtain high resolution; (2) replacing the artificial approximate boundary condition, we use an exact integral equation on the boundary to greatly reduce numerical noise; (3) we decompose the full matrix into several small sparse matrices and one small full matrix, we solve these small matrices, in parallel, and greatly reduce computational time and storage; (4) we can use the SGILD method for large-scale oil exploration, marine exploration, and atmosphere prediction. The basic frame of our SGILD coupled inversion is the GILD modeling and inversion method.

**New Magnetic integral equations in the time domain:** Because most hydrological data is measured in the time domain, we develop the joint inversion in the time domain. We derive a new integral equation

\[
\mathbf{H}(t, \mathbf{r}) = \mathbf{H}_b(t, \mathbf{r}) - \mathbf{N} \int \left( \frac{1}{\varepsilon} \mathbf{\sigma}_t - \frac{1}{\varepsilon_b} \mathbf{\sigma}_b \right) d\mathbf{r},
\]

and differential equation

\[
\nabla \times \mathbf{H}_t \left( \nabla \times \mathbf{G}^M_b \right) d\mathbf{r},
\]

for the magnetic field in the time domain (Xie et al., 1999) where \( \mathbf{N} \) is the unit that makes the integral quantity unit of the right-hand side of the equation a magnetic unit, \( \mathbf{G}^M_b(r', r) \) is the magnetic Green tensor, \( \mathbf{E}^M_b(r', r) \) is the electric tensor, and \( *t \) is a convolution.

Similarly, we derive the integral equation for seismic and hydraulic inversion in the time domain. The new integral equation (1) will be important progress in electromagnetic theory and application.

We use Bayes theory, the new integral equations in the selected subdomain and differential equations in the remainder subdomain to develop the SGILD geophysical and hydrological modeling and coupled inversion in the time domain.

**GILD regularizing:** We find that the ill-posed property of the inverse problem is relative to the constitutive law. We use a new constitutive term to construct the new GILD regularizing operator.
Results

We use the SGILD algorithm for hydrological conductivity, electric conductivity and seismic velocity imaging. An axis symmetric SGILD conductivity code is tested primarily using synthetic data. Mean conductivity imaging and standard deviations are presented. In Figure 1, 18 injection point sources are located in a single hole. The 72 point receivers are located in the same hole.

We use the synthetic model to create head response synthetic data with Gaussian noise in one and two months; the maximum standard deviation of data is 5%. The imaging of the mean conductivity is obtained (Figure 1c). The total maximum standard deviation (TSTD) of the conductivity is 11.8%. The local standard deviation (LSTD) of the conductivity of the target at the left side corner is 6%. The local standard deviation of conductivity on the right side is 18.6%; that is because the left side is closed to the area of the data site in the single hole. The 2-D mesh is 148 x 128, 16 x 18 CPU minutes in MPP and 68 iterations are used. The optimized mean regularizing parameter is 0.687456E-6. A coupled acoustic, electromagnetic and flow head inversion is used to obtain conductivity imaging as shown in Figure 1b. It is obvious that the conductivity imaging from the coupled inversion has higher resolution than the single inversion imaging shown in Figure 1c. SGILD resistivity imaging from practical field data in the geothermal exploration site is obtained. The maximum standard deviation of the resistivity is 18.8%; the local standard deviation of resistivity near the borehole area is 11%.

Significance of Findings

The preliminary tests show that the SGILD modeling and inversion is a high-resolution, robust, stable and high-performance parallel imaging algorithm. There are obvious improvements of resolution of the moments from the field data. We use these moments to estimate the uncertainty and construct confidence intervals and consistent conditions. The GILD and SGILD method discussed here is capable of overcoming the limitations of the conventional inversion and can accurately handle high-resolution through the joint nonlinear inversion of coupled hydrological and geophysical data. The GILD method can become a powerful imaging tool for DOE environmental remediation, geophysical exploration, CO2 sequestration and atmosphere sciences.

Related Publications


Funding

This work has been supported by the Office of Science, Office of Basic Energy Sciences, Division of Engineering and Geosciences of the U.S. Department of Energy under Contract No. DE-AC05-76SF00098.
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 and Sweden. The program has established the Center for International Radioactive Waste Studies, the main purpose of which is to foster relationships with other countries in order 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 will be located about 350 m below the surface within a thick unsaturated zone (UZ). The subsurface rocks at Yucca Mountain consist primarily of fractured volcanic tuffs that vary in the degree of welding. To date, a total of 60 deep surface boreholes have been drilled in the area. In addition, an 8-km-long underground tunnel, the Exploratory Studies Facility (ESF), was completed at Yucca Mountain in 1996.

Berkeley Lab's work at Yucca Mountain consists of solving many ground-breaking problems related to multiphase, nonisothermal flow and transport through the UZ. Some of the key questions 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 matrix blocks?
- How much of this water will seep into the waste canister emplacement drifts?
- How will the water containing radionuclides migrate from the repository to the water table?
- How will coupled TH (thermo-hydrological), THC (thermo-hydrologic-chemical) and THM (thermo-hydrologic-mechanical) processes affect flow and transport?

The Nuclear Waste Program is organized into three main groups — Ambient Testing, Thermal Testing and Modeling — to address these questions, with support from geophysical 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 the fracture/matrix interaction test, the drift-to-drift test, the Paint Brush Unit test (PTn test), and niche testing. The fracture/matrix interaction test is a relatively small-scale (several meters) test that focuses on the components of water flow in fractures and matrix blocks and the interaction between the two continua. The drift-to-drift test addresses 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, being above the potential repository, is key to dispersing fracture flow from the above fractured units and buffering the transient behavior of episodic flow. The niche studies address perhaps the most crucial problem of Yucca Mountain; i.e., deter-
mining the fraction of water that will flow into the emplacement drifts. The niche studies are carried out by introducing water into boreholes above the 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 thermo-dynamic 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 drift over 80 m long. This second heater test is intended to resemble the actual in-place conditions when the high-level radionuclide waste is placed in the emplacement drifts. Berkeley Lab’s role in the tests is 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 perform predictive thermo-hydrological and thermo-hydrologic-chemical calculations.

The initial characterizations of the heater test areas are performed with air injection tests that yield the 3-D permeability structure of the fracture network. Continued air-injection testing during the heating and cooling phases of the heater test yielded changes that can be attributed to changes in fracture saturations or mechanical effects.

Cross-hole radar tomography has also yielded very promising results regarding change in global saturations of the system due to heating. Detailed 3-D thermo-hydrologic and thermo-hydrologic-chemical calculations were used to predict the behavior of the tests. These will be refined to better fit observations as the test progresses. Finally, Berkeley Lab scientists are involved with measurements of the isotopic compositions of condensate water that have seeped into the boreholes.

**Modeling Group**

Berkeley Lab has the primary responsibility for the development of the UZ flow and transport model. This is a comprehensive 3-D, dual permeability numerical model that represents the entire unsaturated zone 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 the model predictions and the subsequent observations gives a measure of the reliability of the model and guidance to what additional data need to be collected and incorporated.

A very important sub-model 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, in a similar fashion as the UZ model, predicts the results of the niche tests, and is modified subsequently to match the actual observations. Another sub-model of the UZ model is the Coupled Process THC model, which is calibrated using the heater test data and used to estimate the chemistry of water and gas entering the drifts. All three 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**

Research Objectives

The potential exists for a capillary barrier to form in unsaturated porous media at the boundary between a fine-grained unit, such as a highly fractured rock, and an underground cavity. Conditions such as these exist at the proposed radioactive-waste repository located at Yucca Mountain, Nevada. If licensed and constructed, the monitored geologic repository will include 117 km of mine openings or waste emplacement drifts housing containers of radioactive waste. The repository would be constructed in the unsaturated zone at least 200 meters (m) below the land surface and at least 200-250 m above the regional water table within the fine-grained Topopah Spring Tuff (Tpt), a densely welded, intensely fractured, ash-flow tuff.

It is important to determine whether a capillary barrier will exist above a waste emplacement drift because such a barrier can have a direct impact on waste isolation and repository performance. Water introduced at the land surface during a natural precipitation event, assuming it migrates to the repository level, may be excluded from seeping into the drift and instead may be diverted laterally around the opening if a capillary barrier exists. In contrast, if a capillary barrier does not form, then water may drip into the opening and come in contact with the waste packaging, hastening canister corrosion and failure, and potentially leading to radionuclide migration to the accessible environment.

An extensive series of liquid-release tests was performed above a specially constructed drift, called a niche, located in the Exploratory Studies Facility at Yucca Mountain to determine whether a capillary barrier exists. In addition, the tests were used to quantify the seepage threshold flux, defined as the liquid-release flux at and below which water will no longer seep into the opening.

Approach

Seven 10-m-long boreholes were drilled at the niche to gain access to the rock for air injection and liquid-release tests prior to mining the niche. Three of the borings (shown in Figure 1) were installed approximately one meter apart, 0.65 m above the crown of the niche in the same horizontal plane. The remaining boreholes were drilled within the limits of the proposed niche and were subsequently removed when the niche was constructed and before the seepage tests were performed. All the boreholes were installed parallel to the axis of the niche.

More than 200 air-injection tests were conducted in the boreholes prior to excavation to determine the distribution of air permeability within the rock mass and to select test intervals for subsequent liquid-release tests. Next, a series of liquid-release tests were conducted by pumping water containing colored or fluorescent dyes at a constant rate into a select number of packed-off zones previously tested with air. A finite amount of dye-spiked water was introduced into each test interval, with essentially no pressure buildup, to document the relatively undisturbed flow path traveled by the wetting front.

The niche was excavated dry using a mechanical excavator to observe and photograph the distribution of fractures and dye within the rock. Dye was observed along individual fractures as well as along intersecting fractures to depths ranging from 0 to 2.6 m below the release points. Two primary types of flow paths were observed during the mining operation, including: (1) flow through individual or small groups of high-angle fractures, and (2) flow through several interconnected low and high-angle fractures creating a fracture network.

Air-injection tests were repeated in the upper boreholes after the niche was excavated to determine the post-construction distribution of air permeabilities. The geometric mean air permeability for all the boreholes tested increased dramatically by nearly two orders of magnitude after the niche was excavated, probably due to mining-induced damage to the formation.

Forty short-duration seepage tests were conducted after the niche was excavated by pumping water at a constant rate into the boreholes located above the niche. After water appeared at the niche ceiling and dripped into a specially constructed capture system located within the niche (Figure 2), it was collected and weighed. The mass of water captured ranged from 0 to 568.6 grams per test. The seepage percentage, defined as the mass of water that dripped into the capture system divided by the mass of water released, ranged from 0% for very low permeability zones to 56.2% for

Figure 1. Test configuration above the niche representing a waste emplacement drift.
predominately gravity driven flow through highly saturated fractures.

**Results**

The seepage threshold data were interpreted using an analytical solution describing the exclusion of water from a buried cylindrical cavity analogous to a niche. The resulting analysis produced estimates of the quantity $2\alpha^{-1}$ defined as the sorptive length, a useful parameter that characterizes the capillary properties of the unsaturated medium. Values of $2\alpha^{-1}$ equal to 19.6 and 981 Pascals were measured and believed to be representative of flow through two types of in-situ fractures, including individual or small groups of high-angle fractures and fracture networks, respectively. The sorptive number $\alpha$ was used along with wetting front arrival times to estimate fracture-water characteristic curves (volumetric water content, $\Theta$, versus water potential, $\Psi$) for several test zones. These curves indicate that the residual $\Theta$ may be on the order of 0.1% and that the saturated $\Theta$ (i.e., effective porosity) may be as high as 2.4% for the seepage flow paths tested.

**Significance of Findings**

Direct field observation, indirect field evidence and analytical and numerical models were used to confirm that a capillary barrier exists above an underground cavity. In addition, the seepage tests demonstrated that a seepage threshold flux does exist below which water will not seep into the opening. The results of this investigation and future studies will be used in part to design and construct the monitored geologic repository.

**Related Publications**


**Funding**

This work has been supported by the Director, Office of Civilian Radioactive Waste Management, through Memorandum Purchase Order EA9013MC5X between TRW Environmental Safety Systems, Inc., and Ernest Orlando Lawrence Berkeley National Laboratory for the Yucca Mountain Site Characterization Project under U.S. Department of Energy Contract No. DE-AC03-76SF00098.
Spatial and Temporal Flow Variability in the Paintbrush Nonwelded Tuff

**Research Objectives**

An understanding of processes influencing percolation flux, and the partitioning of flow between the matrix and fractures and/or faults, is important for the development of an appropriate conceptual model of flow for Yucca Mountain, Nevada. Of particular importance is the role of the Paintbrush Nonwelded Tuff (PTn), through which downward percolation must pass prior to reaching the potential repository horizon (i.e., the fractured Topopah Spring Welded (TSw) unit). A fundamental question is whether the PTn is effective in dampening pulses of localized infiltration, providing a generally uniform percolation flux to the TSW, or whether flow is localized through preferential flow paths in the PTn.

We have carried out field studies of flow through the variably altered, nonwelded PTn. The overriding objective of this effort was to gain insight into flow dynamics along a fault and within the altered matrix of the PTn. Specifically, the objectives were to measure flow velocities, seepage rates and wetting front migration within a fault and in the matrix of the PTn. The tests were designed to mimic conditions analogous to the introduction of focused flow to the PTn from the overlying fractured Tiva Canyon (TCw) unit during transient high infiltration events.

**Approach**

Field experiments were conducted in the north face of Alcove 4 within the Exploratory Studies Facility (ESF). In the north face of Alcove 4, the PTn is cut by a normal fault with a small offset (~0.25 m) and a high angle fracture (Figure 1). In-situ flow experiments involved the release of different volumes and rates of tracer-tagged water in intervals 0.3 m in length along horizontal boreholes intersecting the fault and matrix. Twelve 0.075-m diameter boreholes were drilled perpendicular to the plane of the north face of Alcove 4 for liquid release and monitoring. Changes in percolation rates and saturation were monitored using a nest of boreholes installed with psychrometers and electrical resistivity probes (ERPs). A slot 4 m wide, 4 m deep and 0.3 m high was excavated below the test bed to collect any injected fluid percolating downward.

The nature of matrix flow in the PTn was investigated using boreholes 5, 6, 7 and 8 (Figure 1), located in a section of the test bed that was determined to be free of fractures and faults. Water was continuously injected under constant head conditions into a zone located between 2.44 and 2.74 m from the collar in borehole 5, for a period of 29 days, while changes in saturation and water potential were monitored along the lengths of boreholes.

![Figure 1. Geological sketch and borehole/slot layout for the north face of Alcove 4.](image-url)
Two boreholes (11 and 12) were positioned to intercept the fault at a distance of ~1.4 m from the alcove face and used to determine specific flow characteristics of the fault. Here, water was injected under a constant head condition in borehole 12 at a distance of 1.4 m from the collar (i.e., along the fault) during seven separate release events. During and after the release events, changes in saturation and water potential were continuously monitored in borehole 11.

**Results**

Liquid-release tests suggest that a large variability exists in the hydrologic response between the fault and matrix in the Alcove 4 test bed. Two components of the test that demonstrate this variability are the measured rates of liquid release and the capacities of the matrix and fault to transmit water.

**Flow dynamics in the matrix:** When water was released into the matrix in borehole 5, the rates at which the matrix absorbed water rapidly decreased from >50 ml/min to <1 ml/min in less than five hours. During this early stage of the test ~1.7 liters of water had been released to the formation. During the next eight days the liquid release rate to the formation continued to decrease, asymptotically approaching 0.14 ml/min after ~4.0 liters of water had been released. This rate then persisted for the remainder of the test.

The wetting front in the matrix was detected 0.5 m below the point of release 10 days after the test was started. Here changes in saturation were detected by a single ERP located 2.9 m from the collar in borehole 6.

**Flow dynamics in the fault:** Liquid-release rates in the fault gradually fell from ~200 ml/min to 50 ml/min over a period of 41 hours, during which 200 liters of water percolated into the fault. A wetting front was observed along borehole 11 over a distance of 1.5 m following the seven release events in borehole 12. This wetting front can be inferred from the decrease in resistivity at various distances from the collar (as shown in Figure 2). Initially, wetting was observed along the projected fault, but with subsequent tests the wetting width increased. At the fault (i.e., at a distance of 1.4 m from the collar), the ERPs responded to individual release events, showing a wetting trend during fluid injection and a drying trend between and after the release tests. Further from the fault, the probes detected gradual increases in moisture for the duration of the tests. The travel time of the wetting front within the fault from the injection zone in borehole 12 to borehole 11, a distance of 1.0 m, was initially 3.3 hours and gradually increased to 10 hours.

**Significance of Findings**

These series of experiments have demonstrated for the first time that active flow tests can be conducted within a fault in the vadose zone of Yucca Mountain. Techniques developed during the design of these experiments have permitted investigations of specific hydrologic properties of a fault located within the PTn.

Results to date suggest that the variably altered PTn matrix at Alcove 4 dampens flow pulses. Tests in the fault suggest that as increasing amounts of water are introduced into the fault, the rate at which water can be released to the fault continuously decreases. Travel times within the fault were found to be dependent both on the release rates (i.e., for fast release rates the travel times were faster), and wetting history (i.e., in successive injections travel was faster, but with delays of 4-6 days between injections, travel times were significantly slower).

**Funding**

This work has been supported by the Director, Office of Civilian Radioactive Waste Management, through Memorandum Purchase Order EA9013MC5X between TRW Environmental Safety Systems, Inc., and the Ernest Orlando Lawrence Berkeley National Laboratory for the Yucca Mountain Site Characterization Project under U.S. Department of Energy Contract No. DE-AC03-76SF00098.
Research Objectives

The view of fractures as primary conduits for flow in the unsaturated zone of Yucca Mountain, Nevada, has replaced the belief of the last decade, which held that flow primarily occurred through the rock matrix under ambient conditions. This shift in paradigm has resulted from indirect evidence of fracture flow as suggested by a relatively young perched water table below the Topopah Spring Welded (TSw) unit, mineral deposits on fractures, and the detection of bomb-pulse $^{36}$Cl in isolated locations within the mountain. However, direct evidence of fracture flow remains elusive, largely because of technical difficulties encountered in locating and measuring fracture flow in this underground site.

This paper presents the results of a field investigation of fracture flow in the Exploratory Studies Facility (ESF) at Yucca Mountain. The objective of this effort was to estimate hydraulic parameters such as formation intake rates, flow velocities, seepage rates and fracture porosities using techniques developed for in-situ testing of flow in fractured rock. Field tests were designed to mimic conditions analogous to releases of contaminated fluid from the rupturing of containers or from transient high infiltration events leading to focused flow (i.e., point source releases of 5–20 liters of fluid).

Approach

Field experiments were conducted on the right rib of Alcove 6 in the Main Drift of the ESF (Figure 1a). The test bed was situated in the middle nonlithophysal portion of the Topopah Spring Tuff. Two distinct features defined the layout of the field experiment: horizontal boreholes and a slot (Figure 1b). Four boreholes were drilled perpendicular to the alcove wall. Of these, one (borehole A) was used for fluid injection while the other three (boreholes B, C and D) were monitored for changes in moisture conditions. A slot excavated below the test bed was used to observe the location and amount of water seeping from the formation above. There were three distinct components to the flow investigation: (1) controlled release of water into isolated zones, (2) borehole monitoring for changes in saturation and water potentials, and (3) monitoring of seepage from the slot ceiling.

Experiments were conducted to determine flow dynamics resulting from liquid release in two zones of different permeabilities within a single borehole (borehole A). These zones were identified from air-permeability measurements to lie 0.75–1.05 m (low permeability) and 2.30–2.60 m (high permeability) from the borehole collar. In both the high permeability zone (HPZ) and low permeability zone (LPZ), a series of tests were conducted to determine the temporal changes in the rate at which the formation could take in water. In the HPZ, a second series of tests was conducted during which the injection rates were changed and the seepage rate into the slot was monitored. During the entire duration of the experiments, saturation and water potential changes along the monitoring boreholes were continuously measured, and water that seeped into the slot was periodically sampled and analyzed for tracer concentrations.

Results

The rate at which water moved into the LPZ steadily decreased with time, asymptotically approaching a steady rate (~0.35 ml/min). In the HPZ, the rates varied significantly during
Field Investigations of Fracture Flow in Welded Tuffs

Figure 2. Seepage response observed in the slot in Alcove 6 in the ESF

and between tests. In the two monitoring boreholes located below the injection borehole (C & D), changes in saturation were detected both by the electrical resistivity probes (ERPs) and psychrometers in response to liquid releases in both the LPZ and HPZ. For releases in the LPZ, large changes were detected between 0.9 and 1.9 m from the collar; for releases in the HPZ, changes were observed between 1.7 and 3.4 m from the alcove face.

Seepage into the slot was observed directly below the injection zone during all eight tests in the HPZ. In the first test, after 0.41 liters of water had been introduced to the formation, water was first seen on the slot ceiling after five minutes. In the second and third tests, water appeared in the slot within three minutes after 0.17 and 0.14 liters, respectively, had been injected. In the final test in this batch, after 1.50 liters of water had been injected at a rate of 5 ml/min, water appeared in the slot after five hours.

In the second batch of experiments, travel time for the first drop of water during the first injection (0.14 liters at a rate of ~69 ml/min) was three minutes. In the two subsequent tests, after 0.26 and 0.20 liters of water were injected at a rate of 38 and 29 ml/min, the arrival time of the wetting front was seven minutes. In the final test in this batch, after 0.90 liters had been injected into the formation at a rate of 14 ml/min, water appeared in the slot after just over one hour.

The amount of water recovered in the slot continued to increase as each test progressed. However, significant variability existed in the percentage of water recovered (Figure 2a) and the seepage rate (Figure 2b) during and between tests. This variability was a function of both the amount of water injected and the rate at which water was released into the formation. Early in each test, the amount of water recovered sharply increased until approximately 10 liters of water had been injected, after which the percentage of injected water recovered approached a relatively constant value. The amount of injected water recovered was consistently higher for all injected volumes at release rates of 28 and 38 ml/min.

In all of the tests during which there was seepage, 0.5-1.3 liters of water entered the slot after water supply to the formation was switched off. The constant head test had a "stepped" nature to the post-injection recovery; here, during the first 15 minutes, the 0.8 liters of collected water appeared in four bursts, each containing 0.1-0.3 liters of water.

Significance of Findings

From these experiments, we were able to establish the effectiveness of new techniques developed for in-situ characterization of certain fundamental flow parameters (e.g., travel times, percolation and seepage rates). Results from liquid-release tests in the LPZ and HPZ suggest the presence of both open- and close-ended fractures and provide estimates of the volume of water occupied by both fast flow paths and close-ended fractures. This data, when coupled with data from the seepage response to different liquid injection rates, has led to certain hypotheses, which, when tested, should provide new directions for conceptualization of flow within these unsaturated, fractured systems.

Funding

This work has been supported by the Director, Office of Civilian Radioactive Waste Management, through Memorandum Purchase Order EA9013MC5X between TRW Environmental Safety Systems, Inc., and the Ernest Orlando Lawrence Berkeley National Laboratory for the Yucca Mountain Site Characterization Project under U.S. Department of Energy Contract No. DE-AC03-76SF00098.
Research Objectives

In-situ measurements of hydrologic parameters at Yucca Mountain, Nevada, form an integral part of efforts directed towards characterization of flow and transport in the unsaturated zone of this potential site for high-level nuclear waste disposal. An important feature in this environment is the fractured, consolidated rock formation, which contains fractures of varying densities, orientations, spatial extents and apertures. Because of this, unique problems arise with regard to instrument placement and sampling techniques. While theories, methods and experimental results developed from unconsolidated media have initially formed the basis for the characterization of unsaturated consolidated media, new techniques are now required (in addition to those established) to monitor fractured rocks.

The primary objective of this effort was to develop a reliable tool for monitoring the migration of a wetting front in boreholes located within fractured rock environments. In this paper we present the design of Electrical Resistivity Probes (ERPs) and Borehole Sensor Trays (BSTs). We also include some results from experiments conducted to evaluate the ERPs in the laboratory and in boreholes within the Exploratory Studies Facility (ESF) at Yucca Mountain.

Approach

Electrical Resistivity Probes: The basic concept defining the working of ERPs is that increasing water saturation results in decreasing electrical resistance. Probes were developed using a piece of filter paper across which changes in electrical resistance could be measured. The paper permits a flexible sensing surface that could be molded to the contours of the boreholes. These probes comprised two electrical leads sandwiched between pieces of filter paper (Figure 1a). To maintain a consistent geometry between probes, all electrical leads were cut to the same length and meshed through a nylon fabric such that the distance between wires was the same for all sensors. Meshed nylon fabric was also used to provide a protective outer sleeve for the probes. The size of the probes was determined by the type of application and ranged from squares with 0.02-m sides used for laboratory column experiments to 0.075 m for borehole monitoring.

Borehole Sensor Trays: To locate ERPs and psychrometers in multiple locations along borehole walls, trays were designed to permit multiple arrays of sensors to be easily installed and removed in the boreholes, independent of borehole orientation. These trays were fabricated from PVC pipes. The outer diameter of each tray was selected to match the diameter of the borehole being instrumented (Figure 1b). Psychrometers were located in small diameter holes (~ 3 mm ID) drilled through the trays. ERPs were attached to the outer surface of the trays with strips of Velcro. This assembly permitted extensive contact between the ERPs and the borehole wall while allowing the psychrometers to contact the borehole wall through a small cavity. On each tray, psychrometers were installed at typical distances of 0.25-0.5 m along the borehole while ERPs were located at 0.25-m intervals.

Two BSTs were located along each section of borehole to permit sensors to be located on opposite sides. To improve the contact between probes and the borehole wall, an adjustable wedge system was used.

Results

Water imbibition in a basalt column: To test ERP
function in the laboratory, six ERPs (each a square with 0.02 m sides) were attached to the walls of a basalt column (0.20 m height, 0.06 m diameter) after the column had been placed in a pool of water 0.01 m deep. As the column imbibed water, resistance changes along the surface were continuously measured.

Temporal changes in resistance measured across the six ERPs show the migration of a wetting front along the basalt column (Figure 2a). The initially low resistance measured in the two lower ERPs reflects the close proximity of the water table. The difference in the temporal response observed in the two higher zones suggests that despite the wetting front reaching the higher probes, a gradient in saturation developed with the bottom of the column being wetter than the higher zones.

Wetting front detection following tunneling activities: At the ESF, plumes of water resulting from tunneling activities (cutter head cooling, dust control, etc.) in the vicinity of a new tunnel were tracked with ERPs and psychrometers. To monitor the plumes, a 30-m-long borehole (0.10 m ID) was constructed sloping downwards at an angle of 30° under the proposed path of the tunnel. Twenty-seven psychrometers and 54 electrical resistivity probes located on nine BSTs were installed in this borehole. Changes in water potential and electrical resistance were monitored along the entire length of the borehole using psychrometers and ERPs located on BSTs as tunneling activities progressed through the formation above.

The ERPs responded in a pattern similar to that of the psychrometers located adjacent to the probes. For example, at a depth of 9.4 m where the water potential increased steadily from -400 m to -70 m, the corresponding ERP measurements followed a similar pattern (Figure 2b). Large fluctuations in water potentials in relatively short periods of time (~200 m in four days) were detected by both types of probes. The slower, more gradual recovery observed by psychrometers deeper in the formation was also well tracked by the ERPs (e.g., at 21.3 m; Figure 2c).

Significance of Findings

We were able to establish that ERPs are effective for laboratory scale experiments looking at water movement in the rock matrix, in which both the test bed and the sampling resolution can be relatively small. From field investigations, the response of the ERPs compared well with the performance of psychrometers, suggesting that these probes (with their current design) can be effectively used as a qualitative tool to detect the arrival (or departure) of wetting fronts in rock matrix, fractures and faults. Unlike psychrometers, these probes are relatively inexpensive, easy to maintain and have a low failure rate. This makes them particularly useful for extensive down-hole monitoring applications in unsaturated fractured rock environments such as that found at Yucca Mountain.

When installed on BSTs along with psychrometers, these ERPs provide an effective compilation of sensors, which provide data on relative wetness and water potential changes at high spatial resolution. With ERPs, the arrival (and departure) of a wetting front can be measured at time intervals of less than a minute, while the spatial extent can be measured to a resolution of less than 0.10 m. Backfill is not needed, increasing the accuracy of measurements and the relative ease of installing and removing sensors. The BSTs have the potential for further improving our abilities to measure flow parameters in the unsaturated zone of fractured rocks.

Funding

This work has been supported by the Director, Office of Civilian Radioactive Waste Management, through Memorandum Purchase Order EA9013MC5X between TRW Environmental Safety Systems, Inc., and the Ernest Orlando Lawrence Berkeley National Laboratory for the Yucca Mountain Site Characterization Project under U.S. Department of Energy Contract No. DE-AC03-76SF00098.
Research Objectives

Contaminant transport in arid climates is often controlled by thick vadose zones. The in-situ determination of hydraulic conductivity and other relevant transport parameters in these unsaturated systems has been hampered by the lack of practical methods for reliably making measurements and interpreting the results. The Restricted Interval Guelph (RIG) permeameter has been developed to fill this void by making measurements in saturated/unsaturated systems. Whereas the original Guelph permeameter is known to produce unreliable results for heterogeneous systems, the RIG permeameter was developed specifically to overcome this limitation. A simple analytical method for reducing the data has been developed based on saturated/unsaturated flow theory. The analytical data analysis approach is compared with a numerical simulation that more accurately reproduces actual test geometry. Finally, sensitivity analysis is used to verify the applicability of the RIG methodology for determining transport parameters for a field application in a rhyolitic tuff.

Approach

The RIG permeameter is similar to the original Guelph permeameter, in that it uses a Mariotte Siphon reservoir to produce a constant head injection test. However, unlike the Guelph permeameter, the region tested is isolated using either a single pneumatic packer or a straddle packer (Figure 1). This results in a fixed interval to be tested, which will not change even when changing the applied head. The applied head, H in Figure 1, is equal to the difference in elevation between the air reference line in the Mariotte Siphon reservoir and the elevation of the borehole zone being tested.

A test is conducted by first isolating the region of interest with the pneumatic packer(s). It should be noted that the borehole can be oriented in any direction. The air exit line is opened as water is introduced through the water line. When only water flows out from the air exit line, the line is closed and the test is underway. The volume of water introduced into the formation is read off a scale on the Mariotte Siphon reservoir and recorded as a function of time until a steady-state flow rate is reached.

By performing two injection tests at the same location using different applied heads, a method has been developed that allows for the determination of both the field-saturated hydraulic conductivity and the sorptive number. A closed-form expression for flow from a saturated sphere using dimensionless spatial coordinates, neglecting the influence of gravity, has been derived by A.W. Warrick, and is used here:

\[ K_f = \frac{\alpha q}{8 \pi \Psi \left( r - \frac{1}{r} \right)} \]  

(1)

The above equation is based upon a solution of Richards equation where water is the mobile liquid phase, and air is immobile. \( \Psi(m) \) is the head applied during testing and \( q (m^3/s) \) is the measured steady-state volumetric flow rate. The field saturated hydraulic conductivity, \( K_f (m/s) \), and the sorptive number, \( \alpha (m^1) \), are the unknowns to be determined through the simultaneous application of Equation 1 for two injection tests conducted with different heads at the same location. The radius at which the pressure head is applied, taken as an equivalent spherical radius, is \( r \), and \( r_0 \) is the radius of the saturated region (\( \Psi = 0 \)). The equivalent spherical radius corresponds to a sphere with the same surface area as is wetted during the actual field test. The radial coordinates are nondimensionalized by \( \alpha/2 \).

Forward simulations of RIG permeametry were carried out using the general multiphase and multicomponent porous media transport simulator TOUGH2. Similar to the analytical approach, the single-phase equation of

Figure 1. Schematic of Restricted Intervals Guelph permeameter. N.O.—normally open and N.C.—normally closed.
Table 1 Results of RIG permeametry in an unsaturated rhyolitic tuff showing a comparison between a simple analytical model and a numerical model which more accurately depicts testing geometry.

<table>
<thead>
<tr>
<th>Borehole</th>
<th>Interval Length (cm)</th>
<th>Head (cm)</th>
<th>Steady State Q (ml/sec)</th>
<th>Analytical $K_f$ (m/s)</th>
<th>Analytical $\alpha$ (m$^{-1}$)</th>
<th>Numerical $K_f$ (m/s)</th>
<th>Numerical $\alpha$ (m$^{-1}$)</th>
</tr>
</thead>
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<tr>
<td>G1</td>
<td>6.75</td>
<td>33.0</td>
<td>0.0488</td>
<td>1.6x10$^{-7}$</td>
<td>1.3</td>
<td>2.0x10$^{-7}$</td>
<td>2.5</td>
</tr>
<tr>
<td>G2</td>
<td>8.65</td>
<td>25.0</td>
<td>0.0037</td>
<td>7.5x10$^{-9}$</td>
<td>0.73</td>
<td>1.0x10$^{-8}$</td>
<td>1.6</td>
</tr>
</tbody>
</table>

The Restricted Interval Guelph Permeameter

Results

RIG permeametry was used to estimate the field-saturated hydraulic conductivity and sorptive number for an unsaturated rhyolitic tuff at Yucca Mountain, Nevada. Measurements were carried out at the ends of two 2.54-cm-diameter, 1-m-deep, horizontal boreholes. The first borehole, which we refer to as G1, was drilled into a high porosity ($\phi=0.44$) rhyolitic tuff, containing abundant coarse pumice and lithic fragments. Borehole G2 was drilled 0.7 m higher in elevation at the argillically altered upper portion of the same stratigraphic unit, which had a significantly reduced porosity of 0.25.

Table 1 lists relevant test conditions for each injection as well as the steady-state flow rates recorded. Simultaneous application of Equation 1 was used for each of the two applied heads and measured steady-state flux rates to solve for the hydraulic conductivity, $K_f$, and the sorptive number, $\alpha$. Although the actual injection geometry is cylindrical, the test interval is small enough that we use an equivalent spherical radius based on the surface area of the cylinder. The G1 borehole was determined to have a field-saturated hydraulic conductivity two orders of magnitude less than the hydraulic conductivity calculated for the G2 borehole, which is located in the argillically altered layer. The numerical model provided similar results. Table 1 also shows that the value for $\alpha$ is in good agreement between the analytical and numerical model.

ITOUGH2 simulations were used to determine the sensitivity of the volume of water released to porosity, capillary pressure parameters, sorptive number, absolute permeability and the initial liquid saturation. It was determined that the most sensitive parameter was absolute permeability, $k$, followed by sorptive number, $\alpha$. Both initial liquid saturation and formation porosity were shown to play a secondary role in determining the amount of water introduced into the formation. The capillary pressure parameters were shown to have minimal effect on test results.

Significance of Findings

The RIG permeameter has shown itself to be a versatile instrument for vadose zone characterization. Its simplicity and low cost make it an attractive method for measuring in-situ field-saturated hydraulic conductivity and estimating the sorptive number. Good agreement between the analytic and numerical results indicates that the analytical spherical flow model used is a valid approach for analyzing the data collected. Furthermore, the sensitivity analysis shows that RIG permeametry as carried out here is an effective method for estimating $k$ and $\alpha$ for the nonwelded rhyolitic tuff that was tested.

Related Publication


Funding

This work has been supported by the Director, Office of Civilian Radioactive Waste Management, through Memorandum Purchase Order EA9013MC5X between TRW Environmental Safety Systems, Inc., and Ernest Orlando Lawrence Berkeley National Laboratory for the Yucca Mountain Site Characterization Project under U.S. Department of Energy Contract No. DE-AC03-76SF00098.
Research Objectives

The partitioning of water between fractures and matrix is determined by the relative rates of imbibition and fracture flow. This partition is very important for the repository design and performance assessment for the proposed high-level waste repository at Yucca Mountain, Nevada. In this work, laboratory imbibition experiments were developed to accurately measure water imbibition into welded tuff of low permeability. For water flow through fractured rocks with low matrix permeability, the fast flow component is through the fracture network. Some water flowing along the fractures will imbibe into the matrix blocks because of strong capillarity from the extremely small-sized pores of the matrix. Imbibition of water into a porous medium typically proceeds in proportion to the square root of time, with the proportionality constant denoted as the sorptivity. Sorptivity is jointly controlled by the permeability and capillary pressure, and is a useful parameter for characterizing transient imbibition processes, especially when the influence of gravity is insignificant.

Approach

Rock cores (5.08 cm in diameter and 2.0 cm in length), oven-dried at 60°C, were used for the imbibition experiment. Cores were cut and machined from a sample block, which was collected within the middle non-lithophysal zone of the Topopah Spring welded unit at Yucca Mountain, where the potential repository for waste canister emplacement will be located.

To measure imbibition rates into cores, the rock core was placed in a holder that was connected to a bottom-weighing electronic balance. The rock core was suspended inside a constant humidity chamber, with the core bottom immersed into water in a reservoir at about a 1-mm depth. A PC and LabVIEW program were used to acquire and store the balance readings, at a user-specified logging interval, over time.

The water level in the reservoir fell because of imbibition and evaporation, and the core submergence depth decreased. This reduced the buoyant force on the sample. As a result, the sample appeared (from the balance reading) to gain more water than it actually did. A mathematical formulation for the buoyant force change was developed and employed to correct the experimental results to obtain “true” water mass imbibed into the core sample.

Results

An example of cumulative imbibition versus time for a tuff sample is shown in Figure 1. The measured data without corrections are compared with (1) evaporation correction, and (2) both evaporation and imbibition corrections. The data agree with the final weighing of the core sample, which was independently measured. Over a total of 109 imbibition tests, the average difference between the corrected mass for water imbibition and the balance-indicated mass is 20.7% (with a standard deviation of 2.3%). Thus it is important to account for buoyant force decrease in imbibition measurements.

Plots of cumulative imbibition versus the square-root of time are shown in Figure 2, with the sorptivity determined from the slope of the linear segment. Linear segments are evident only for the “early” times, which differ between the two cores: a relatively uniform Core-A and a fractured Core-1. Deviation from linearity in Figure 2 can arise from several sources, including (1) the leading edge of the wetting front reaching the opposite boundary, (2) heterogeneities in hydraulic properties along the length of the sample, and (3) gravitational effects. For these tuff samples under initially dry conditions and short core length, gravitational effects can be neglected.

The measured porosity for is 0.160 for Core-1 and 0.0821 for Core-A; the difference is attributed to the presence of the fracture and the altered band regions around the fracture in Core-1. During imbibition tests for Core-1, it was observed that water was imbibed preferentially into the band regions, which presumably possess a higher permeability. The wetting front reached the core top in less than 30 minutes (which corresponds to a water saturation of 35% for the whole core); this corresponds very well to the time when the cumulative imbibition starts to show curvature (Figure 2B). Wetting front propagation for Core-A imbibition was more or less uniform, travelling less than 0.3 cm from the core bottom in 30 minutes. For Core-A, the linear segment ends after 29 hours, which is likely related to the arrival of the wetting front to the top of the core.
Laboratory Measurement of Water Imbibition Into Low-Permeability Welded Tuff

At this time, the water saturation of Core-A is about 80%.

The corrected increase in mass of water includes not only water imbibed but also water transported by vapor-phase diffusion into pore space and condensation in pores. The core sample, treated by coating the core walls and covering the core top (but leaving a small hole for air to escape), was hung above the water reservoir inside the humidity-controlled chamber. Core weight gain by condensation was compared to the non-treated case. The results indicate that the coating and coverage can control/minimize capillary condensation into the core. For Core-A, the condensation component could be as large as 18%.

The measured sorptivity difference for the core sample with different coverages is found to be consistent with the contribution from capillary condensation. The average sorptivity is $3.395 \times 10^{-3} \text{ (m s}^{-0.5})$ for the fractured Core-1, and $3.58 \times 10^{-6} \text{ (m s}^{-0.5})$ for the non-fractured Core-A, with the sorptivity ratio ($S_{Core-1}/S_{Core-A}$) equal to 9.49. Since permeability is correlated to the 4th power of sorptivity, the permeability for Core-1 is about 8,100 times greater than that for Core-A. Hence, the permeability for the fracture surface zones that have undergone permeability-enhancing alterations is as large as 8,100 times that of the underlying rock matrix.

**Significance of Findings**

A well-controlled method has been developed for measuring imbibition rates and determining sorptivities for low permeability media. Automatically recorded balance readings were used to quantify the imbibition of water into rock cores, even when the total mass of imbibed water was small and the duration of the experiment was long. A formulation was developed to correct for the apparent balance increase because of the buoyancy force decrease. Weight readings corrected for this effect agreed very well with independently measured total uptake. High contrasts in sorptivities between fractured and unfractured cores are related to high contrasts in permeabilities between fractures and the tuff matrix. Capillary condensation can provide a significant contribution to the water uptake into cores during imbibition experiments. Rock cores were treated by coating and coverage to reduce this effect. The method developed resulted in an accurate measurement of sorptivity, as exhibited from the consistent and reproducible results of multiple measurements. The method is expected to be very useful for measuring imbibition rates of very low permeability materials and/or materials with initial partial saturation.

**Related Publication**


**Funding**

This work has been supported by the Director, Office of Civilian Radioactive Waste Management, through Memorandum Purchase Order EA9013MC5X between TRW Environmental Safety Systems, Inc., and Ernest Orlando Lawrence Berkeley National Laboratory for the Yucca Mountain Site Characterization Project under U.S. Department of Energy Contract No. DE-AC03-76SF00098.
Research Objectives

Field evidence suggests that in semi-arid environments such as Yucca Mountain, Nevada, water is able to migrate downward rapidly along preferential paths through fracture networks in partially saturated rocks, without being imbibed into the rock matrix. This raises concerns for the disposal of nuclear waste because nuclides may transport downstream with water. To help understand mechanisms of fast preferential flow in unsaturated fractures, we have developed a high-resolution numerical model for simulating fluid flow and transport in unsaturated fractured rocks. Such a numerical model requires a detailed description of fracture heterogeneity. Therefore, the objectives of our research are to develop a statistical simulator that is able to capture realistic heterogeneities of natural fractures and to provide a better understanding of water seepage behavior in unsaturated fractured rocks by simulating flow in large ensembles of synthetic heterogeneous fractures.

Approach

In this research, we focus on small-aperture fractures in hard rocks, such as tuffs, granites and basalts. Fractures are conceptualized as two-dimensional heterogeneous porous media that can be characterized by a heterogeneous permeability field. Elements that are essential for a synthetic fracture to replicate natural fractures include the presence of asperity contacts, a gradual change from asperities towards larger aperture, small-scale wall roughness, and a finite-size spatial correlation length. We have developed a statistical simulator based on the algorithm of simulated annealing for generating realizations of natural fractures. Simulated annealing (SA) is an algorithm that operates in analogy to the physical process of annealing, moving a system towards a state of global minimum energy through successive perturbations. The classic Metropolis algorithm is commonly used as a perturbation mechanism, but we found that this is not adequate to capture the correlation structure near asperity contacts. Therefore, we have developed enhancements to the Metropolis algorithm that can better represent the neighborhood of asperity contacts.

Flow simulations were carried out with the general-purpose flow simulator TOUGH2, using a special equation-of-state flow module EOS9 which solves Richards' equation; that is, it is assumed that the gas phase acts as a passive bystander with negligible pressure change during variably saturated water seepage.

Results

Figure 1 shows two realizations of permeability fields annealed to the same variogram with the standard and modified Metropolis algorithms. It is obvious that the permeability field annealed with the modified Metropolis algorithm shows more consistent correlation near asperity contacts than that annealed with the standard Metropolis algorithm.

In the subsequent flow simulations, water is injected uniformly over the entire top boundary at a constant rate of $10^3$ kg/s. To model the effect of normal stress on water seepage, we generated fractures with increasing fractions of asperity contacts. One realization of water seepage at steady state is shown in Figure 2. Also shown in Figure 2 are the corresponding breakthrough curves (BTCs) for the seeps in Figure 2, as well as for other seeps with different fractions of asperity contacts.

Typical phenomena seen in our numerical seepage experiments include flow bypassing, ponding, fingering and flow exclusion. For each fraction of asperity contacts, we generated 30 realizations of synthetic fractures and calculated their effective permeability. Plotting the arithmetic mean of these effective permeabilities shows that effective permeability decreases nonlinearly with increas-
High Resolution Studies of Water Seepage in Unsaturated, Heterogeneous Rock Fractures

Distance (m)

(a) 25% asperity contacts

(b) 40% asperity contacts

(c) BTC's

Figure 2. Liquid seeps at steady state in fractures subject to increasing normal stress. Water is injected uniformly at a constant rate of $10^{-3}$ kg/s over the entire top boundary. BTCs are also shown.

Combining these two findings suggests that water seepage in unsaturated fractures may be faster than in saturated ones, and seepage may become faster as normal stress increases. On the other hand, the asymptotic decrease of effective permeability with normal stress implies the existence of residual flow in fractures subject to large normal stress.

Dispersion at asperity contacts may have significant effects on water seepage and solute transport. It will in general delay downward seepage and cause the breakthrough time to increase. Dispersion may either increase or decrease due to ponding, depending on the geometric connection between ponded and flowing regions.

Related Publications


Funding

This work has been funded by the Office of Science, Office of Health and Environmental Sciences, Biological and Environmental Research Program, of the U.S. Department of Energy under Contract No. DE-AC03-76SF00098.
Research Objectives

Fracture/matrix (F/M) interaction is a key factor affecting flow and transport in unsaturated fractured rocks. In classic continuum approaches, it is assumed that flow occurs through all the connected fractures and is uniformly distributed over the entire fracture area, which generally gives a relatively large F/M interaction. However, fractures seem to have limited interaction with the surrounding matrix at Yucca Mountain, Nevada, as suggested by geochemical nonequilibrium between the perched water (resulting mainly from fracture flow) and pore water in the rock matrix.

Because of the importance of the F/M interaction and related issues, there is a critical need to develop new approaches to accurately consider the interaction reduction inferred from field data at the Yucca Mountain site. Motivated by this consideration, we have developed an active fracture model based on the hypothesis that not all connected fractures actively conduct water in unsaturated fractured rocks.

Approach

Physically, the F/M interaction reduction can result from three mechanisms. First, because of gravitational instability and a heterogeneous aperture distribution, water flow through an unsaturated fracture is likely to be channelized, which can considerably reduce the F/M interface area. Second, fracture coating can reduce imbibition into the matrix, significantly in some cases. Third, because of the combination of the large nonlinearity involved in an unsaturated system and heterogeneities of fracture structure at different scales, significant fingering flow can occur even in a well-connected fracture network. In other words, only a portion of fractures in a connected network contribute to water flow, while other fractures are simply by-passed. For large-scale flow and transport, the third mechanism is the most important. The portion of the connected fractures that actively conduct water are defined as active fractures.

It is important to note differences between the active fracture model and the conventional, capillary equilibrium-based, fracture water distribution model. The latter assumes that liquid water occupies fractures with small apertures first and then fractures with relatively large apertures as water potential increases. In contrast, the active fracture model presumes gravity-dominated, non-equilibrium, preferential liquid water flow in fractures. The water distribution is not controlled by the capillarity.

The fraction of active fractures in a connected fracture network, $f_a$, should be determined by flow and transport conditions and fractured rock properties. An expression for $f_a$ must satisfy the following conditions: (1) all connected fractures are active if the system is fully liquid saturated; (2) all fractures are inactive if the system is at residual saturation; and (3) $f_a$ should be related to water flux in fractures. Based on these considerations, we express $f_a$ as a power function of effective water saturation in connected fractures, $S_e$,

$$f_a = S_e^\gamma$$

where $\gamma$ is a positive constant depending on properties of the corresponding fracture network and can be considered as a measure of the "activity" of connected fractures.

A generalized version of van Genuchten capillary pressure and relative permeability relations for the fracture continuum were developed based on the above equation for $f_a$ and the following considerations: (1) van Genuchten relations are assumed to be valid for active fractures; (2) inactive fractures are filtered out from the fracture continuum in describing flow and transport in fractures; and (3) the apparent F/M interface area reduction factor (R) results not only from the actual interface area reduction, but also from the difference between active fracture spacing and fracture spacing, determined from the geometry of the corresponding fracture network. Note that the derived relation for the F/M interface area reduction factor (R) is used as an additional constitutive relation. Figure 1 shows the factor as a function of the effective water saturation.

Results

An inverse modeling approach was used to determine the "activities" of connected fracture net-
An Active Fracture Model for Unsaturated Flow and Transport

The estimated $\gamma$ values are about 0.43, indicating that about 18-27% of connected fractures are active in the TSw unit under ambient conditions. This relatively high percentage is consistent with various field observations, including the relatively uniform matrix water saturation and in-situ water potential values measured for most of the units. Furthermore, calcite coatings, signatures of water flow history in fractures, were found in about 10% of the fractures within the welded units.

Tracer transport simulations were also performed to check the consistency of the model with geochemical data. The calculated 50% tracer concentration breakthrough times of fracture continua at the bottom of the TSw unit are between 3,500 and 5,000 years, and are generally in agreement with the perched water age data.

Significance of Findings

Fingering flow in a fracture network is a common flow mechanism in an unsaturated fracture-matrix system. This makes it necessary to formulate the fracture water flow differently from water flow in unsaturated porous media. This study introduced a new model to incorporate fingering flow at a fracture network scale into the dual continuum approach. The simulation results based on the new model are generally in agreement with the field observations at the Yucca Mountain site.

Related Publications


Funding

This work has been supported by the Director, Office of Civilian Radioactive Waste Management, through Memorandum Purchase Order EA9013MC5X between TRW Environmental Safety Systems, Inc., and Ernest Orlando Lawrence Berkeley National Laboratory for the Yucca Mountain Site Characterization Project under U.S. Department of Energy Contract No. DE-AC03-76SF00098.
Research Objectives

Accurate and efficient simulation of chemical transport processes in the unsaturated zone of Yucca Mountain, Nevada, is important to evaluate the performance of the potential repository. The scale of the unsaturated zone model domain for Yucca Mountain (50 km² area with a 600-m depth to the water table) requires a large gridblock approach to efficiently analyze complex flow and transport processes. The conventional schemes based on finite element or finite difference methods perform well for dispersion-dominated transport, but are subject to considerable numerical dilution/dispersion for advection-dominated transport, especially when a large gridblock size is used. Numerical dispersion is an artificial, grid-dependent chemical spreading, especially for otherwise steep concentration fronts.

One effective scheme to deal with numerical dispersion is the random walk particle method (RWPM). While significant progress has been made in developing RWPM algorithms and codes for single-continuum systems, a random walk particle tracker, which can handle chemical transport in dual-continuum (fractured porous media) associated with irregular grid systems, is still absent (to our knowledge) in the public domain. This is largely due to the lacking of rigorous schemes to deal with particle transfer between the continua, and efficient schemes to track particles in irregular grid systems.

The main objectives of this study are to (1) develop approaches to extend RWPM from a single-continuum to a dual-continuum system; (2) develop an efficient algorithm for tracking particles in 3-D irregular grids; and (3) integrate these approaches into an efficient and user-friendly software, DCPT, for simulating chemical transport in fractured porous media.

DCPT: A Dual-Continuum Random Walk Particle Tracker for Transport

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Figure 1. Comparisons between DCPT and analytical solutions:
(a) 1-D dual continuum with linear sorption; (b) 2-D convection and dispersion transport, and (c) particle trail in a concentration field with an irregular grid.

Approach

In RWPM, chemical transport is represented by the movement of a large number of particles. In addition to advection determined by the corresponding velocity field, dispersion/diffusion is simulated by random walks of particles. In DCPT, RWPM is directly adopted to simulate particle movement in each continuum. Unlike a single continuum, however, a dual-continuum system is associated with two very different velocity fields at a given "physical point." The mass transfer between the fracture and matrix continua is one of the critical processes that control the movement of chemicals. The mass transfer process between the fracture and the matrix is simulated by the particle transfer probabilities (PTP) which determine if a particle will leave the current continuum at the next time level. Determination of PTP is one of the key and unique elements in DCPT.

The challenge is to convert the net mass flow between the fracture and the matrix (in the Eulerian point of view) into the particle transfer probabilities (the Lagrangian point of view). An analytical solution of the mass conservation equation of the particles in the Lagrangian point of view is found, based on which a new scheme to calculate the PTP is developed and incorporated into DCPT (Pan et al., 1999).

In most of the currently available RWPM codes, regular grids are generally used. For many subsurface contaminant problems, such as those in the unsaturated zone of Yucca Mountain, the related subsurface media can be highly heterogeneous. To capture these heterogeneities, irregular grid systems are required. An efficient scheme to track particle locations in irregular grids was developed for DCPT (Pan et al., 1999). The main idea of this scheme is to establish a secondary structure of the original 3-D irregu-
lar grid so that only a very small portion of the whole grid has to be searched each time. In this way, decaying of the computational efficiency due to increases in the number of grid blocks can be avoided.

DCPT can be used to simulate reactive transport with linear sorption. For a single-continuum system, the retardation factor method has been widely used in RWPM. However, this approach cannot be directly used for a dual-continuum system, because of the coupling of transport processes in the two continua with different retardation factors. In the light of the imaginary porosity method proposed by Liu and Bodvarsson (1999), a physically based conditional probability approach (Pan et al., 1999) was incorporated into DCPT to describe the effects of the linear sorption process on either the transfer probability between two continua or the advection/dispersion processes in each continuum.

DCPT was developed using FORTRAN 90 and following the principle of the objective-oriented programming technologies.

Results

Figure 1 shows comparisons between simulation results of DCPT and several typical analytical solutions in 1-D and 2-D domains. The comparisons were designed to verify DCPT’s capability to (1) calculate particle transfer between the two continua and consider the sorption (Figure 1a); (2) incorporate dispersion and diffusion in multi-dimensional domains (Figure 1b); and (3) track particle movement in an irregular grid (Figure 1c). Particularly, Figure 1c depicts a trail of a particle in a concentric velocity field (radial velocity is zero everywhere) simulated by DCPT, which is a circle theoretically. The satisfactory matches indicate that the methodologies and algorithms developed are valid and successful.

Figure 2 shows the comparison between simulation results obtained from DCPT (2000 particles) and T2R3D (Wu et al., this report) for two 1-D problems under unsaturated conditions. The corresponding 1-D column is extracted from the 3-D grid of the site-scale unsaturated zone (UZ) model for Yucca Mountain. The comparison is fairly good, and DCPT gives a steeper concentration front, resulting from its ability to deal with numerical dispersion.

All the simulations of DCPT mentioned above were performed on a Pentium II 300 MHz PC and took a few seconds up to about 10 minutes of CPU time, depending on the particle numbers used.

Significance of Findings

Based on the newly developed methodologies to extend RWPM from a single continuum system to a dual continuum system, a new software program, DCPT, has been developed. Comparisons between DCPT simulation results with analytical solutions and results obtained from T2R3D show that DCPT could be used to simulate chemical transport processes associated with linear sorption in fractured continua without numerical dispersion.

Related Publications


Funding

This work has been supported by the Director, Office of Civilian Radioactive Waste Management through Memorandum Purchase Order EA9013MC5X between TRW Environmental Safety Systems and the Ernest Orlando Lawrence Berkeley National Laboratory for the Yucca Mountain Site Characterization Project under U.S. Department of Energy Contract No. DE-AC03-76SF00098.
Research Objectives

The site characterization and modeling studies continued in 1998 for investigating the feasibility of using the unsaturated zone (UZ) at Yucca Mountain, Nevada, as a permanent storage facility for the geologic disposal of high-level nuclear waste. As part of these efforts, the 3-D site-scale UZ flow and transport model developed at LBNL has been improved significantly during the fiscal year. The primary goals of this model are to simulate and investigate the existing natural state of the mountain's hydrogeological system, and to predict possible future system responses in support of the Yucca Mountain Project. In 1998, modeling studies and development efforts focused on supporting the total system performance assessment-viability assessment (TSPA-VA) and license application (LA) activities. The UZ model and simulation results of flow fields were used directly in the current TSPA-VA efforts by the Yucca Mountain Project.

Approach

In developing the UZ model, the UZ hydrogeological system of the site is represented using a 3-D numerical model grid; model conditions are described based on the most updated geological framework model and observed data. The model domain encompasses a 5,000-m by 9,000-m area, as shown in Figure 1, with a 500-700 m depth to the water table. Model parameters are estimated using a combined, inverse and direct modeling approach, dual-permeability concept for fracture-matrix interactions and several infiltration rates. During inverse modeling, the state variables are calibrated using observed matrix liquid saturation, water potential, pneumatic and temperature data from boreholes. The parameter sets estimated from these simultaneous 1-D inversions are further modified, when necessary, to account for spatial heterogeneities, such as perched-water occurrences, geochemical data and groundwater travel times through the 3-D modeling studies.

Continual Development Of the UZ Model for Yucca Mountain, Nevada

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The general approach of the UZ model development consists of the following major steps:

1. Development of a conceptual hydrogeological model for moisture, gas and heat flow, and tracer/chemical transport processes in the UZ system;
2. Representation of the hydrogeological system using a 3-D discrete computer model;
3. Integration and incorporation of all available field and laboratory observation data into the model;
4. Model calibration and sensitivity studies, including both inverse and forward modeling efforts to estimate model input parameters and conditions;
5. Model applications, including predictive studies.

Results

A comprehensive summary of the development and results of the 1998 UZ model was reported by Bodvarsson et al., 1998. The major achievements and emphases of the year have been to incorporate all new site data into the model, update the UZ flow and transport conceptual models, and focus on specific features and processes that may be important to repository performance. A summary of these achievements follows:

- New data have been incorporated from the new boreholes, the ESF and East-West Cross Drift.
- Matrix and fracture properties were updated with a new set of calibrated hydrologic properties.
- Submodels of the Ghost Dance Fault and the Solitario Canyon Fault were developed to evaluate flow within and near faults.
- The 3-D UZ model was updated with a new hydrogeological property set, improved geological and mineralogical models, and a refined model grid, as shown in Figure 1. The UZ model utilizes a dual-permeability concept with a dual porosity representation of faults. Simulations were completed that predict ambient...
continuum Development of the UZ Model for Yucca Mountain, Nevada

A 2-D cross-sectional, drift-by-drift model was used to evaluate the impact of coarse-grid averaging.

Conceptual models for perched water and flow below the repository were evaluated with a detailed model of the Calico Hills nonwelded unit. Large effects on lateral flow are found from the permeabilities of zeolites, the degree of fracturing within zeolites, and the extent of perched-water bodies. One of the model-predicted perched water bodies is shown in Figure 2.

A detailed model of the Paintbrush bedded tuff has been developed and showed that lateral flow may be limited to less than 100 m.

Significance of Findings

The UZ model provides estimates of important parameters and processes for the TSPA-VA and LA. Updated modeling efforts render more realistic representations of the 3-D nature of flow within the unsaturated zone and of the relevant processes occurring at Yucca Mountain. In addition, the model provides input to various other models, such as the ambient and thermal drift-scale model, the mountain-scale thermohydrological model and the UZ transport model used for LA.

Related Publication


Funding

This work has been supported by the Director, Office of Civilian Radioactive Waste Management, through Memorandum Purchase Order EA9013MC5X between TRW Environmental Safety Systems, Inc., and Ernest Orlando Lawrence Berkeley National Laboratory through U.S. Department of Energy Contract No. DE-AC03-76SF0098.
Development of WinGrider: An Interactive Grid Generator For TOUGH2

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Research Objectives

Designing a proper numerical grid is one of the major efforts in modeling flow and transport processes in complex, heterogeneous systems using the TOUGH family of codes. The problem becomes even more difficult when using an irregular grid, such as in the case of modeling studies of unsaturated zone (UZ) flow and transport for Yucca Mountain, Nevada. The development of an efficient meshmaker was motivated by the requirements of the TOUGH codes for simulating the subsurface processes of high-level nuclear waste isolation in partially saturated geological media of the Yucca Mountain site. A mountain-scale model often involves various geological and engineering objects in the complex hydrogeological settings. Designing and generating a suitable irregular grid for such a system has been a tedious and error-prone process, especially when the number of gridblocks and connections becomes very large. Inspecting the grid or extracting some sub-grids or other specific information or use from the grid has also been a time-consuming task. Therefore, user-friendly, efficient grid-generating software is a critical part of successful application of the TOUGH codes to solve real-world problems. Our objective is to develop user-friendly and integrated software for generating grids that best represent the geological and engineering features within 3-D model domains for given computing resources.

Approach

WinGrider was primarily written in the Visual Basic language following the principles of object-oriented programming to provide graphical user interfaces, interactive operation and visualization functionality. Advanced database techniques were incorporated to handle a large number of grid blocks and connections efficiently.

Development of the new grid system starts with assignment of nodes in map view for each object [e.g., the domain (base nodes), repository or faults] with specified orientation and density. Based on the information of these nodes, a primary 2-D grid is generated with Voronoi tessellation techniques. The 2-D grid is then improved systematically and/or interactively by deleting physically incorrect or unnecessary connections. A few iterations of these steps, including adding and deleting some nodes, are taken to create a final 2-D grid (a column scheme) that serves as the basis for generating the third dimension of the grid. All 3-D cells and vertical connections between adjacent cells are generated column by column to ensure that each vertical connection connects only adjacent cells and that each cell has at least one vertical connection. Lateral connections are then generated segment by segment with each segment joining two neighboring columns. This ensures that only cells in two adjacent columns have lateral connections and that no connections...
between two adjacent columns are missing.

Three-dimensional cells are created for each hydrogeological unit in each column and then are laterally connected within the same layer except where the layer is interrupted by faults or repository drifts. An approach using the three parallel, fault-related columns is used to ensure that the grid represents faults correctly. In particular, this scheme preserves three important roles of faults: (1) separator between geological layers that may serve as a structural barrier to lateral flow across it; (2) continuous zone that may serve as a fast path for flow along the fault depending on its hydraulic properties; and (3) dipping feature with angles of inclination varying spatially.

Results

WinGrider is Windows-based software for designing, generating and visualizing numerical grids used in reservoir simulation and groundwater modeling using the TOUGH2 code (Pan et al., 1999). Figure 1 shows an example of the graphical user interfaces provided by WinGrider. WinGrider has been used for various numerical simulations in the Yucca Mountain project. The generated grids were verified independently in terms of accuracy in representing the geological and engineering systems as well as correctness of connections. Figures 2a and 2b show a map view of the UZ98 grid and a 2-D cross-section grid for grid spacing analysis, respectively.

Significance of Findings

We have developed a user-friendly, efficient grid-generating software that should provide an important tool for successful applications of the TOUGH family of codes to solve real-world problems. WinGrider can be used to generate complex, irregular 2-D or 3-D grids with high quality and efficiency. Many important features, such as inclined faults with offset, layering structure, local refinements and repository drifts can be represented in the grid. This gridmaker has been used as a primary tool for designing model grids in modeling efforts for the Yucca Mountain project.

Related Publications


Funding

This work has been supported by the Director, Office of Civilian Radioactive Waste Management, through Memorandum Purchase Order EA9013MC5X between TRW Environmental Safety Systems, Inc., and Ernest Orlando Lawrence Berkeley National Laboratory for the Yucca Mountain Site Characterization Project under U.S. Department of Energy Contract No. DEAC03-76SF00098.
Research Objectives

Even with the continual progress made in both computational algorithms and computer hardware, it remains a challenge to simulate transport of a tracer or radionuclide in heterogeneous fractured porous media with a numerical method. It becomes even more difficult when dealing with tracer transport in a multiphase and non-isothermal flow system using a general 3-D, irregular grid. One of the primary problems in solving advection-diffusion type transport equations in a complex geological medium is determining how to approximate the diffusion/dispersion tensor in order to estimate the dispersive terms of mass transport accurately. Most numerical modeling approaches in the literature use schemes that are based on regular grids and the partial dispersion tensor. Very few studies have addressed transport using an irregular 3-D grid for large, complex geological systems.

T2R3D, a TOUGH2 module, has been developed to model radionuclide or tracer transport in heterogeneous, fractured porous media (Wu et al., 1996). The model formulation incorporates a full dispersion tensor with a 3-D, irregular, integral finite difference. It takes account of the physical processes of tracer or radionuclide transport in a non-isothermal, multi-phase, multi-dimensional flow environment in the subsurface.

Approach

T2R3D is built on the framework of the TOUGH2 code (Pruess, 1991). The basic mass and thermal energy balance equations for three components of water, air and a radionuclide/tracer, and heat solved by T2R3D are similar in form to those for the standard TOUGH2 EOS3 module. Also, the integral finite difference method and a first-order, backward finite difference scheme are used for spatial and temporal discretization, respectively. The tracer transport mechanisms include molecular diffusion and hydrodynamic dispersion in the liquid or gaseous phase, in addition to advection terms. First-order decay is taken into account and adsorption of a tracer on rock matrix and/or fractures is described by an equilibrium isotherm with a constant distribution coefficient.

The model formulation considers advection/dispersion transport processes of a liquid or gas tracer and incorporates a full dispersion tensor, based on a 3-D velocity field on a 3-D, regular or irregular, integral finite-difference grid in a heterogeneous geological system. In addition to advection terms for the tracer transport, the dispersive and diffusive mass flux, $F_D$, is described by

$$ F_D = -\rho_\beta \vec{D} \cdot \nabla X_\beta \quad (\beta=\text{liquid or gas}) \quad (1) $$

Figure 1. Model grid and simulation results of T2R3D for radionuclide transport through the unsaturated zone of Yucca Mountain, Nevada.
where $\mathbf{D}$ is the combined diffusion-dispersion tensor accounting for both molecular diffusion and hydrodynamic dispersion; $\rho_f$ is fluid density; $X_b$ is mass fraction of the tracer in phase $\beta$. We have incorporated a general dispersion model for 3-D tracer transport into the T2R3D code.

$$\mathbf{D} = \alpha_T |V_{\beta}| \delta_{ij} + (\alpha_L - \alpha_T) \frac{V_{\beta} V_{\beta}}{|V_{\beta}|} + \phi \delta_{\beta} \tau d_m \delta_{ij}$$  \hspace{1cm} (2)

($\beta =$ liquid or gas)

where $\alpha_T$ and $\alpha_L$ are the transverse and longitudinal dispersivities, respectively; $V_{\beta}$ is the Darcy velocity vector of phase $\beta$ through fractures or matrix; $\tau$ is the tortuosity of the medium; $d_m$ is the molecular diffusion coefficient in phase $\beta$; and $\delta_{ij}$ is the Kronecker delta function. ($\delta_{ij} = 1$ for $i=j$, and $\delta_{ij} = 0$ for $i \neq j$).

One of the key issues in implementing the general 3-D dispersion tensor of (2) is how to interpolate velocity fields for determining the dispersion tensor. The averaging or weighting scheme used to evaluate a velocity vector at the interfaces between element blocks is called "projected area weighting method" (Wu and Pruess, 1998). In this method, a velocity component, $v_{n,i}$, of the velocity vector element $n$ is determined by the vectorial summation of the flow components of all local connection vectors in the same direction, weighted by the projected area in that direction:

$$v_{n,i} = \frac{\sum_m (A_{nm} [n_1] v_{nm} n_1)}{\sum_m (A_{nm} [n_1])} \hspace{1cm} (i=x,y,z)$$

where $m$ is the total number of connections between element $n$ and all its neighboring elements $m$, $v_{nm}$ is the flux along connection $nm$ in the local coordinate system, and $n_i$ are the directional cosines of connections. The velocity vector $v$ at the interface of element $n$ and $m$ is then evaluated by harmonic weighting to preserve total transit time for solute transport travelling between the two blocks.

The mass fraction gradient of the tracer/radionuclide is evaluated at the interface between gridblocks $n$ and $m$ as

$$\nabla X_{nm}^{(k)} = \left( n_x \Delta X_{nm}^{(k)}, n_y \Delta X_{nm}^{(k)}, n_z \Delta X_{nm}^{(k)} \right)$$

with

$$\Delta X_{nm}^{(k)} = \frac{X_m^{(k)} - X_n^{(k)}}{D_m + D_n}$$

(5)

The net mass flux of diffusion and dispersion of a tracer/radionuclide along the connection of element $n$ and $m$ is determined by equation (1).

**Results**

As a new member of the TOUGH2 family of codes, T2R3D (Wu et al., 1996) provides a capability for modeling liquid or gas tracer or radionuclide transport in multiphase and non-isothermal flow systems. In particular, T2R3D can be used to simulate tracer transport in complex, heterogeneous fractured rock using a general, irregular 3-D grid. In addition to incorporation of a full dispersion tensor in evaluating dispersive tracer transport, the code takes into account linear adsorption and first-order decay effects. The model formulation and numerical scheme make it easy to include any other transport mechanisms, such as non-adsorption, multi-decay chains, or thermal/mechanical effects. Figure 1 shows an example application, in which T2R3D is used to assess radionuclide transport in the unsaturated zone of Yucca Mountain along a 2-D cross section with an irregular finite-difference grid.

**Significance of Findings**

The T2R3D code has found a wide range of applications in field characterization studies of the unsaturated zone transport of environmental isotopic tracers and radionuclides at the Yucca Mountain site, a potential underground repository for high-level radionuclide wastes. The special capability of modeling tracer transport processes through heterogeneous fractured rocks under multi-phase and non-isothermal conditions with full consideration of hydrodynamic dispersion will make T2R3D a very useful tool in modeling studies of tracer transport in oil, gas and geothermal reservoirs.

**Related Publications**


**Funding**

This work has been supported by the Assistant Secretary for Energy Efficiency and Renewable Energy, Geothermal Division, and by the Director, Office of Civilian Radioactive Waste Management, through Memorandum Purchase Order EA9013MC55x between TRW Environmental Safety Systems, Inc., and the Ernest Orlando Lawrence Berkeley National Laboratory under U.S. Department of Energy Contract No. DE-AC03-SF760098.
Laboratory Studies on Heat-Driven Multiphase Flows In Rock Fractures

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Research Objectives

Water and vapor flow through non-isothermal, fractured, porous rock environments are important in a number of fields, including the geologic disposal of high-level nuclear waste and geothermal reservoir development. Here we present the results of a number of visualization experiments that were performed to gain a better understanding of liquid and vapor flow in non-isothermal fractures, and imbibition into the fracture wall.

Approach

Several types of experiments have been performed to investigate the behavior of liquids in boiling fractures, including introducing liquid into natural and saw-cut fractures in Topopah Spring tuff from Yucca Mountain, Nevada. In each experiment, heat was applied to create a temperature gradient and boiling zone. Two types of experiments are described here.

In the first experiment, we introduced water at three different flow rates into the top of a 22-cm natural fracture oriented vertically. Heat was applied at the bottom, creating a boiling zone near the center of the rock with temperatures of about 120°C at the rock bottom and 80°C at the top. Water was introduced at a point in the center of the fracture top at 7, 14 and 28 mL/hr, and a different non-volatile dye was added for each flow rate. The dyed water flowed through the heated fracture, and where it boiled, the non-volatile dye was left on the rock.

Two experiments of the second type were performed in an assembled rock/glass fracture to simultaneously observe (1) liquid flow through a fracture, (2) imbibition into the porous rock, and (3) temperature in a heated fracture. Direct visualization and video recording were used to observe flow phenomena in the fracture; an infrared camera and thermocouples were used to monitor temperature, and x-ray attenuation was used to monitor imbibition. The fracture was made by placing a saw-cut slab-shaped block of Topopah Spring tuff (15 x 23 x 2.6 cm) with a porosity of 10% next to a glass plate. The rock and the glass plate were placed in a frame and held apart by gold shims, providing a 12.5-micron nominal aperture. Heaters were installed both in the rock slab and on the assembly such that the fracture was heated on the bottom, with a thermal gradient from about 140°C near the rock bottom to about 80°C at the top. Water containing potassium iodide to enhance x-ray attenuation contrast was introduced into the aperture. Solid potassium iodide was precipitated upon boiling, identifying regions of active boiling. The experiments extended over 24 and 72 hours with flow rates of 2.5 ml/min initially that were reduced to 0.55 ml/min in the first experiment and 0.3 ml/min in the second.

Results

In the first experiment, dyes stained the rock as the water boiled off. At the lowest flow rate with red dye, water did not penetrate significantly below the boiling isotherm (Figure 1). Water evaporation occurred in two bands: near the horizontal boiling isotherm and near the injection point. Yellow dye was introduced with water at the medium injection rate. Some evaporation occurred in the same locations where the water introduced at the lowest flow rate evaporated, however flow also extended downward beyond the centrally located nominal boil-

Figure 1. Fracture faces following infusion of water with dyes. The boiling isotherm for each case is shown.
Water to flow through these regions. In the first experiment, partial clog-

becoming permanently confined to particular pathways. Water
pathways were visible as cooler areas extending from water introduced at the highest
flow rate was visible in most cases beyond the extent of the yellow dye, and
an apparently wider finger, or several fingers, extended to the bottom of the fracture.

In the second type of experiments investigating fracture flow and imbibition, the time scale of fracture flow was on the order of minutes and the time scale of imbibition was hours. Upon introduction into the fracture, water flowed in fingers and films downward toward the heated region, with broader fingers occurring in the first experiment with the higher flow rate. As water penetrated the above-boiling region, boiling occurred and vapor began to condense in cooler regions (Figure 2a). Intermittent unstable boiling events called rapid evaporation events (REEs) frequently occurred in both experiments when liquid water superheated and boiled rapidly. These REEs caused pressure pulses that affected flow and often triggered REEs in other parts of the sample. Solid potassium iodide accumulated in the boiling region at temperatures exceeding the boiling point and hindered liquid flow, but the salt buildup was intermittently washed out by flow through these regions. In the first experiment, partial clogging of the aperture by salt caused a buildup of heat, which was reduced during washouts.

Temperature monitoring showed cooling upon introduction of water. Water pathways were visible as cooler areas extending through the boiling region in the thermal images. At the higher flow rate, water flowed through the heated region without becoming permanently confined to particular pathways. Water flowed first through one side, cooling it, then the middle, then the other side, intermittently oscillating from side to side on a time scale of hours. At the lower flow rate (Figure 2b), water generally flowed around the hottest regions, but intermittent boiling events of water accumulating in the apparatus bottom caused water to flow through these regions.

Water imbibition into the rock increased over time, but was spatially non-uniform. X-ray attenuation in the boiling region was much higher than elsewhere, indicating both salt-crystal build-up and imbibition (Figure 2c). In some locations, video images and radiographs show salt crystal buildup in the same locations, but even greater x-ray attenuation (darker spots

Figure 2. (a) Visual, (b) temperature and (c) x-ray attenuation images of water flow through a non-isothermal fracture. The single arrow in (a) indicates condensing water; the double arrow indicates solid potassium iodide also seen in (c). In (b), the heated zone is at the bottom with red representing 140°C, cyan 100°C, and purple <80°C. Darker regions in (c) show greater x-ray attenuation, indicating higher imbibition or precipitation.

We have identified and observed several important phenomena which occur in boiling fractures. Water flow into boiling-hot regions was hindered by heat and the accumulation of mineral precipitates. Higher flow rates allowed deeper penetration into the boiling region, and allowed washout of precipitated minerals. Imbibition was not uniform across the sample; more permeable regions and hotter regions showed greater x-ray attenuation, indicating increased imbibition into the rock and salt deposition. REEs occurred frequently in the boiling region, affecting liquid and vapor flow in their vicinity. Flow paths were variable through the heated region, particularly at the higher flow rates, with flow rate influencing flow paths.

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**Significance of Findings**

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**Related Publications**


**Funding**

This work has been supported by the Director, Office of Civilian Radioactive Waste Management, through Memorandum Purchase Order EA9013MC5X between TRW Environmental Safety Systems, Inc., and Ernest Orlando Lawrence Berkeley National Laboratory for the Yucca Mountain Site Characterization Project under U.S. Department of Energy Contract No. DE-AC03-76SF00098 and by Lawrence Livermore National Laboratory under contract W-7405-ENG-48.
Research Objectives

The Drift Scale Test (DST) is the second of the two in-situ heater tests being carried out in the underground Exploratory Studies Facilities at Yucca Mountain, Nevada (the Single Heater test, SHT, was the first). The primary objective of the DST, as it was with the SHT, is to develop a better understanding of the effect and influence of thermal-loading on the coupled thermal, mechanical, hydrological and chemical (TMHC) responses of the surrounding rock mass.

Approach

The primary difference between the DST, located in the middle non-lithophysal unit of the Topopah Spring welded tuff of Yucca Mountain, and the SHT is that of scale. Whereas the heating element of the SHT was only 5 m long and placed in a 9.6-cm diameter borehole, the heated drift of the DST is 47.5 m long and 5 m in diameter. Heating is provided by nine canister heaters, which are placed on the floor of the heated drift. In addition, there are 25 wing heaters, placed perpendicular to the longitudinal axis of the heated drift, on each side of it. The wing heaters are used to emulate the effects of adjacent heat-generating waste-storage drifts. Each wing heater is about 9.5 m long (consisting of an inner and outer section, each about 4.5 m long), and the spacing between each wing heater is about 1.83 m. The canister heaters and wing heaters together have a heat output of approximately 185 KW. The TMHC responses from the DST are measured by approximately 3,500 sensors, which are placed in 147 boreholes. Numerous variables, including heater power, temperature, thermal expansion, moisture and mechanical displacements are measured by these sensors, which are connected to an automatic data collection system.

The heating phase in the DST started on Dec. 3, 1997. The planned duration for the heating and cooling phases is four years each. The heating phase has been planned to elevate temperatures of a substantial rock volume (more than 10,000 cubic meters) above 100°C, while allowing the temperatures along the heated drift wall to reach as high as 200°C. The heat output of the canister and wing heaters can be adjusted over the full range to achieve these targets.

Thermal-hydrological simulations of the DST are being performed with the TOUGH2 simulator, an integrated finite difference simulation program for nonisothermal flow of multicomponent, multiphase fluid in porous and fractured media. We use the EOS4 module, which supports the thermodynamics of nonisothermal two-phase flow of components air and water, with vapor-pressure-lowering capabilities.

The configurations, parameters, and initial and boundary conditions of the numerical model are designed to resemble the actual test conditions of the DST as closely as possible. The DST model domain encompasses three different stratigraphic layers of Yucca Mountain; i.e., the upper lithophysal, the middle non-lithophysal, and the lower lithophysal units of the Topopah Spring fractured welded tuff. The heated drift itself is in the middle nonlithophysal unit. The material properties within each layer are assumed homogeneous. As far as feasible, the input parameters of thermal and hydrological properties for the DST numerical model have been derived from laboratory and field pre-test characterization data of the DST block. When site-specific measurements are not available, properties are derived from mountain-scale calibration to measured data from numerous surface-based boreholes.

The results presented below are based on the hydrology property sets, which are calibrated to an infiltration rate of 0.36 mm/yr. While different conceptual models have been utilized for simulating the TMHC responses from the DST, here we will present only the three-dimensional dual-permeability model, which assumes two separate continua for the fractures and the matrix. The details of the model can be found in Birkholzer and Tsang (1997, 1998).

Results

The key processes involved in the thermal-hydrological response of the unsaturated fractured tuff to heat are as follows. As formation temperature approaches 100°C around the heater,
matrix pore water boils and vaporizes. Most of the vapor generated moves into the fractures, where it becomes highly mobile and is driven by the gas pressure gradient away from the heat source. Upon further heating, the zone near the heating plane develops a "dry-out" area. However, away from the heating plane, when the vapor encounters cooler rock, it condenses, and the local fracture liquid saturation builds up.

Part of the condensate then may imbibe into the matrix, where it is subject to a very strong capillary gradient towards the heat source, giving rise to a reflux of liquid to the dry-out areas. Some fraction of the condensate in the fractures may also flow back towards the boiling zone, however, as capillary forces are relatively weak in the fractures, a substantial amount of liquid may drain by gravity. As a result, liquid saturation builds up below the heated drift. Figure 1 shows the simulated liquid saturation in the fractures after one year of heating in a vertical plane about 10 m from the west end of the heated drift. The signatures of all the physical processes described above can be observed in this figure.

Figure 1 also shows that the drying region is about 4 m thick after 12 months of heating. Beyond the drying region is the condensation zone, where the liquid saturation increases from preheat values. The redistribution of the moisture content described by the numerical model is consistent with data (not shown here) obtained from active testing by neutron logging, electrical resistivity tomography, cross-hole radar tomography and air-permeability tests.

Temperature data have been continuously collected in about 40 boreholes, which allows the display of data either as a snapshot or as time evolution at a particular spatial location. Figure 2 shows a snapshot of temperature after 12 months of heating. Temperature data from boreholes 139 and 143 are displayed as a function of radial distance from their collars at the heated drift wall. The simulated matrix temperatures are also plotted along with measured data. Observe that the temperature at the heated drift wall is around 150°C. After a small dip in temperature thereafter, it rises to about 165-170°C over a distance of about 4.5 m. Then the temperature dips slightly again, before going back up over another 4.5 m or so. Beyond this point, the temperature decreases as one moves farther away. The interpretation of such a temperature profile is as follows. Boreholes 139 and 143 are located parallel to the wing heaters on either side of the heated drift. The wing heater starts at a distance of 1.67 m from the heated drift wall, explaining the first dip in temperature. Since the wing heater is about 4.5 m long, one observes the upward trend in temperature after the first dip. The inner and outer parts of the wing heaters are separated by a gap of 0.67 m, resulting in the second dip. Notice also the small temperature plateau at the nominal boiling point, at about 12 m from the heated drift wall, indicating that a small two-phase zone exists at the tip of the wing heaters. Figure 2 confirms that our simulation results are able to mimic the thermal and hydrological processes taking place in the DST quite closely.

**Significance of Findings**

The agreement between measured data and simulation results indicates that the thermal-hydrological responses of the DST are well represented by the coupled thermal-hydrological numerical model. While heat conduction accounts for most of the temperature rise, thermal-hydrological coupling contributes to the heat transfer by convection, resulting in better agreement between simulations and measured data. The thermal-hydrological coupling also accounts for the moisture redistribution seen by the active testing data.

**Related Publications**


**Funding**

This work has been supported by the Director, Office of Civilian Radioactive Waste Management, through Memorandum Purchase Order EA9015MC5X between TRW Environmental Safety Systems, Inc., and Ernest Orlando Lawrence Berkeley National Laboratory for the Yucca Mountain Site Characterization Project under U.S. Department of Energy Contract No. DE-AC03-76SF00098.
Research Objectives

Yucca Mountain, Nevada, is the site of a proposed high-level nuclear waste repository. To test the effects that heat generated by the nuclear waste may have on the host rock for the repository, a drift-scale heater test (DST) is being carried out in the underground Exploratory Studies Facility at Yucca Mountain. The DST began in December 1997 and is designed to continue for a total of eight years. During the initial heating phase, which will last for the first two years of the project, the rock at the drift wall is being heated to 200°C. Over the next two years the temperature of the wall rock will be maintained at 200°C. For the last four years the heaters will be turned off and the system will be allowed to cool. As part of the monitoring efforts for this project, the concentrations and stable carbon isotope ratios ($\delta^{13}C$) values) of CO$_2$ in gas samples from the rock around the heated drift are being measured. CO$_2$ and associated dissolved inorganic carbon compounds (DIC) in the porewaters in the rock have a strong influence on the chemistry of the porewaters, which in turn controls mineral reactions in the system.

Approach

The host rock for the thermal test is the Topopah Springs welded tuff unit. The rock is a highly fractured unit containing approximately 10% matrix porosity, which is about 90% filled with water. The thermal test alcove is located about 250 m below the surface.

The heater drift for the DST is 47.5 m long and 5 m across. Heat is provided by a series of canister heaters in the center of the drift and wing heaters that extend 10 m into the rock on either side of the drift. The entrance to the heater drift is isolated from the observation drift (OD) by a thermally insulated bulkhead. Gas samples are collected from a series of 12 hydrological monitoring boreholes drilled into the rock around the drift. High-temperature, inflatable packers placed at approximately 10-m spacing divide the boreholes into three or four intervals. One-half-liter gas samples were collected for analysis from the packed-off intervals after purging approximately three times the volume of the interval. The CO$_2$ concentrations in the samples were measured using an infrared analyzer (Li-Cor). The CO$_2$ was then separated out of the samples and the stable carbon isotope ratio analyzed using the VG Prism Series II isotope ratio mass spectrometer at Berkeley Lab's Center for Isotope Geochemistry. Where possible, aliquots of the CO$_2$ collected for $\delta^{13}C$ analyses were saved for $^{14}C$ analyses. To date, six of those samples have been analyzed at the Center for Accelerator Mass Spectrometry at Lawrence Livermore National Laboratory.

Results

The concentration of CO$_2$ in the rock has increased significantly since heating began. The CO$_2$ concentration of a gas sample collected from a borehole drilled into the unheated side of the access/observation drift (AOD) was 919 ppm. Figure 1 is a plot of the concentrations and $\delta^{13}C$ values of CO$_2$ in samples collected from boreholes 74 through 78 during December 1998 (slightly over one year after heating began). The CO$_2$ concentrations in several of the hotter intervals are in excess of 20,000 ppm. By contrast, the concentration of CO$_2$ in the AOD was 375 ppm and in

![Figure 1. The $\delta^{13}C$ values of CO$_2$ in samples collected from boreholes 74-78 at the DST during December 1998. Given in parentheses are the concentrations of CO$_2$ (in ppm) and the temperatures (in °C) for the sampling intervals.](image-url)
Evolution of CO₂ From Heated Rock at Yucca Mountain

The δ¹³C values of the CO₂ are also increasing as the rock is heated. The δ¹³C value of the CO₂ in the gas sample collected from the borehole into unheated rock opposite the heater drift was -13.1‰. The δ¹³C values of the borehole samples on Figure 1 range from -12.3‰ to -1.5‰. The ¹⁴C contents of a limited number of the CO₂ samples were also measured. The data for samples from borehole 78, interval 3, are plotted in Figure 2. The general increase in CO₂ concentrations and δ¹³C values with temperature is clear in this interval. The ¹⁴C values of the CO₂ decreased from 40.0% of the concentration of modern atmospheric CO₂ in February to 10.5% of modern in October.

**Significance of Findings**

The shifts observed in the δ¹³C values and ¹⁴C contents of the CO₂ in the heated rock suggest that the increased concentrations of CO₂ are derived from two sources. One source is the porewater DIC. As the temperature rises, the partitioning of inorganic carbon between the gas and liquid phases shifts, with a higher proportion going into the gas phase. When the rock reaches the boiling point of water, the CO₂ concentrations will increase even more quickly until the rock dries out and all the inorganic carbon is converted to CO₂. Therefore, as the temperature rises and the DIC is converted to CO₂, the δ¹³C value of the gas-phase CO₂ will increase.

The other source of CO₂ is dissolution of secondary calcite deposited in the fractures in the rock. As the temperature increases, calcite will tend to precipitate rather than dissolve. However, in areas of the system where steam generated from boiling of the porewaters is condensing or draining (e.g., interval 3 of borehole 78), hydrolysis can occur, and will produce increased concentrations of CO₂. The δ¹³C values of calcite in the rock are high (between -6‰ and +10‰) and will also produce high δ¹³C CO₂ when it is dissolved. This makes it difficult to distinguish from CO₂ derived from porewater DIC. However, the ¹⁴C content of CO₂ derived from calcite will be lower than that derived from porewater DIC. The ¹⁴C content of CO₂ (which will be close to equilibrium with the porewater DIC) at this depth is about 50% of modern, whereas the ¹⁴C content of the calcite in the fractures is essentially 0% of modern. Therefore, the trend towards lower ¹⁴C contents observed for CO₂ from borehole 78, interval 3, indicates a shift from degassing of porewater DIC to hydrolysis of calcite.

The isotopic compositions of the CO₂ in the rock present a powerful tool for quantifying factors such as the degree of degassing of porewater DIC and for identifying areas and rates of calcite dissolution. These factors can have significant impacts on variables such as the pH of the porewaters and mineral equilibria in the rock. In turn, mineral precipitation and dissolution may influence the permeability of the rock and the movement of water within the system, which are important issues for ensuring safe, long-term storage of nuclear waste.

**Funding**

This work has been supported by the Director, Office of Civilian Radioactive Waste Management, through Memorandum Purchase Order EA9013MC5X between TRW Environmental Safety Systems, Inc., and Ernest Orlando Lawrence Berkeley National Laboratory for the Yucca Mountain Site Characterization Project under U.S. Department of Energy Contract No. DE-AC03-76SF00098.
Research Objectives

The Drift Scale Test (DST) is the second underground thermal test that is being carried out in the Exploratory Studies Facility at Yucca Mountain, Nevada. The purpose of the test is to evaluate the coupled thermal, hydrological, chemical and mechanical processes that take place in unsaturated fractured tuff over a range of temperatures from ambient (approximately 25°C) to nearly 200°C. The DST was begun on Dec. 3, 1997, with a planned four-year period of heating, followed by four years of cooling.

Our objectives were to make predictions of the coupled thermal, hydrological, and chemical (THC) processes, followed by model refinement and comparison to measured data. We expected that some water (formed by condensation of steam in fractures) would be collected as was the case for the completed Single Heater Test. Throughout 1998, samples of water and gas were collected from boreholes that enabled us to further refine our models and understanding of the complex rate-limited chemical interactions between rock, water and gas.

Approach

Here we describe our conceptual model for coupled THC processes at the DST and their treatment by numerical modelling. A conceptual model for reaction-transport processes in the fractured welded tuffs at the DST must account for the different rates of transport in very permeable fractures, compared to a much less permeable rock matrix. Transport rates greater than the rate of equilibration via diffusion leads to disequilibrium between waters in fractures and matrix. Because the system is unsaturated and undergoes boiling, the transport of gaseous species is an important consideration. The model must also capture the differences in initial mineralogy in fractures and matrix and their evolution.

To handle these separate yet interacting processes in fractures and matrix, we have adopted the dual permeability method. In this method, each grid block is broken into a matrix and fracture continuum, characterized by its own pressure, temperature, liquid saturation, water and gas chemistry, and mineralogy.

Coupled THC simulations of the DST were carried out with the TOUGHREACT code (Xu et al., 1998), which was enhanced to handle regions of complete dryout, and chemistry under boiling conditions (Sonnenthal et al., 1998; Spycher et al., 1998). The geochemical module in TOUGHREACT solves simultaneously a set of chemical mass-action and mass-balance equations to compute the extent of reaction and mass transfer between aqueous species, minerals and gases at each grid block. Mineral-water reactions take place under kinetic and/or equilibrium conditions, whereas gas-water and aqueous species interactions are assumed to be at equilibrium. Equations for transport and chemical reactions are carried out sequentially once the equations for heat, water and vapor flow are solved.

The two-dimensional dual-permeability grid, the thermal and hydrological properties, and pressure-temperature-liquid saturation boundary conditions were developed by Birkholzer and...
Tsang (1997) for their predictions of the thermohydrological behavior of the DST. This provided an excellent starting point on which to build the model for the mineralogy, water and gas chemistry of the DST. The mineralogy of the rocks at the DST was derived from studies done at Lawrence Livermore and Los Alamos National Laboratories. The initial water and gas chemistry were based on data from the U.S. Geological Survey.

**Results**

The predictive modeling for the DST indicated that the pH of waters was controlled primarily by CO₂ degassing during boiling, redissolution in condensate waters in fractures, and interaction with calcite (Sonnenthal et al., 1998). However, to capture the full chemical character of condensate waters it is necessary to consider several primary and secondary minerals (feldspars, clays, zeolites, silica phases, calcite and gypsum). This is apparently the result of the extremely small effective reaction rates for the aluminosilicates, such as feldspars, that have a measurable, yet minimal, effect on the water chemistry over the time scale of days to weeks.

A simulation illustrating the outgassing, transport, and redissolution of CO₂ and the precipitation and dissolution of calcite, silica phases and gypsum is presented here. Minerals, aqueous and gaseous species are given in Table 1.

Simulation results for CO₂ and temperature in fractures after one year of heating are contoured in Figure 1. Regions of decreased CO₂ are evident near the drift wall, and along the wing heaters where dryout has occurred, or where water has mostly boiled away. A large halo of increased CO₂ starts at about the 90°C isotherm and extends well into the region of ambient temperature (below 30°C). The water in fractures, which started with a pH of about 8.3, has dropped to less than 7 in the condensate areas (Figure 2). The boiling zone, within the wide interval between 90°C and 100°C, is characterized by higher pH waters and reduced CO₂.

Numerous measurements of CO₂ concentrations in gas collected from hydrology boreholes around the DST (Conrad, 1998) have shown a large region of increased partial pressures of CO₂ (over 50,000 ppmv CO₂), compared to the atmospheric concentration (around 375 ppmv CO₂). In terms of the magnitude and distribution of PCO₂ around the DST, these data compare remarkably well to the model results. Some local differences are thought to be related to heterogeneity in the fracture system.

<table>
<thead>
<tr>
<th>Minerals</th>
<th>Primary Aqueous Species</th>
<th>Gaseous Species</th>
</tr>
</thead>
<tbody>
<tr>
<td>Cristobalite-a</td>
<td>SiO₂ (aq)</td>
<td>CO₂</td>
</tr>
<tr>
<td>Quartz</td>
<td>Ca²⁺</td>
<td>H₂O</td>
</tr>
<tr>
<td>Amorphous silica</td>
<td>Na⁺</td>
<td></td>
</tr>
<tr>
<td>Calcite</td>
<td>Cl⁻</td>
<td></td>
</tr>
<tr>
<td>Gypsum</td>
<td>HCO₃⁻</td>
<td></td>
</tr>
<tr>
<td></td>
<td>SO₄²⁻</td>
<td></td>
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<tr>
<td></td>
<td>H⁺</td>
<td></td>
</tr>
</tbody>
</table>

**Table 1** Mineral phases, aqueous and gaseous species used in the DST model simulation.

**Significance of Findings**

Previously, there has been little work on modeling reaction-transport processes in unsaturated systems under boiling conditions. The DST presented an unprecedented opportunity to test the conceptual models and codes on a well-constrained system over time and spatial scales greater than simple lab experiments. The agreement of CO₂ concentrations between model results and field measurements gives confidence that essential aspects of the coupling between thermal, hydrological, and chemical processes have been captured. The methodology developed for the modeling of the DST can then be applied with more certainty to predictions of the long term behavior of a potential nuclear waste repository.

**Related Publications**


**Funding**

This work was supported by the Director, Office of Civilian Radioactive Waste Management, through Memorandum Purchase Order EA9015MC5X between TRW Environmental Safety Systems, Inc., and the Ernest Orlando Lawrence Berkeley National Laboratory under U.S. Department of Energy Contract No. DE-AC03-76SF00098.
Research Objectives

ROCMAS is a three-dimensional finite-element computer code developed at LBNL for analysis of coupled thermohydromechanical (THM) processes in fractured rock. Recent interests in coupled THM processes associated with nuclear waste repositories in geological media and, in particular, the issue of resaturation of a clay buffer around a waste canister has encouraged major developments of the ROCMAS code in the past three years. The main objective is to develop a tool for analysis of THM processes in practical field scale, including unsaturated rock masses and also detailed behavior of near-field fractures and an unsaturated clay buffer. This development is accompanied with validation of the relevant processes through modeling of laboratory and field experiments.

Approach

The ROCMAS code has been extended from analysis of fully saturated media to partially saturated media. This development is based on Phillip and de Vries’ work on moisture and heat transport in hysteretic, inhomogeneous porous media. In the new development, ROCMAS considers both liquid-water flow and vapor flow in air-filled pores due to molecular diffusion; both are coupled with temperature and mechanical deformation. The liquid flow is driven by the pressure gradient and depends on the relative permeability, which is a function of saturation. The vapor flow is driven by the vapor density gradient and depends on an effective molecular diffusion coefficient, \( D_v \). Airflow and convection of vapor with bulk airflow are not considered. Thus, this approach may be limited to relatively low-temperature or low-permeability systems where the steam convection can be neglected.

The new algorithms of ROCMAS are verified against existing analytical solutions and by code-to-code comparison with the independently developed thermohydrological two-phase flow computer code TOUGH2. Further code-to-code verifications and validations against laboratory and field experiments are provided by participation in the international cooperative project DECOVALEX (Development of Coupled models and their Validation against Experiments in nuclear waste isolation). Within this project, the fundamental responses of a bentonite clay material were investigated in a number of laboratory tests conducted by the Japan Nuclear Cycle Development Institute (JNC). The following tests were included:
- Suction test
- Infiltration test
- Thermal gradient test
- Swelling pressure test

First, a number of suction tests were conducted to determine the relationship between suction pressure and saturation; that is, the water retention curve. Second, several infiltration experiments were conducted on compacted bentonite specimens of 20- by-20 mm to determine the relative permeability, \( k_r \), and the effective molecular diffusion coefficient, \( D_v \). The samples were initially dry and water was supplied through a metal filter at the bottom. After various infiltration periods, the specimens were sliced into 2-mm sections for measurement of the water content.

The third type of experiment was the thermal gradient test for determination of the thermal vapor diffusion. These tests were conducted on compacted bentonite samples of 68% saturation, 50 mm in diameter and 100 mm in height (Figure 1). Applying an elevated temperature at the lower boundary of the samples creates a thermal gradient. Temperature was monitored at various distances along the sample and water content was measured from the weight loss during a subsequent oven drying. The fourth test was conducted to determine the relationship between total stress and saturation due to swelling of the bentonite clay material were investigated in a number of laboratory tests conducted by the Japan Nuclear Cycle Development Institute (JNC). The following tests were included:

![Figure 1. Schematic view of thermal gradient test.](image-url)
Testing of a Coupled THM Model for Unsaturated Media Against Laboratory Experiments

Figure 2. Experimental and modeling results of the thermal gradient test after 400 hours of heating.

Results

The suction tests resulted in water retention curves that cannot be exactly represented by any standard function. Therefore it is used exactly as is, and tabulated into the ROCLMAS code. From the infiltration test, the relative permeability, \( k_r \), and the effective molecular diffusion coefficient, \( D_m \), were determined directly from the test results by an analytical method. Thereafter, the actual experiment was modeled with ROCLMAS for validation of the code. The results of the modeling show that the liquid water flow and the relative permeability are important at saturations above 30%. Relative permeability at full saturation is \( k_r = 1.0 \) and decreases to \( k_r = 0.01 \) at about 30% saturation. Below 30% saturation, \( k_r \) is so low that the vapor flow due to molecular diffusion becomes dominating, and the effective molecular diffusion coefficient is determined to be \( D_m = 2.0 \times 10^6 \) m^2/s.

With the properties for isothermal diffusion known from the infiltration test, the properties for thermal diffusion can be back-calculated from the thermal gradient test. Figure 2 presents the results of modeling and experimentation for one of the tests after 400 hours of heating. The moisture transport in this experiment is dominated by the vapor flow due to the thermal gradient. As the temperature increases at the hot end of the sample, liquid water vaporizes, increasing the density of vapor. In response to the increased vapor density, the vapor is transported towards cooler regions, where it is again condensed into liquid water. Thus, the bentonite becomes drier at the hot end and wetter at the cooler end. The vapor flow due to the thermal gradient is opposed by a liquid flow that is driven by the liquid pressure gradient, which wants to transport water back from wet toward dry areas.

The experiments were matched using a thermal diffusion enhancement factor, \( f_{Th} = 1.0 - 1.7 \).

The swelling pressure test could be well matched with a Bishop type of effective stress law. However, the experiment was conducted by increasing the saturation from 68% toward full saturation. The results may therefore not be relevant for very low saturation where the Bishop's effective stress law probably is not valid.

Significance of Findings

The agreement between the data and simulated results indicates that the THM responses of the experiments are well represented by the new algorithms simulating coupled THM processes in unsaturated media. Furthermore, the results indicate that the approach of Phillip and de Vries is appropriate for the bentonite material and for the circumstances of these experiments. Thus, convection of vapor with gas flow seems to be minor in comparison to the molecular diffusion.

Related Publications


Funding

This work has been supported by a grant from the Swedish Nuclear Power Inspectorate.
Coupled Analysis
Of a THM Field Experiment
In an Unsaturated Buffer-Rock System

Jonny Rutqvist, Jahan Noorishad and Chin-Fu Tsang

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Research Objectives

The Kamaishi Mine Heater Test is a major field test case in the international cooperative project DECOVALEX (DEvelopment of COupled models and their Validation against EXPERiments in nuclear waste isolation). The heater experiment was conducted in the fractured hard rock and clay buffer system of a potential nuclear waste repository design. A major objective of the test is to observe near-field coupled thermohydromechanical (THM) phenomena in-situ and to build confidence in coupled mathematical models of these processes.

Approach

The experiment was conducted in a 5-by-7-m alcove excavated off an existing drift located at a depth of about 300 m. In 1995, a test pit 1.7 m in diameter and 5 m in depth was drilled in the floor of the alcove. In 1996, a heater was installed into the test pit and surrounded by a buffer of bentonite-clay which had an initial water content of 16% (66% saturation). The temperature of the heater was set to 100°C for eight and one-half months followed by a six-month cooling period. The bentonite and the rock surrounding it were extensively instrumented for monitoring of system response. Data included temperature, moisture content, fluid pressure, stress, strain and displacements. The experiment was completed in the beginning of 1998 and thereafter the monitoring sensors were calibrated.

The heater test is modeled with the computer code ROCMAS (Noorishad and Tsang, 1996), which is a finite-element program for analysis of coupled THM processes in fractured and unsaturated rocks (see article, this report). The three-dimensional model of the test environment consists of 11,158 elements and includes 13 materials, with the nearby drifts explicitly defined (Figure 1). The rock mass is simulated as an equivalent continuum, but in the near field a few important shear fractures are defined discretely. The in-situ permeability of these fractures could be determined by model calibration using measurements of water inflow through the wall of the open test pit. The property values of the buffer and intact rock matrix, including relative permeability, molecular diffusion coefficient, thermal conductivity, thermal expansion coefficient, heat capacity and Young's modulus, were determined from laboratory tests of small samples.

Results

Figure 2a shows a comparison of the predicted and measured temperatures at three key points at mid-elevation of the heater. The agreement of the temperature is very good in these points as well as at other monitoring points in both the bentonite and surrounding rock. After turning on the heater, the temperature rises in the bentonite and approaches an apparent steady state after about one month, with a temperature of about 55°C at the bentonite-rock interface. The elevated temperature is a major driving force for the moisture flow in the bentonite and gives rise to thermal stresses.

There are two main processes controlling the water flow in the unsaturated bentonite. First, there is vapor flow from the...
inner hot region towards cooler regions of the bentonite driven by the temperature gradient. Second, there is a liquid flow from the fully saturated rock-bentonite interface towards the inner dryer regions of the bentonite, which is driven by the pressure gradient. The overall agreement of the time history of water content in the bentonite is satisfactory with all measured general trends captured in the modeling (Figure 2b). Near the heater (BW5) the water content gradually decreases to a few percent (10% saturation) at the end of the heating phase and thereafter increases slowly during the cooling phase. In the mid-section between the heater and the rock (BW4) the water content increases during the first few months and thereafter decreases. This temporary increase of water content is due to a condensation zone that is moving outwards during the heating phase. At BW3, which is located in the bentonite about 1 cm from the bentonite-rock interface, the water content increases to the maximum of about 25% (full saturation) within 10 days. Both the modeling and the field experiments indicate that there is no influence of high permeability fractures on the wetting of the bentonite. This indicates that the rock permeability was sufficient over the entire rock-bentonite interface to supply an unlimited amount of water for wetting of the bentonite. However, the inflow from the rock into the bentonite was slightly over-predicted at locations above and below the heater. This may be due to the fact that the permeability of the rock matrix is overestimated or that there is a sealing effect at the bentonite-rock interface that is not captured in the modeling.

There are two main processes controlling the changes in mechanical stress during this experiment. The immediate response is that the thermal expansion of the rock and bentonite gives rise to thermal compressive stresses in both the rock and the bentonite. Thereafter, as the water content changes, the bentonite either swells or shrinks. It swells and creates increased compressive stresses (swelling pressure) in regions near the rock-bentonite interface where the water content increases. On the other hand, the bentonite shrinks near the heater where the water content is reduced and tensile fracturing may occur. Both the modeling and the field measurements show that the swelling pressure in this case is low (less than 0.5 MPa). However, there are considerable uncertainties in the measurements of the swelling pressure as well as modeling of the mechanical behavior of the bentonite, especially when the degree of saturation is low.

**Significance of Findings**

The good agreement between the predictions and measured results regarding temperature and water content indicates that the thermal-hydrological responses of the Kamtishi heater test are well represented by the coupled numerical model. Uncertainties remain in the hydromechanical behavior of the bentonite and the influence of the rock-bentonite interface on the wetting process.

**Related Publications**


**Funding**

This work has been supported by a grant from the Swedish Nuclear Power Inspectorate (SK). The work was also partially supported by the National Energy Research Scientific Computational Center (NERSC) through U.S. Department of Energy Contract No. DE-AC03-76SP00098.
Research Objectives

The primary role of geophysical studies at Yucca Mountain, Nevada, has been the measurement and imaging of physical rock properties. Properties such as density, conductivity, bulk and shear moduli are used to estimate other geologic properties such as stratigraphy, structure, saturation, fracturing and permeability. Although boreholes and tunnels in the Exploratory Study Facility (ESF) will allow direct examination of physical properties, there is a need to detect and characterize subsurface features away from and between these access points. Boreholes and tunnels to date have given a very small window into the entire repository volume. In addition, the lateral variability and heterogeneity in the Topopah formation make it difficult to extrapolate between observation points. It is necessary to know the location of significant faults and fracture zones as well as variations in lithology and rock type to help design and predict the performance of the potential repository. The current experiment was undertaken to broadly detect and characterize subsurface faults, fracture networks and lithological features within the potential repository, the middle-nonlithophysal zone (Tptpmn) and its vicinity.

Approach

To achieve these goals a surface-to-tunnel seismic imaging survey was designed. A total of 180 vibroseis (vibrating) sources with a spacing of 30 m were deployed along Yucca Mountain Ridge over a total length of 5 km, while 224 two-component geophone sensors were grouted in the tunnel with a separation of 15 m between 2680 and 5970 m, producing more than 5 km² of interpretable images. In order to investigate and image the repository area, the first arrival times and associated amplitudes of the seismic waves are interactively determined. To better understand the wave propagation in this survey, a 2-D elastic program with parameter adjustment allowing a simulation of 3-D geometry is used. Such a reduction is justified for the cases of 3-D problems with cylindrical symmetry where medium properties are laterally homogeneous and change only along the vertical z coordinate (i.e., horizontal layering). The first step is to apply a 2-D velocity model, as derived from VSP studies at UZ-16 (Majer et al., 1996) and project the velocities for the lithologic units onto a 2-D cross-section of the 3-D site scale geologic model. This original 2-D velocity model has to be adjusted to match the arrival times and waveform between the elastic waveform simulations and the recorded field data. The modeling efforts produce evidence that first arrivals at far offsets are reflected waves from lower structures rather than direct waves. Thus, to eliminate the larger offset travel times in the tomographic imaging inversions, only angles of less than about 45 degrees are used.

Results

In order to estimate the variations in seismic wave properties, the seismic traces, when aligned along their first arrival travel times and corrected for geometrical spreading, reveal significant lateral variation in the amplitudes across the tunnel length. In order to quantify this variation, the root mean square (rms) values of the amplitudes associated with the first arrival are determined. To support this comparison, the fracture density, determined along the tunnel walls, is presented alongside the amplitude values in Figure 1. Both curves are normalized (the fracture density to 1, the rms amplitudes to 2) to separate them in the plot. It is evident that the correlation is good, particularly in the sections with increased fracture intensity where the rms amplitudes rise above their background value.

To prove the hypothesis that this result is caused by site amplification due to a decrease in velocity and density within the fracture zone, a noise investigation is performed. If the increase in seismic amplitudes is due to site amplification, the noise should be amplified in the same way. Therefore, the rms amplitude of the noise is determined and the values displayed in Figure 1 (upper curve). It is evident that the noise is not amplified in the same way as the seismic waves, and therefore,
The presence of the Sundance fault seems to be manifested by an interruption of the unfractured area at about 23,300 m Northing (northerly direction).

### Significance of Findings

Surface-to-tunnel tomographic imaging seems to be suitable to produce estimates of large-scale velocity, attenuation and fracture density distributions at Yucca Mountain. It is found that certain geometries of fracture distribution may lead to constructive interference and consequently to an increase in amplitudes of the propagating waves. The repository horizon appears to be heterogeneous regarding the degree of fracturing, with the more intensely fractured areas in the southern part, while the northern end of the survey area seems to be less fractured. Furthermore the alignment of fractures may vary from the south towards the north. The East-West drift appears to be located in an area of relatively unfractured rock.

### Related Publications


### Funding

This work has been supported by the Director, Office of Civilian Radioactive Waste Management, through Memorandum Purchase Order EA9013MC5X between TRW Environmental Safety Systems, Inc., and Ernest Orlando Lawrence Berkeley National Laboratory for the Yucca Mountain Site Characterization Project under U.S. Department of Energy Contract No. DEAC03-76SF00098.
Research Objectives

Inca rulers were held accountable by their subjects for provisions during times of adverse conditions. For example, a local ruler in Lambayeque, Peru, was put to death by his subjects during an especially severe drought. As a result, the Inca developed sophisticated systems for the storage and distribution of goods such as textiles, maize, beans and other agricultural products. In much of southern Peru, precipitation occurs primarily during the monsoon season, and the ability to store and retrieve water is necessary to ensure consistent supply. Inca water storage systems consisting of reservoirs, cisterns and aqueducts are known from many sites. The focus of the present research is to demonstrate that the stonework at the site of Tambomachay, about 5 km north of Cuzco, is not merely ornamental, as has been assumed by previous authors, but rather forms the basis of a sophisticated geologic water storage system not as yet described in the literature.

Approach

The site of Tambomachay is dominated by a series of masonry walls, ranging from 1 to 3 m in height (Figure 1). The upper two stone courses are of high-quality masonry, with finely fitted stone joints and smoothly finished faces, while the lower two courses are of slightly lower-quality fieldstone construction with mud mortar. The tiers are separated by terraces of flagstone and pounded earth. Aside from such ubiquitous features of Inca architecture as trapezoidal niches and vertically tapered walls, the principal features of the site are the fountains, which originate from a small opening in the main stone course. From this discharge point, outflow is led through a series of channels to feed first a single and then a double fountain. On either side of the masonry walls, the land surface slopes down from a limestone ridge that marks the rear of the site to a small stream (the Rio Cachimayo) that flows in the valley bottom in front of the stone construction.

The site receives approximately 950 mm of rainfall per year, almost all of which falls during the monsoon season. During and shortly after the monsoon season, the toe of the slope is the site of numerous springs that discharge ground water from the hill slope to the Rio Cachimayo. Although these springs dry up shortly after the rainy season, the fountains continue to run year-round.

In order to determine whether the stone walls act to intercept and store groundwater in-situ, a field examination of the site for evidence of increased groundwater levels behind the stone retaining walls was conducted. Following the field survey, a numerical model was constructed using the TOUGH2 flow simulator code to illustrate the concept of geologic water storage at Tambomachay and gain insight into the effectiveness of this storage system.

Results

Inspection of the site yielded abundant evidence that the stone walls act to intercept and store groundwater. The site visit occurred during the monsoon season. At that time, the soils behind the walls were obviously at field capacity, and in areas where foot or livestock trails were incised below the general land surface, standing water was in evidence. Soils to either side of the stone walls were damp from recent rains, but appeared well drained. This observation suggests that recharge entering the aquifer from precipitation mounds up behind the stone construction, resulting in high saturations behind the walls. To either side of the stone walls, recharge is free to discharge through the coarse alluvial sediments to the Rio Cachimayo. Further evidence of increased water table elevations behind the masonry comes from inspection of the walls themselves. Although the joints between the individual stone blocks are too tightly fitted to allow significant seepage, precipitate encrustation (presumably CaCO3) and moss growth near the top of the highest tier indicate that the water table regularly rises to the height of the stone retaining walls.

Because the results of the field survey appeared to confirm the hypothesis that the stone walls intercept discharge from ground water, a model of the site was devised to illustrate the general concept of geologic water storage and to give some bounds on the efficiency of the system. To this end, the system was modeled in two cases. Case I represented the hydrologic sys-
Investigation of Geologic Water Storage Near Cuzco, Peru

The results of modeling for these two scenarios can be seen in Figure 2, which represents a cross section through the aquifer directly behind the discharge point. In the figure, distance from the discharge point (x-axis) and potentiometric head (y-axis) have been normalized on the aquifer characteristic length and the maximum potentiometric head, respectively, while the time is shown as the hydrologic equivalent of the Fourier number (the square of the characteristic length times time, divided by the aquifer diffusivity). By comparing the curves for the two cases, it can be seen that the Case II scenario (post-construction) contains significantly greater quantities of water in storage at all times than the Case I scenario. By assuming reasonable values for specific storage, hydraulic conductivity, characteristic length, etc., it can be shown that potentiometric head values in the pre-construction aquifer would reach a value of 1% of the original value approximately 19 days after cessation of the monsoon rains. Using the same parameter values for the Case II aquifer yields a value of about two years to decrease heads to 1% of their original values. In addition, although both cases exhibit exponential decay of discharge rate, dimensionless discharge for the Case I aquifer decreases by more than two orders of magnitude by a dimensionless time of two units. Over the same period of time, the Case II aquifer dimensionless discharge decreases by only about 10%. The effect of this discharge leveling is a nearly constant flow rate over the entire year for the post-construction aquifer.

**Significance of Findings**

A comparison of the pre- and post-construction system models clearly indicates the dilemma of the ancient hydrologists: the natural system contained adequate resources for one or more years of human use, but under pre-construction conditions, this water was exhausted in a minimal amount of time. The elegant solution of instituting a control on the discharge boundary allowed the groundwater resources to be stored in-situ and used at a rate more suitable for human needs.

It is presently unknown how prevalent geologic storage of water was in pre-Columbian Latin America. Although the example presented in this paper is the only one observed by the author to date, the archaeological literature contains several references to "elaborated springs," which may refer to Tambomachay-style water storage systems. The prevalence of this type of storage method is important because cultural development in South America was heavily influenced by the availability of water. Geologic water storage would allow colonization of otherwise marginal areas and could therefore comprise an important control on settlement patterns not only in South America, but possibly across cultures. For example, a correspondence has been noted between geologic water storage at Tambomachay and the seeps at the feet of shallow escarpments that provided water for Mesa Verde in the Four Corners region of the United States (V. Scarborough, personal communication). As at Tambomachay, many geologic water storage systems may still be operational, impacting land use patterns from pre-Columbian through modern times.

**Related Publication**


**Funding**

This work has been supported by a grant from the Stahl Foundation and by the Director, Office of Civilian Radioactive Waste Management, through Memorandum Purchase Order EA9013MC5X between TRW Environmental Safety Systems, Inc., and Ernest Orlando Lawrence Berkeley National Laboratory under U.S. Department of Energy Contract No. DE-AC03-76SF00098.
The Energy Resources Department (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, Energy Resources Department researchers seek to transform these concepts into tangible products of use to the industry within a time-frame consistent with today's rapid growth in technology. Reservoir characterization and monitoring involve development of new seismic and electromagnetic techniques focused at the inter-well scale. Optimization of reservoir performance involves application of reservoir engineering and geomechanics principles to enhance production. The next major step in research will focus on methods to optimize performance through integration of monitored geophysical data, production data and reservoir simulation.

Principal research activities include:

- Development of single-well seismic technology, including instrumentation, acquisition and processing;
- Applications of seismic methods for characterization of fractured reservoirs;
- Use of converted waves in cross-well applications;
- Development of magnetotellurics for marine applications;
- Development of mid-frequency electromagnetic techniques with a focus on imaging through casing;
- Improved inversion methods for reservoir characterization, with a focus on combining production and geophysical data;
- Application of X-ray C7 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.

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 multi-program 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
- Development of magnetotellurics for marine applications;
- Development of mid-frequency electromagnetic techniques with a focus on imaging through casing;
- Improved inversion methods for reservoir characterization, with a focus on combining production and geophysical data;
- Application of X-ray C7 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.
- Diagnostics and imaging technology
- Drilling, completion and stimulation
- Environmental technologies
- Downstream technologies

International and national concern about the variable climactic 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, the Energy Resources Program is initiating research in methane hydrates and geologic sequestration of CO₂. These studies are focused on development of technologies which will minimize the impact of fossil fuel usage on the environment.

Projects are typically multi-year, 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, etc.). With these goals in mind, existing tools and methodologies are upgraded and new techniques and instrumentations are developed for use in the areas of geology, geophysics, geochemistry and reservoir engineering.

The program encompasses theoretical, laboratory and field studies, with an emphasis on a multidisciplinary approach to solving the problems at hand. 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 a significant part of the Berkeley Lab effort has been directed toward industry assistance, especially in the area of technology transfer and in understanding the nature and dynamics of 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:
- Development and enhancement of computer codes for modeling heat and mass transfer in porous and fractured rocks;
- Laboratory investigations of the hydraulic and thermal properties of fractured and intact reservoir rocks;
- Isotopic and noble gas studies to characterize geothermal fluids and to identify their sources, their potential migration paths and the connectivity within the geothermal reservoir;
- Documentation of the behavior of geothermal fluids under commercial production and injection operations (e.g., field case studies), with specific emphasis on The Geysers field.

**Funding**

The Oil and Gas Exploration and Development program receives funding from the Fossil Energy, Natural Gas and Oil Technology Partnership Program and Office of Science of the U.S. Department of Energy. Support is also provided by the Gas Research Institute (GRI) and direct industry contributions. Industrial collaboration is an important component of the DOE Fossil Energy and GRI programs.

Research Objectives

Crosswell seismic-imaging applications have yielded a variety of tools and approaches over the past several years. It has become clear that it is possible to leverage this technology to address the next frontier in borehole seismology—that of single-well seismic imaging (SWSI). A multi-participant research program in SWSI is being led by Berkeley Lab and includes Idaho National Engineering and Environmental Laboratory, Sandia National Laboratories and Stanford University. The continuing objective of this project is to identify and provide solutions to fundamental issues surrounding single-well seismic imaging in order to evaluate and develop the technology in a timely and cost effective fashion.

Approach

The current work consists of four interdependent activities which comprise facets of the technology required for the ultimate, successful development of single-well seismic imaging (and required for improvements in crosswell imaging). They are (1) Hardware: sources/receivers, telemetry/recording, borehole noise effects, deployment; (2) Modeling: synthetic seismograms, parametric studies, inversion, optimal designs for hardware/surveys; (3) Field Testing: quality data sets, evaluation/validation at well characterized sites; 4) Data Processing and Interpretation: algorithms, 3-D imaging, noise reduction, visualization.

We are working closely with the industry's 12-company Salt Imaging Consortium, which is focused on the use of single-well surveys to image salt dome flanks and the leveraging of resources from the Uni-well project in the United Kingdom. The project is designed around four major tasks representing the technologies described above.

Task 1 – Instrumentation Design and Development

The objective of this task will be to design and develop prototype instrumentation to augment current technology. The project team draws on past industrial experience, together with computer and laboratory experiments and analysis, to design, fabricate and field test hardware concepts for enhancing the signal-to-noise ratio for different single-well source/receiver combinations.

Task 2 – Modeling of Wave Propagation in Complex Media

Algorithms for performing computational modeling of the seismic wavefield expected in a single-well recording environment will enable us to investigate a large variety of factors that may influence the success of this imaging technique. Efforts include (1) development of elastic or viscoelastic wave propagation algorithms to generate realistic synthetic seismograms, and (2) investigation of the influence of geologic factors (e.g., curved strata, overhung salt flanks, diffuse reflectors) on the quality/utility of acquired data and on various data acquisition issues, such as source-receiver offset.

Task 3 – Field Testing and Data Acquisition

In order to evaluate and develop a useful methodology, it must be tested in environments representative of the sites of eventual application. The ongoing objective of this task is to validate and test current available methodologies as well as test new instrumentation concepts to identify optimal data collection systems, modeling needs and data-processing schemes. Initially, DOE-sponsored efforts concentrated on interfacing a diverse set of sources and receivers in order to allow field testing.

Task 4 – Development and Application of Software to Process Single-Well Data

The processing and interpre-
Development of Single-Well Seismic Imaging

The task is to evaluate and aid in the development of processing techniques that will be needed for single-well seismic imaging, including analysis of various borehole seismic sources such as the orbital vibrator.

Results

Our efforts at LBNL have focused on tasks 1, 3 and 4.

Task 1 – Instrumentation Design and Development

The borehole hardware originally available was limited by data transmission rates possible with standard wirelines, so a fiber optic design was chosen to increase communication rates and bandwidth. Successfully addressed were the design, fabrication and testing of fiber optic connectors, including transmission through a seismic source (Conoco AC orbital vibrator) in a borehole environment. In addition, Sea Con Inc. completed the adaptation of the AC orbital vibrator such that it can now be used with the commercially available P/GSI fiber optic wireline (20,000 ft) in addition to the LBNL fiber-optic wireline (10,000 ft). Also acquired by Berkeley Lab was a OYO fiber-optic system, which will accommodate the Exxon multilevel receiver system, the Conoco five-level geophone string or the Conoco 15-level hydrophone string. This provides great flexibility in data acquisition capability. A schematic of the current system is shown in Figure 1.

Task 3 – Field Testing and Data Acquisition

The second salt dome field test was carried out by Berkeley Lab in November 1998 using the AC orbital vibrator in conjunction with the CONOCO five-level 3C wall lock receiver string in well Wilbert =28 inside of the salt dome. The well exited the salt, giving ground truth on the location of the edge. Three offsets were acquired (167, 184 and 204 ft), giving a maximum of 15-fold. An example of this data is shown in Figure 2. A full single-well reflection survey was acquired over 1000 ft of a zone including salt and sediments near the base of the salt dome.

Task 4 – Development and Application of Software to Process Single-Well Data

Travel-time analysis of the axial vibrator seismic data at the Bayou Choctaw test site has been initiated. The goal of this modeling/analysis is to identify events that are potential reflected arrivals from the nearby salt dome flank. Several events in the vertical and horizontal component recorded data have nearly linear moveout at large source-receiver ranges, and can be modeled as mode-converted reflected arrivals.

Significance of Findings

The successful acquisition of single-well imaging data with a powerful borehole source (the AC orbital vibrator) and a modern multi-channel borehole acquisition system in an oil production environment leads the way to a new technique in exploration geophysics. There are immediate applications for imaging the flanks of salt domes. Another important application will be imaging around horizontal boreholes to find sub-horizontal horizons. The technology developments of this program will also improve the state-of-the-art in cross-well seismic imaging.

Related Publications


Funding

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

The Rye Patch Reservoir area in northern Nevada has had preliminary geothermal resource exploration. Initial exploration in the late 1980s and early 1990s resulted in only one successful well (44-28). Other wells were either too cold or had no flow. In 1997 TransPacific Geothermal Inc. (TGD) proposed a 3-D seismic survey to determine the geologic structure of the potentially fault-controlled reservoir. This would be possibly the first application of the 3-D seismic method to a geothermal field and therefore of interest to the entire geothermal community. The 3-D seismic method has proven an integral part of modern oil and gas exploration efforts; however, the heterogeneous and hydrothermally altered nature of geothermal reservoirs makes all seismic imaging more difficult. It was not known if the methods used in the petroleum industry could be directly transferred to the geothermal industry.

Before conducting a full-scale 3-D survey, DOE contracted LBNL to investigate the viability of seismic imaging in the Rye Patch area. LBNL obtained a vertical seismic profile (VSP) in nonproducing well 46-28 to test the seismic reflectivity in the area and to obtain velocity information for designing and potential processing of the proposed 3-D seismic survey. This initial borehole seismic study would provide a go/no-go decision for the larger, costlier 3-D study.

Approach

A vertical seismic profile (VSP) was recorded in Rye Patch by LBNL between Dec. 11 and Dec. 13, 1997. The VSP in well 46-28 used LBNL's vibroseis source and a single-level, high temperature, hydraulic wall-locking, three-component seismometer. The source was a P-wave vibrator. The source sweep was 10 to 80 Hz, 10 seconds (s) long, with a 0.2 s cosine taper. The borehole geophone used 14-Hz vertical and horizontal geophones. Six data channels were recorded: the three geophones, the source pilot, the vibrator reference and the vibrator baseplate accelerometer. The record length was 12,288 samples at a 1-millisecond (ms) sample rate, giving a 2.3-s correlated record length. A 10-Hz low-cut filter was used; no high-cut filter was used except for the anti-alias filter.

Data was acquired from a 600-ft offset location northwest of the well, spanning the depth range in the well from 1000 to 4200 ft at 40-ft intervals. Four sweeps were summed in the field to produce one record. One to three sets of four were recorded at each depth. Well depths were measured from the ground level of 4,418 ft. Because of borehole fluid pressures, a lubricator and packer were used to place the borehole geophone in the well. The geophone had a temperature monitor, which showed a maximum temperature of 259°F.

The VSP dataset was processed to obtain accurate seismic velocity as a function of depth and to image any reflections in the data. The first step in reflection processing was to balance trace amplitudes with an automatic gain control (AGC) of 200 ms, followed by a frequency-wave number (F-K) filter to remove the downgoing energy. After this process, there still was some coherent tube wave noise that was removed using a median dip filter. This was followed by a 200-ms AGC. After these processing steps, two prominent, coherent reflectors were present.

Results

Using the velocity model obtained from the first arrival times, the VSP reflection data are mapped to depth. The results are superimposed upon a cross-section traversing the VSP well (46-28) and the producing well (44-28); see Figure 1. The upper reflector correlates with the sandstone/siltstone (upper member) of the Natchez Pass Formation. This is the main permeable clastic unit which produces the thermal fluids at the Rye Patch wells. It spans the elevation range of 1300-1500 ft above sea level and is strongly coherent to about 180 ft northwest of the well. At this point, there is a loss of the reflection, possibly due to changes in rock properties or the presence of a fault.

The deeper reflector appears within the lower
member of the Natchez Pass Formation, and may occur at a limestone/siltstone interface. This reflector is about 400 ft below sea level and is coherent over 285 ft northwest of the well. This spans the entire CDP transform range, indicating that this reflector is more continuous and may continue beyond the mapped extent. The depth of this reflector is not certain because it occurs below the last sensor and there is no velocity control from direct arrivals.

**Significance of Findings**

The VSP data collected at well 46-28 did produce a coherent reflection from the permeable clastic unit, which is the main production unit in this geothermal field at a depth of about 3,000 ft. Also, seismic attenuation at this borehole was not extreme enough to limit a 3-D survey.

Based on this information, a "go" decision was made, and a three-square-mile 3-D seismic survey was collected in August 1998. The processing of this dataset is ongoing, and will be reported at a later date.

**Related Publication**


**Funding**

This work has been supported by the Assistant Secretary for Energy Efficiency and Renewable Energy, Geothermal Division, of the U.S. Department of Energy under Contract No. DE-AC03-76SF00098.
Research Objectives

Numerical modeling is an essential tool for the design and optimization of production and injection operations at geothermal reservoirs. The response to production and reinjection is governed by the coupling between fluid flow in fractures and heat transfer from adjacent matrix blocks. Furthermore, flow of water, steam, gas and heat are strongly affected by the geometric and hydrological characteristics of the fracture network.

The reliability of model predictions depends on the accuracy with which these coupled processes are accounted for. Moreover, the salient features of the geothermal reservoir must be captured, including the development of an appropriate conceptual model and the determination of thermal and hydrologic parameters. Inverse modeling—automatic calibration of the numerical model against field data—is a means to obtain model-related parameters that can be considered optimal for the given conceptual model. However, the large number of parameters needed to fully describe coupled nonisothermal multiphase flow in fractured-porous media often leads to an ill-posed inverse problem, which is predisposed to yielding nonunique and unstable solutions.

The general objective of this research is to assess the usefulness of inverse modeling for the calibration of geothermal reservoir models. More specifically, we try to identify the data that contain relevant information regarding fluid and heat flow in the reservoir. Effective fracture properties will be estimated, potentially improving the accuracy of long-term model predictions.

Approach

The most important element in geothermal inverse modeling is a sophisticated multiphase flow simulator, capable of capturing the coupling between fluid flow and heat transfer. As an example, extraction of hot fluids and reinjection of cold water leads to vaporization and condensation effects near production and injection wells, respectively. Furthermore, as a result of pressure and temperature variations during production and injection in high-salinity geothermal reservoirs, precipitation or dissolution of salt may occur, changing fracture porosity and thus the overall permeability of the reservoir. Changes in sodium chloride concentrations may therefore contain information about fluid flow in the fracture network, indicating potential connections between injection and production wells, which may eventually lead to unwanted thermal interference.

The next step is to develop an optimization routine to automatically improve the match between the observed data and the model calculation. A number of nonlinear minimization algorithms have been incorporated into the iTOUGH2 inverse modeling code (Finsterle, 1999). By performing synthetic data inversions, the contribution of each potential observation to the estimation of relevant input parameters can be determined. For example, temperature data obtained in production and observation wells contain aggregate information about hydrologic and thermal properties of the reservoir, which govern the conductive heat exchange from the matrix blocks to the flowing fluids in the fractures. Steam production and flowing enthalpy data as well as tracer data are likely to contain information about effective fracture properties on the relevant field scale.

An error analysis is performed after calibration to assess the uncertainty of the estimated parameters and to reveal unwanted parameter correlations. Using inverse modeling, the layout of the monitoring system can be optimized to reduce estimation uncertainty. The approach was tested using data from a synthetic geothermal reservoir, and by simultaneously matching field data from a well completion test and subsequent production.

Results

The iTOUGH2 code was used to simulate production from a hypothetical geothermal reservoir with high salinity and CO2 as the non-condensible gas. Due to precipitation of salt near the production well and the depletion of fluid reserves in the
reservoir, the production of steam declines rapidly and almost ceases within a relatively short period of time. After five years of exploitation, condensate is reinjected a few hundred meters from the production well. Injection of cold water leads to a reduction of steam saturation in the immediate vicinity of the injection wells. Evaporation of injectate, however, increases the reservoir pressure, driving steam towards the production well, enhancing both the rate and enthalpy of the produced fluid. Time series of simulated temperatures, steam production rates, flowenthalpies and NaCl concentrations in the production well are considered to be the data available for model calibration. The parameters studied include fracture spacing, fracture absolute permeability, porosity, initial reservoir temperature, heat conductivity and an exponent that describes the change in permeability as a function of porosity change due to salt dissolution and precipitation. Figure 1 shows contours of the objective function—an integral measure of misfit between all available data and the corresponding model output—in the parameter space spanned by log-permeability and intrinsic fracture porosity. A unique parameter set was accurately identified by the minimization algorithm within a few iterations, as indicated by the green search path.

In the field study, pressure data from multistep cold water injections into the high-temperature well KJ-31 at the Krafla geothermal field, Iceland, were matched simultaneously with enthalpy data observed during the initial discharge period after well completion (Finsterle et al., 1999). Figure 2 shows the enthalpy data (red symbols), along with the simulation results obtained with an initial parameter set from a conventional well test analysis (dashed line), and the best match obtained using iTOUGH2 (solid line). The estimated fracture properties and initial steam saturation also honor the pressure data observed during the multistep completion test (not shown). While the pressure data alone can easily be matched using either a single- or dual-porosity model, the inclusion of fractures is essential to adequately account for the boiling of large quantities of cold drilling water, as evidenced by the enthalpy data.

**Significance of Findings**

The iTOUGH2 analyses show that a joint inversion of all available data greatly improves the identifiability of key hydrologic and thermal properties affecting geothermal field performance. Adding tracer concentration data to the analysis considerably reduces the correlation among some of the parameters, allowing for a more independent and more stable estimation of reservoir properties.

Inverse modeling is a powerful tool for the design of field tests, for the optimization of reinjection operations and for the evaluation of prediction uncertainties from geothermal reservoir simulations. Combining the characterization efforts from a variety of disciplines and making use of all available data obtained during testing or production provides the basis for a better understanding of nonisothermal multiphase flow processes, for the development of an appropriate conceptual model and for the estimation of the properties required to perform reliable model predictions.

**Related Publications**


**Funding**

This work has been supported by the Assistant Secretary for Energy Efficiency and Renewable Energy, Office of Geothermal Technologies, of the U.S. Department of Energy, under Contract No. DE-AC03-76SF00098, with in-kind contributions from the National Energy Authority, Reykjavik, Iceland.
Research Objectives

The Salton Trough is host to the most prolific geothermal power production area in North America. It includes the Imperial Valley of southern California (U.S.) and the Mexicali Valley of Baja California (Mexico), where a number of high-temperature (above 180°C) geothermal areas are under commercial production. At present, the installed electrical generation capacity in the area exceeds 1,000 MW (i.e., in Mexico, 620 MW at Cerro Prieto (CPGF); and in California, 248 MW at Salton Sea (SSGF), 105 MW at East Mesa and 84 MW at Heber).

The existence of these geothermal fields is due to the region's particular geologic environment. The Salton Trough is a broad structural basin, characterized by high heat flow, tectonic deformation and seismicity, as well as volcanism resulting from tectonic activity that created a series of pull-apart basins and transform faults linking the East Pacific Rise to the San Andreas fault system (Figure 1).

As is typical of geologic systems, all geothermal fields have unique characteristics; however they also have underlying similarities. The CPGF and SSGF were compared because of their large size and high temperature. The purpose was to establish the similarities and differences between these two Salton Trough fields from the earth sciences and developmental points of view.

Approach

Data published in reports, conference articles and journal papers were assembled and analyzed to determine the main characteristics of the Cerro Prieto and Salton Sea geothermal fields. Additional information was obtained from the California Division of Oil, Gas and Geothermal Resources.

Results

As described by Lippmann et al., 1999, the comparison between CPGF and SSGF shows that they are alike in certain aspects and quite different in others. Both have similar geologic frameworks and maximum measured temperatures (350-370°C). They differ slightly in lithology (more continental, especially lacustrine sediments at the SSGF) and ultimate energy capacities (more than 800 MW at CPGF; more than 1000 MW at SSGF).

However, there are large differences in the chemistry of their geothermal fluids (Figure 2) and in the amount of evaporites and sulfides in their sedimentary columns, both being higher at SSGF. Different conceptual models apply to the two fields.

The contrast in fluid chemistries is explained by the positions of the fields with respect to the crest of the Colorado River delta. South of the crest, in an area in good communication with the

Figure 1. Generalized map showing the location of the Cerro Prieto (CPGF) and Salton Sea (SSGF) geothermal fields within the Salton Trough, Gulf of California, and the East Pacific Rise tectonic regime.

Figure 2. Chemical compositions of aquifer fluids from Cerro Prieto well M-5 and Salton Sea SSSDP well State 2-14 compared to those of normal seawater and Reykjanes, Iceland, well 8 (geothermal fluid compositions calculated for reservoir conditions).
Comparison of the Two Most Important Salton Trough Geothermal Fields

North

Salton Depression

SSGF

Colorado River Delta

South

CPGF

Gulf of California

mean sea level

Rising Plumes of Brine

No mixing with groundwater

Mixing with groundwater

Contiguous Saline

Brine (~20 wt%)

Hot Intrusive Rocks

Marine Hypersaline

Brine (~30 wt%)

Hot Intrusive Rocks

Figure 3. Schematic model of the Salton Trough when the pull-apart basins “moved” into the areas of the Salton Sea (SSGF) and Cerro Prieto (CPGF) geothermal fields.

sea (i.e., the Gulf of California to the south), salts do not accumulate in the deltaic sediments because surface and groundwaters tend to flow toward the gulf. On the other hand, at the SSGF located in the closed Salton depression north of the delta crest, salts have accumulated because waters can only leave the basin by evaporation.

In both areas concentrated brines infiltrated and accumulated in deep sediments of the Salton Trough. At SSGF the brines had higher salinities and were of continental origin, while at CPGF they were less concentrated and mainly marine. When the pull-apart basins “moved” into these two areas and the areas were heated by igneous intrusions, the brines were mobilized, forming diapirs (domes) which did not reach the ground surface (Figure 3). At CPGF mixing of the ascending brines with less saline groundwaters was significant, while at SSGF, because of the higher density contrast between the brines and the local groundwaters, mixing was minor.

The need to solve the problems of handling the higher salinity (and corrosivity) of the SSGF fluids, as well as differences in U.S. public policy and economic considerations were the main factors that delayed the development of SSGF compared to that of CPGF in Mexico.

Significance of Findings

From the exploration and development points of view it is important to recognize differences and similarities between geothermal areas and understand the underlying causes.

The presently installed electrical generation capacities at CPGF and SSGF are 620 and 248 MW, respectively, making them the largest developed liquid-dominated geothermal systems in Mexico and the United States; additional power plants are planned in both fields. A good conceptualization of the geohydrologic systems will help optimize the expansion of the wellfields and reduce the impact of large-scale fluid production and injection on the geothermal reservoirs.

Further expansion of geothermal electricity production in the Salton Trough will depend on economic factors, although public policy in favor of renewable energy—e.g., to meet Kyoto global warming goals—may foster development. Therefore in the future, the comparison will be extended to other fields in the region.

Related Publication


Funding

This work has been supported by the Assistance Secretary for Energy Efficiency and Renewable Energy, Office of Geothermal Technologies of the U.S. Department of Energy under Contract No. DE-AC03-76SF00098.
Research Objectives

The objective of this project is to offer easy-to-use graphical software to monitor waterflood performance and show ways of increasing oil production while limiting reservoir damage from water injection. The software should be data-driven, but it should have several process-dependent plug-in models of water infectivity, oil and gas productivity, waterflood response, spatial relationships in injection and production data and their cross-correlations. We also should be able to perform simple inversions of field data. Finally, the software should be intuitive, simply point-and-click and robust.

We have focused on waterflood in low-permeability rock with close well spacing, where fluid flow is linear and transient and all wells are hydrofractured. The injection fractures may grow, catastrophically at times, and production hydrofractures may shrink. For each injector, the injection rate and pressure can be inverted into the hydrofracture area as a function of time. Our approach is object-oriented, making it relatively easy to switch to other types of waterflood or altogether different fluid injection processes.

Approach

Supervisory control of waterflood requires continuous surveillance of the water injection-oil production relationships. Accordingly, we have developed an interactive software tool called Analyzer using the Matlab® 10 programming environment. This software has been developed for waterfloods in low-permeability reservoirs where all wells are hydrofractured. Analyzer lets us:

- Examine the producer and injector well histories, develop maps of field productivity and injectivity, and quantify injector-producer interactions.
- Model cumulative oil, water and gas production of individual wells, as well as the field as a whole.
- Estimate the reservoir properties based on the primary production data.
- Analyze the oil, water and gas responses to waterflood.

Waterflood failures are caused by direct injector-producer coupling, water breakthrough in some layers, poor displacement efficiency and reservoir damage due to catastrophic hydrofracture extensions. Excessive waterflooding, under an assumption that maximizing water injection will maximize oil production, leads to well-failure and causes reservoir damage. Over time, a constant injection rate at constant pressure causes, albeit inadvertently, hydrofracture extensions and reservoir damage. In order to operate the injection wells successfully and prevent catastrophic hydrofracture extensions, reservoir damage and well failures, we need to measure the dynamics of hydrofracture growth in response to fluid injection. We have used two different approaches for the characterization of injection hydrofractures. One is based on an inversion of the injection data, while the other is based on periodic hydraulic impedance testing of the injection wells.

Hydraulic impedance testing involves monitoring the transient response of the injection well-hydrofracture system to a short-duration pressure pulse generated at the wellhead. The fracture size is then estimated from the pressure response.

Results

In this project, we have had access to complete production and injection data from several large waterflood projects in the South and Middle Belridge Diatomite and Lost Hills. These fields are located in the San Joaquin Valley, Calif. The field data were used to test the various features of Analyzer.

When we choose a particular field for analysis, Analyzer displays a map of the field showing all its producers and injectors. A user can click on any given well and examine its production or injection history. In addition, Analyzer allows comparisons of the performances of several producers or injectors through an interactive plot option. Analyzer can also quantify interactions between a sin-
gle injector and its neighboring producers. By cross correlating the injection and the production data, Analyzer identifies injector-producer linkage as water breakthrough at a producer caused by a given injector. In addition, Analyzer lets us examine the domain of influence of injectors and producers. The influence diagram helps to identify improper well placements, and inefficiencies, if any, of waterflood and oil production.

One of the important issues is to identify the influence of waterflood on oil production. Analyzer provides various options for examining the injection-production relationship. One of them is a three-dimensional animation of the field-wide water injection and oil production profiles. We illustrate this in Figure 1, which shows a snapshot in time of the field-wide water injectivity and oil productivity for a diatomite waterflood. The peaks represent injection highs, whereas the shading represents oil production. Regions of low oil production are marked in blue, while high production regions are marked in red. Note that maximum oil productivity is in regions of low-to-moderate water injection, while high injection is associated with low oil productivity. This suggests that the injection policy for the field is sub-optimal and needs to be improved.

Successful operation of water injectors requires knowledge of the dynamics of injection hydrofracture growth. Analyzer estimates this growth through an inversion of injection data, as shown in Figure 2.

Our research has shown that an injection well and its associated fractures can be modeled as a lossy transmission line network. The model parameters for the well are determined completely by the well geometry and the fluid properties. The fracture characteristics are determined either by matching the measured hydraulic impedance test response of a well with the simulated response or by model-based inversion of the transient response data. An independent measure of the dynamics of hydrofracture growth is, therefore, obtainable through periodic hydraulic impedance testing of injection hydrofractures.

**Significance of Findings**

We have developed Analyzer, an interactive software tool for complete surveillance of waterfloods. Our software allows one to identify deficiencies in water injection policies, imminent injector-producer linkage and water breakthrough at producers. Analyzer also provides an estimate of the hydrofracture size. In addition, we have shown that an independent measure of the dynamics of hydrofracture growth can be obtained through periodic hydraulic impedance testing at the injection wells. It is expected that the surveillance software, along with the hydraulic impedance testing methodology, will provide adequate inputs for a supervisory control system that strives to optimize the performance of waterfloods.

**Related Publications**


**Funding**

This work has been supported in part by the Assistant Secretary for Fossil Energy under the Advanced Computational Technology Initiative of the U.S. Department of Energy under Contract No. DE-AC03-76SF00098. Partial support has been provided by CalResources and Chevron Petroleum Technology Company, Inc., as gifts to U.C. Oil Consortium.
Control of Fluid Injection
Into a Low-Permeability Rock

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Research Objectives

About one-third of the world’s crude oil and a comparable fraction of oil reserves in the United States are locked in low-permeability rocks. Low-permeability fractured oil reservoirs, such as the Austin Chalk, the West Texas carbonates or the California diatomites hold tens of billions of barrels of oil. For example, in the diatomites, 10 years of primary recovery yield only 2.5-6% of estimated original oil in place. Primary production leads to reservoir compaction and well damage, and must be stopped.

The low-permeability diatomite reservoirs present a tremendous target for incremental recovery by water and steam injection. Steam can displace oil without contacting it directly, but it is very expensive, and its low density makes stable control of injection a very difficult task. Thus, we have focused our efforts on the analysis, modeling and control of water injection into low-permeability fractured rocks.

The purpose of this project is to design and implement a “smart” controller of water, steam or CO₂ injection into a low-permeability fractured rock. Analysis of the reasons of poor past performance of such controllers in critical situations led us to a new design. Our controller is based on optimal control principles; it “understands” the dynamics of fluid injection and remains stable even during catastrophic hydrofracture extension.

Approach

Current waterflood projects maintain a field-wide injection rate at a constant level. Thus, the growth of injection hydrofractures is inevitable. Very low permeability rocks require specific techniques for modeling the propagation of pressure away from the hydrofracture, as well as boundary conditions on the hydrofracture that differ from those used currently.

We propose to apply the Gordeev-Entov self-similar solution for characterization of pressure propagation. Since this solution is exact, it helps in comprehending the most important features of the process. Moreover, it can be used to build stable numerical schemes of high precision in spite of singularities at the tips of the fracture. The results of this modeling have been plugged into the controller design.

We have also developed the capability of inverting the pressure and rate into controller input. The controller requires three basic input parameters: the history of cumulative injection, the history of injection pressure and the history of hydrofracture growth. The first two parameters are normally collected and stored anyway, whereas the technique for the estimation of the last one is more complicated. We use inverse modeling to estimate the last parameter. Such an approach may require some experimental calibration, but after that the fracture size will be provided as the controller input at no additional cost.

Results

Pressure propagation model—
The Gordeev-Entov self-similar solution is an exact two-dimensional solution of the boundary-value problem for pressure propagation from a growing hydrofracture. Using Duhamel’s principle we have enhanced this solution to include time-dependent injection pressure.

As an example, we have modeled a portion of Section 33 in the South Belridge Diatomite Field. As we can observe from Figures 1 and 2, the pressure propagates almost perpendicularly to the fracture face. The pressure changes very little at a distance of 150 ft from the fracture face and remains almost unperturbed even after 10 years of injection (Figure 3).

Accounting for the layered structure of the rock, we have compared the pressure propagation rates in different layers (see Figure 4). One can observe that although the pressure propagation in some layers is very slow, in others there is a real danger of establishing links between the injector and the neighboring producers (compare layers I and K.)

Fracture size estimation—We have developed an inversion procedure, which allows us to obtain one of the controller input-parameters
without additional measurements and therefore at no extra cost. Comparison of the results of inversion and the results of other fracture estimation techniques will allow us to scale and tune up the model and the controller. For this purpose we have considered the dimensionless relative fracture size instead of absolute dimensions. In order to obtain the estimate, we solve a Volterra integral equation generated from a Carter-like mass-balance model. Figure 5 illustrates application of this procedure to real data. The top plot shows cumulative injection versus time. The second plot shows the injection pressure history versus time. The bottom plot shows the relative effective hydrofracture size estimate. Since the estimated parameter itself incorporates the fracture size along with the changes in the formation permeability, we call it "effective fracture area."

**Significance of Findings**

Our analysis of pressure propagation in low-permeability rocks has provided insights crucial to the design and implementation of a "smart" controller of water, steam or CO₂. Our inversion technique for estimating the effective hydrofracture size allows obtaining an additional controller input parameter at no extra cost. Practical implementation of the results described here—combined with our Waterflood Analyzer software—will lead first to the creation of a cradle-to-grave automated or semi-automated system of control and management of waterflood projects.

**Related Publications**


**Funding**

This work has been funded by the Assistant Secretary for Fossil Energy, Office of Gas and Petroleum Technology, of the U.S. Department of Energy under Contract No. DE-AC03-76FS00098.
Research Objectives

The objective of this project is to develop a methodology to characterize a reservoir through the use of surface expression data such as displacements and surface tilts induced by pumping or injection. An inversion algorithm that jointly inverts such surface data and the pressure data is being developed. The results of the inversion will be the map of the pressure changes in the reservoir. This can be a cost-effective remote-sensing technology for obtaining information regarding the reservoir flow geometry, which is a critical piece of information for successful reservoir development/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 the reservoir is horizontal and homogeneous, the induced displacements will be distributed concentrically around the production/injection borehole. In the case of the surface tilts, tilt vectors will be radially convergent to or divergent from the borehole. If a preferential flow path such as a fault zone exists in the reservoir, which is often the case in geothermal reservoirs, the flow will mostly occur along the fault. The distribution of the volume change and subsequent surface displacements will be skewed. An inversion algorithm can then 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 at a particular location, the more fluid has likely moved into or out of the location. The distribution of volume change is tightly coupled with that of the reservoir flow properties: permeability and compressibility. A joint inversion of surface displacements and reservoir pressure should satisfy both constraints.

Surface expressions of such reservoir dynamics can be monitored by using high precision tiltmeters, GPS (global positioning system), laser level gages and even SAR (synthetic aperture radar), depending on the magnitude of the displacements. A large number of measurement points are necessary to reliably estimate the distribution of reservoir volume changes to infer the flow geometry. Monitoring of the surface expressions at or near the surface, however, costs very little compared to drilling a corresponding set of boreholes and installing pressure sensors in them. This remote-sensing approach also provides independent data of the reservoir dynamics that can be used to confirm/refute the reservoir model based on the borehole data alone.

A series of fluid injections were conducted in a geothermal reservoir at Hijiori, Japan, as part of the JAPEX-LBNL collaborative research project. Ten high-precision tiltmeters (Pinnacle Technologies, Inc.) were installed in shallow boreholes near and around injection well HDR-1, located at the southern edge of the Hijiori caldera. The granodiorite bedrock was encountered at a depth of 1,450 m in HDR-1. The injection interval was from a depth of 2,151 m (bottom of casing) to 2,205 m (bottom of the well). A series of four injections were conducted in November 1998, during which the surface tilts were monitored.

Results

The inversion results of the four injections indicate volume change to the east or to the southeast. This agrees with independent acoustic emission and pump test results. We discuss the results from the stage-4 injection conducted on Nov. 20, 1998, in more detail. The duration was approximately five hours. In total, approximately 110,000 liters of water were injected during the six hours of stages 3 and
There was a clear tilt signal coinciding with the initiation of the injection. The complete set of tilt vectors, corresponding to the first hour of injection, is shown in Figure 1a. There is a fair bit of scatter in the tilt directions and magnitudes. However, the two southeasternmost tiltmeters display consistent and strong tilting to the north. The peak signal, associated with tiltmeter 1, exceeds 0.1 micro-radians and lies well above the instrument noise. The inverted volume increase in the granodiorite, based on the one-layer model with a 20 x 20 grid, is offset to the east by more than 0.7 km from injection well HDR-1. The pattern of volume increase is elongated in an east-west direction. The location of the peak volume change coincides with the southern edge of the volume change associated with the stage-3 injection event. Also, the location of the volume change during stage-4 injection appears to be an eastward extension of the volume change in stage 2. The east-west orientation agrees with acoustic emission information, which suggests east-west flow from HDR-1. In addition, previous analysis of 1995 circulation tests in HDR-1 and surrounding wells indicated an extension of fractures and water loss to the east.

Because the stage-4 injection involved a much larger volume than the other injections and the data appeared to have a higher signal-to-noise ratio, we constructed a more detailed model of subsurface volume change. In particular, we attempted to fit a two-layer model with a deeper layer (1.0-2.0 km) and a shallower layer (0.5-1.0 km). Each layer consisted of a 15 x 15 grid of cells, in which each cell could undergo a distinct volume change. We conducted an inversion of the stage-4 data (Figure 1a) using this model parameterization. The result is shown in Figure 1b and 1c. In the deeper layer (1.0-2.0 km) we still observe the largest volume change to the southeast of HDR-1 as in our one-layer inversion. However, there is a secondary area of volume change to the west of HDR-1, elongated in the north-south direction. In the uppermost layer (0.5-1.0 km) the deep southeast body extends upward in depth. In addition, there is an arm of volume change extending from the western body to the east. Interestingly, this extension in part coincides with a river, which crosses the caldera in a roughly east-west direction. The river is thought to follow a zone of weakness, hypothesized to be a fault, within the caldera. It is an intriguing possibility that some fluid has migrated along this zone of weakness. However, more (and higher quality) data is required to better constrain the volume change. Note that the two-layer model has predicted surface tilt which is very close to the observed data (Figure 1a) both in direction and magnitude. We conclude that some degree of shallow (0.5-1.0 km) volume change is needed to match the high displacement gradients observed in the data.

**Significance of Findings**

High-precision tiltmeters can be used to monitor the surface expression of reservoir dynamics. An inversion algorithm can be used to infer the reservoir flow geometry. The technique can be used to better manage/explore operating reservoirs. It can also be used to track the injected mass of CO₂ during the planned deep geologic sequestration effort.

**Related Publications**


**Funding**

This work has been supported by JAPEX Geosciences Institute, Japan, through Contract No. BG98-071(00).
Research Objectives

Injection of spent production fluids back into geothermal reservoirs from which they are produced is widely recognized as the single-most important factor in maintaining reservoir pressure and extending the productive lives of geothermal fields. Injectate is always colder than reservoir fluids, so eventually returning injectate will cool individual production wells and entire reservoirs. To predict the onset of cooling, it is necessary to develop reliable techniques to determine the volume of injectate co-produced with the reservoir fluid and the rate at which the injectate return increases.

The injected fluids are the brines residual to steam production. Therefore, the injectate is enriched in chloride and heavy isotopes of water (18O and D) and depleted in low-solubility noncondensable gases relative to the production fluids. These natural tracers have been utilized at several geothermal fields to monitor injectate returns. However, their reliability as a quantitative measure of injectate return relies on several assumptions, most notably that there is a single homogenized geothermal fluid into which the injectate is mixed. Since most geothermal systems are comprised of fluids from several sources, this assumption is rarely realized. By comparing different natural tracers, the objective of this study was to evaluate their quantitative reliability.

Approach

Injection into the Dixie Valley, Nevada, geothermal reservoir began in September 1988, about three months after the field commenced production. Since the onset of production the chemistry of the production and injectate fluids has been thoroughly documented, with analyses of quarterly brine samples (Benoit, 1992) and intermittent water isotope analyses. In the past two years, analyses of low solubility noble gases have been obtained to give a complete evaluation of the available natural chemical tracers in a geothermal field that has been well documented.

Almost immediately after injection commenced and continuing over the last 10 years the chloride concentration of the production fluids has increased, suggesting significant return of injectate. However, at Dixie Valley every part of the reservoir that was chemically sampled prior to the onset of injection had a different chloride content. Pre-flash chloride contents ranged from 250 to 400 ppm and showed an inverse chloride/enthalpy relationship: cooler waters have progressively higher chloride contents. Therefore, increasing chloride concentrations may not reflect injectate returns. Any inflow of cooler indigenous water would also increase chloride concentrations.

During the flash process at Dixie Valley, the light water isotopes (16O and H) are preferentially partitioned into the steam fraction, leaving a residual brine enriched in the heavy isotopes. The dominant trend in the isotopic history of the produced fluid between 1986 and 1998 is a progressive enrichment of about 2‰ in \( \delta^{18}O \) and 8‰ in \( \delta^D \) following the start of injection. This is also consistent with co-production of injectate and supports the interpretation of the chloride concentration trends.

The noble gases are particularly well suited for tracing injectate because their solubilities are low, mass-dependent and are known as a function of temperature up to the critical point of water. At Dixie Valley, the concentration of noble gases in the injectate will be about 1-10% of that in the pre-flashed production fluid and the 1997-98 production fluids are significantly depleted in noble gases; consistent with the addition of gas-poor injectate.

The volume fractions of co-produced injectate fluid (\( V_{inj} / V_{total} \)) calculated from all three independent tracers using the 1998 data set, are in very good agreement, despite the assumptions and potential uncertainties. This implies that chloride concentrations at Dixie Valley can be used with confidence to assess the volume fraction of injectate fluid in the production streams. This is very important because chloride data exists for the entire 1988-98 production/injection period.

![Figure 1. The volume fraction of injectate fluid calculated from the \( ^{36}Ar \) abundances, assuming that the well data represent mixtures of \( 20^\circ \)C air-saturated water and spent brine.](image-url)
Natural Geochemical Tracers for Injectate Fluids at Dixie Valley

(Figure 1), which can be used to model the change in the $V_{\text{inj}}/V_{\text{total}}$ ratios (Figure 2) with continued production and injection.

The Section 33 reservoir (dash-dot line in Figure 2) has behaved in a very different manner than the Section 7 reservoir (dotted line). The very rapid rise in the volume of injectate fluid co-produced with Section 33 reservoir fluids suggests a very high degree of connectivity between the injectors and the Section 33 producing wells. However, in late 1992, the volume of co-produced injectate began to decline. This may reflect a change in the hydraulic connectivity induced by water table drawdown isolating the reservoir from the pathway supplying the injectate. Alternatively, the early rise in chloride concentration in Section 33 resulted from the invasion of any of the other known higher chloride indigenous fluids.

The volume of co-produced injectate in Section 7 wells has increased linearly with time at a rate of about 5-7% per year. It is also noteworthy that the range in chloride concentrations between Section 7 wells has diminished over the same period of time, resulting in a rather homogeneous fluid which is about 61% injectate. The true volume fraction of injectate may be as high as 100%, because after 1994 the chloride contents in the Section 7 producers have exceeded the initial injectate concentrations (Figure 1).

Assuming that the injectate fluid gradually replaced the original fluid by pushing the latter out of the fractures and into the production wells, an upper limit on the fracture volume for the system can be estimated from the total volume of fluid injected at Dixie Valley. Once the production fluids reached a chloride content equal to the original injectate concentration, the total volume injected would approximate the local fracture volume. This required about six years and took $206 \times 10^9$ lbs of injectate, corresponding to a fracture volume of about 0.12 km$^3$. If it is further assumed that the porosity provided by the fracture network is about 1%, this implies a reservoir volume of about 12 km$^3$.

**Significance of Findings**

Perhaps the most challenging aspect of geothermal reservoir engineering is to be able to predict thermal breakthrough—the onset of cooling in production wells resulting from cool fluids returning from injection wells. Addressing this challenge requires, among other things, the ability to quantitatively assess and model injectate returns. At Dixie Valley, good agreement between the calculated volume fraction of injectate in the production stream ($V_{\text{inj}}/V_{\text{total}}$), determined using three independent natural tracers (Cl, noble gases and water isotopes), suggests that chloride changes can be used as a viable proxy for monitoring injectate returns. Continued monitoring of the production and injectate fluid chloride, water isotopes, and noble gas concentrations could lead to a better understanding of the relative flux of the indigenous geothermal fluid into the reservoir and provide additional constraints for future modeling efforts.

**Related Publications**

Kennedy, B.M., C. Janik, D. Benoit and D.L. Shuster, Natural geochemical tracers for injectate fluids at Dixie Valley, in Proceedings of the Twenty-Fourth Workshop on Geothermal Reservoir Engineering, Stanford University, Stanford, California, in press.


**Funding**

This work has been supported by the Assistant Secretary for Energy Efficiency and Renewable Energy, Office of Geothermal Technologies, of the U.S. Department of Energy under Contract No. DE-AC03-76SF00098.
Research Objectives

Geothermal reservoir engineering requires accurate numerical solution of advective-diffusive transport equations. The standard weighting scheme used in numerical simulators to approximate saturation or relative permeability at gridblock interfaces is upstream weighting, a scheme that is very stable but also known to produce numerical dispersion. Numerical dispersion degrades the accuracy of strongly advective flow problems by artificially smoothing sharp fronts. Artificial smoothing in reservoir engineering can lead to errors in prediction of thermal breakthrough and tracer arrival times, as well as nonphysical dilution. Phase-front propagation is typically self-sharpening due to the effects of relative permeability and is therefore less prone to numerical dispersion. However, in phase-front propagation problems with boiling, phase saturation is strongly coupled to temperature. In such cases, numerical dispersion of the thermal energy equation can lead to inaccurate modeling of phase-front propagation. Numerical dispersion can be diminished by grid refinement, but this can greatly increase execution times and computer memory requirements.

Another approach for reducing numerical dispersion is to use higher-order differencing schemes. The objective of this research is to develop and test methods of efficiently decreasing numerical dispersion for improved geothermal reservoir simulation. We have implemented total variation diminishing (TVD) higher-order differencing schemes in TOUGH2. Here we demonstrate application of the Leonard TVD (LTVD) scheme to a geothermal flow problem involving phase-front propagation and boiling.

Approach

We compare upstream weighting to the LTVD scheme for a phase-front propagation problem where boiling progressively diminishes the liquid saturation ahead of the reinfected fluid. In the problem, cold water ($T = 300\, ^\circ C$) is injected into a 200-m-long one-dimensional single-continuum flow domain. The system is initially nearly single-phase liquid at the saturated vapor pressure ($P_0 = 85.93\, \text{bar}$) at $T_0 = 300\, ^\circ C$. A schematic diagram of the system and initial and boundary conditions are shown in the upper part of Figure 1. The flow begins by injection of cold water on the left at a rate of 0.4 kg/s and by production of mass at the same rate from the other side. The production at the right-hand side lowers the pressure and induces boiling.

Results

Results for the LTVD differencing scheme with 100 gridblocks are shown in the lower part of Figure 1, through profiles of liquid saturation (dashed lines) and temperature (solid lines). Results for upstream weighting were very similar, except the phase front was approximately 10 m farther advanced to the right-hand side relative to the LTVD result. The advancement of the upstream-weighted phase front relative to the LTVD phase front occurs because upstream weighting produces greater smearing of the temperature front, so that saturation temperature at prevailing pressures is reached at a somewhat larger distance from the injection point. The phase transition to two-phase conditions therefore also occurs farther from the injection point.

The differences between the upstream and LTVD schemes decrease with...
increased spatial resolution. We show in Figure 2 a summary of the results of phase-front location at a time of six months as a function of the number of grid blocks. Note in Figure 2 that the two schemes are converging slowly but that the LTVD scheme is closer to the grid-converged result at much coarser resolution. In this problem, the improved approximations in the thermal energy equation using LTVD give rise to the more accurate phase-front locations.

**Significance of Findings**

The LTVD scheme has proven to be robust and efficient for complex multiphase and multicomponent nonisothermal flow problems relevant to geothermal reservoir engineering. In geothermal injection and production problems where boiling occurs, the location of the phase front may be very sensitive to the choice of weighting scheme. Our simulations show that the LTVD scheme is more accurate for the boiling front problem at a given discretization than upstream weighting, but that temperature and saturation front propagation are sensitive to grid resolution for both schemes.

**Related Publication**

Oldenburg, C.M., and K. Pruess, Simulation of propagating fronts in geothermal reservoirs with the implicit Leonard total variation diminishing scheme, Geothermics, in press.

**Funding**

This work has been supported by the Assistant Secretary for Energy Efficiency and Renewable Energy, Geothermal Division, of the U.S. Department of Energy, under Contract No. DE-AC03-76SF00098.
Fluctuations in Elastic Waves Due to Random Scattering From Inclusions

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Research Objectives

The problem of elastic wave propagation through heterogeneous media is encountered in numerous disciplines. It is particularly important in the discipline of seismology because the earth is heterogeneous on a broad range of scales, so a variety of approaches to this problem have been developed. For a medium that is heterogeneous in only one dimension the problem is essentially solved because exact solutions exist, although estimating and describing the heterogeneity in realistic applications can introduce approximations. For media heterogeneous in 2- or 3-D, the problem is more profound, as it is necessary to combine approximate solutions of the wave equations with approximate descriptions of the media; understanding when a set of approximations is valid is not a simple matter. Because of the complexity of heterogeneity within the earth, it is typically modeled as a random medium in which the effects of the heterogeneity upon elastic waves are treated in a statistical sense. Various approaches to the problem of wave propagation in heterogeneous media have been successful in certain applications, but are accompanied by limitations that can raise questions about the validity and generality of the results. Examples include the lack of conversions between modes of propagation, the failure to conserve energy and the inability to handle strong contrasts in material properties. Our objective is to present a method of handling wave propagation in 3-D heterogeneous media that avoids some of these limitations.

Approach

We followed the basic approach to treat the wave propagation process as a series of forward scattering problems. The medium is described as a random distribution of scatterers, where size, material properties and density can vary. For the case where the scatterers are spherical and homogeneous, exact solutions for the single scattering process are used; multiple scattering effects are only partly included. The use of exact scattering solutions allows a complete treatment of mode conversions between P and S waves and arbitrary strong contrasts in material properties. They also provide a starting point for deriving low- and high-frequency asymptotic solutions that can be compared with other approximate solutions. Analytical results are compared with numerical simulations for elastic waves propagating through a medium containing random spherical scatterers.

Results

To derive basic analytical results we consider a thin slab extending to infinity perpendicular to the direction of incident wave propagation, where both the incidence of compressional and shear waves are treated. Assuming randomness in spatial distribution of scatterers and neglecting their interaction it is possible to obtain formulas for the average values of attenuation and a phase shift for the coherent part of the field. A differential equation for propagation through a layer of arbitrary thickness is derived. The equation gives the same solution to the problem as a stationary phase integral evaluation method. At low frequencies it gives a simple formula for elastic moduli of a composite medium with inclusions of an arbitrary contrast. In similar manner, the effect of fluctuation accumulation is treated, where a differential equation for associated fluctuations is derived. Solutions of this equation allow us to obtain formulas to estimate standard deviations of point measurements of attenuation and phase. For both parameters, the fluctuation level is the same and equal to half the fluctuation of the square amplitude of the field.

The analytical results of this study provide a method of estimating the effects of scattering upon a plane wave propagating through a layer of randomly distributed spherical inclusions. Formulas have been obtained for both the average field and the statistical fluctuations about this average. The general results can be used for inclusions of arbitrary size and contrast and for all frequencies; approximations for small inclusions or low contrast inclusions have also been included. These analytical results have been validated by comparing them with effective media estimates at low frequencies and with numerical simulations over the entire frequency range. In both cases the agreement is satisfactory.

Results show that the relatively simple expressions do an acceptable job over a broad frequency range of describing phase and attenuation effects upon a wave propagating through a region containing scatterers. The fluctuations calculated with derived equations also serve as adequate bounds on the statistical uncertainty of the mean field. Because of the random fluctuations, any attempt to reliably estimate the characteristics of the scattering on the basis of a single seismogram may be a difficult task. Only the phase shift at low frequencies shows a reasonable approximation to the mean field. The non-physical negative values of attenuation are common in the results for a single seismogram. This means that in most cases some sort of spatial averaging of the observational data will be necessary before stable values of the mean phase and attenuation can be estimated.

Assuming that an averaging process has been applied to reduce the fluctuations to a acceptable fraction of the mean value, it is of interest to consider how data can be interpreted in terms of material properties of the scattering medium. Measurements at high frequencies of velocity are only dependent upon the background medium and thus can be used to estimate its elastic parameters. Measurements of velocity at low frequencies can be combined to provide constraints on the properties of the inclusions. The first peak in the phase curve is a well defined feature and constraints on the material properties can be obtained by fitting the analytical results to the data.

The effect of scattering on propagating plane elastic waves
Fluctuations in Elastic Waves Due to Random Scattering From Inclusions

was simulated by using the exact scattering solution for a single elastic sphere (Korneev and Johnson, 1996). A thin slab of a scattering medium was simulated by distributing a large number of spherical inclusions having the same radius and with random spacing. Plane elastic P and S wave pulses containing a broad range of frequencies were propagated in the positive z direction. The calculated transmitted seismograms recorded in linear array of receivers were processed to compute the observed velocity and attenuation. In each case the calculations were performed on a single seismogram and for the average of all 20 seismograms (Figure 1). Also shown are the analytical estimates for the attenuation and the analytical estimates for the fluctuations. The analytical estimates are in reasonable agreement with the numerical results for both the mean and variance. For a single seismogram the statistical uncertainty is so large that only general trends can be identified, but in the case of the averaged seismograms a more quantitative evaluation can be performed.

The agreement is slightly better for the attenuation than for the phase, which contains the additional complication of phase unwrapping. Also, due to the statistical fluctuations, it may be impractical to reliably estimate attenuation and phase from a single seismogram. Furthermore, the results exhibit relatively simple behavior at low frequencies. In this range the numerical and analytical results are in good agreement (even for a single seismogram) and the phase shows a linear dependence upon frequency. Regarding the behavior at high frequencies, although there are both long and short wavelength oscillations associated with the dimensions and properties of the scatterers, the trend in the attenuation is a constant non-zero value and the trend in the phase is a constant value of about zero. Due to the competing effects of conversion of energy from the coherent field and the resultant decay of the coherent field, the amplitude of the fluctuations in the transmitted field has a maximum at a particular propagation distance (Figure 2), and an expression for the maximum is given. It appears that the distance to the maximum decreases as the frequency increases, and the distance to the maximum is greater for S waves than for P waves at low frequencies; the situation is reversed at high frequencies. The phase shift of the coherent transmitted wave can be converted to an effective velocity by interpreting the phase as a time shift. At high frequencies, the velocities approach those of the background.

**Significance of Findings**

Results provide useful estimates for fluctuations of the main measured wave parameters—effective velocity and attenuation. These estimates can be used for receiving array design in order to achieve a desired accuracy and also as inversion data for evaluating a degree of heterogeneity of real elastic media.

**Related Publications**


**FUNDING**

This work has been supported by the Assistant Secretary for Fossil Energy, Office of Oil, Gas and Shale Technologies, Federal Energy Technology Center of the U.S. Department of Energy under Contract No. DE-AC03-76SF00098, and by the Defense Special Weapons Agency under Grant No. DSWA-01-97-1-0026.
Research Objectives

Porosity, absolute and relative permeability and capillary pressure relationships are very important in modeling and calculation of flow in porous media. Considerable effort has been devoted in the petroleum industry to developing correlations between these parameters. The considerable scatter and uncertainty in these correlations is, in large part, attributed to a lack of understanding of the relationship between the microscopic pore space geometry and macroscopic flow properties.

This research project has two objectives. The first is to investigate the relationship between the microscopic pore geometry and the macroscopic flow properties and to advance understanding of the physics of fluid flow in porous media. The second is motivated by the expense and time required to obtain commercial relative permeability measurements needed to support development of petroleum reservoirs. A network model is therefore developed to predict absolute and relative permeability of reservoir rock from measurements of microscopic pore structure. These measurements constitute 2- or 3-D images of the pore space, in combination with gravimetric porosity data and mercury porosimetry data.

Approach

The network model is based on a regular cubic lattice. The nodes of the lattice represent pores while the connections (called branches) represent pore throats. Pores are assumed to be spherical in shape. Different pore throat cross-sectional shapes are incorporated. These are circular, triangular with straight sides, and triangular with concave sides defined by arc segments. The pore throat cross-section is of constant size over the length of the connection between nodes. The ratio of throat size to pore size is a variable.

The pore size at each node in the network was assigned by a random number generator assuming either a normal, log-normal or exponential distribution function.

The coordination number of a completely connected cubic lattice is six. The option of having a lower coordination number is incorporated in the model.

The lattice is further defined by grid spacing. The grid spacing is determined once the porosity and average pore size are specified.

Single-phase fluid flow in a network is analogous to current in an electrical circuit. Therefore, Kirchoff's current law is applied to the mass balance for each node in the network and Kirchoff's second law is applied to the pressure balance in each loop. Using a graph theory representation of network properties (Yang et al., 1994), the relationship between pressure drop and flow rate in each element is found by Hardy cross-iteration. Permeability of the network is then derived using Darcy's law.

Simulation of drainage is performed using the breadth first search graph theory algorithm to determine the interconnectivity among the pores that are filled with the same phase. The priority queue search algorithm is implemented to simulate the nonwetting invasion process. In the process of invasion, at a certain capillary pressure, the distribution of wetting phase and nonwetting phase over the network is determined and the saturation for nonwetting and wetting phase is obtained. Having determined the distribution of phases, subnetworks for each phase are defined.

Relative permeability can be calculated for each phase at each capillary pressure increment in the nonwetting phase invasion process. The effective permeability for each phase is calculated using the same procedure as used in the single-phase problem. Relative permeability is finally obtained by taking the ratio of effective to absolute permeability. The absolute permeability is the permeability of the entire network to one phase.

Results

A number of simulations were performed to evaluate the sensitivity of predicted behavior to the various input parameters. These results provide insight into the sensitivity of absolute and relative permeability to various geometric properties of the pore space. All calculations were performed on a 16x16x16 grid.

The significant effects of the variation in pore and throat sizes are demonstrated by simulations comparing networks with normally and exponentially distributed pore sizes. Figure 1 compares absolute permeability as a function of mean pore size for two distribution types.
pore diameter while holding porosity constant at 20%. Circular cross-section throats are assumed. It is seen that permeability increases much more rapidly if the pores have a normal distribution. The large numbers of small pores associated with an exponential distribution produce flow restrictions which keep the permeability low even though the average size is increasing.

Relative permeability curves corresponding to a normal, log normal and exponential distribution, all with mean pore diameter of 14.4 m, were generated. Curves for normal or log-normal distributions are nearly identical. The greatest differences are in the nonwetting phase relative-permeability curves with the exponential distribution yielding a curve of different shape. The larger numbers of small pores in the exponential distribution limit the number of connections available to the nonwetting phase at low capillary pressures.

Finally, the effect of throat cross-sectional shape was investigated. In this case, the absolute permeability is not very sensitive to the cross-section shape, but the relative permeability is. Figure 2 compares relative permeability curves for circular and curved triangular throat cross-sections. A normal distribution of pore sizes was assumed while keeping other parameters constant for the simulations. At a given water saturation the nonwetting phase relative permeability for a network of curved triangles is greater than for circular throats. The opposite effect is seen in the wetting phase relative permeability. For the curved triangular cross-section, both phases can be present at the same time in the throats. The wetting phase captured in the corners contributes negligibly to the effective permeability but affects the water saturation.

**Significance of Results**

A 3-D pore scale network model has provided insight into the relationship between pore scale microstructure and macroscale flow properties. Simulations show that absolute permeability is strongly related to bulk porosity, the mean pore size, the ratio of throat to pore size and coordination number. Relative permeability is insensitive to these properties. Relative permeability was found to be sensitive to variability in pore sizes reflected in the type of distribution function and standard deviation. Relative permeability was also strongly affected by the cross-section shape assumed for throats.

**Related Publications**


**Funding**

This work has been supported by the Office of Science, Laboratory Technology Research Partnership Program and Office of Basic Energy Sciences, and Assistant Secretary for Fossil Energy, Office of Natural Gas and Petroleum Technologies of the U.S. Department of Energy under Contract No. DE-AC03-76SF00098.
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 involved in 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 (wet lands 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/Other Government Agencies).

DEMONSTRATIONS AND DEPLOYMENT

ERTP supports DOE's Office of Environmental Management in both the areas of Environmental Restoration (EM 40) and the Office of Science and Technology (EM 50). Earth Sciences Division (ESD) scientists directly supervise characterization, remediation and monitoring, and provide regulatory and permitting support to LBNL's Environment, Health and Safety Division for all environmental problems on site. During 1998 the program demonstrated and deployed technologies for trench capture of chlorinated solvents in groundwater, soil vapor extraction of volatile organic contaminants (VOCs) and cryogenic drilling to aid core recovery in fractured rock and coarse overburden.

ERTP research on ferrofluids has shown that they have potential to effectively guide reactants and barrier liquids to contaminated target zones in the subsurface using electromagnetic forces. They also allow the use of geophysical methods to trace the movement and position of liquids injected into the subsurface. This research, combined with earlier work on viscous barriers for containment (patent pending), provides a great opportunity for containing, controlling and predicting solvent, metal and radionuclide contamination at waste sites—DOE's greatest environmental cleanup problem.

In partnership with the Savannah River Technology Center and Florida State University, ERTP is assisting the Institute for Ecology of Industrial Areas in Poland in conducting a full-scale demonstration of biopile (aeration) technologies for clean-up of a petroleum refinery waste lagoon. After nearly a year of operation the demonstration has shown that both passive and active aeration strategies can meet clean-up 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 EM 50 with technical expertise via the Strategic Laboratory Council, the Oakland Site Technology Coordination Group, the multi-agency DNAPL Technology Advisory Group, the SUBCON Vadose Zone Book 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 LBNL, such as the Advanced Light Source, where researchers look directly at the interaction between contaminants, water and minerals at the microscale. This year ERTP also had a new project funded in the Natural and Accelerated Bioremediation Research (NABIR) program. This project 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 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 waste site contaminants. 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 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 San Luis Drain. Microbial studies this year have shown that selenium in-transit losses occur and that the fate of this selenium is bed sediments. 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 LBNL 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 other agency. Several contracts this year were executed for consultation regarding bioremediation and characterization. The Army Corps of Engineers received an award for use of innovative technology from the state of Nebraska for its use of a patented DOE technology to clean up a naval ammunition depot.

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 has continued to be the NABIR program office for the Office of Science. The NABIR program office maintains the 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. The NABIR program office organized the first NABIR annual investigators' meeting in Reston, Va., with more than 120 participants, and produced the NABIR Bioremediation Primer, available in hardcopy or electronically via the NABIR home page. The program office also assisted DOE Headquarters in producing a number of guidance documents for prospective field research centers. This effort enabled DOE-HQ to issue its request for applications for the NABIR field research center in January 1999.

Partners and Funding

ERTP receives support from DOE programs in the Office of Science and the Office of Environmental Management. EM programs include the Environmental Management Science Program, the Subsurface Contaminant Focus Area and the Characterization, Monitoring and Sensor Technology Crosscutting Program. The Office of Science funds the NABIR Program Office at LBNL 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, University of California at Berkeley and U.S. Bureau of Land Management. Other Work for Others in 1998 included: Concurrent Technologies, American Technologies, Radian International, Earhttech, Woodward & Clyde and IT Corporation. Partners include UC Berkeley, Stanford University, Westinghouse Savannah River Company, Idaho National Engineering and Environmental Laboratory, Lawrence Livermore National Laboratory, Pacific Northwest National Laboratory, University of Nevada and University of Illinois.
Experimental Studies Of Ferrofluids for Subsurface Applications

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Research Objectives

Ferrofluids are stable colloidal suspensions of magnetic particles which behave as homogeneous pseudo-single-phase fluids. Ferrofluids can flow through porous media such as natural sediments or fractured rock due to gravitational, pressure gradient, capillary and magnetic forces. The objective of this research is to investigate the potential for the use of ferrofluids in novel subsurface environmental engineering and laboratory applications in the areas of (1) controlling the flow of liquid in the subsurface and (2) detecting ferrofluids using geophysical methods.

Approach

We carried out two broad laboratory-scale investigations using commercially available aqueous ferrofluids and permanent magnets in sand-filled containers and Hele-Shaw cells in a variety of configurations.

The first investigation was designed to demonstrate and quantify the movement of ferrofluid in porous media. This included: (1) measurement of the generation of magnetic forces on a ferrofluid, (2) mobilization of a ferrofluid in homogeneous and heterogeneous porous media in response to an external magnetic field created by a permanent magnet, (3) the static hold that permanent magnets can exert on ferrofluids, and (4) the filtration effects of the porous media on the ferrofluid properties.

The second investigation focused on the ability to detect ferrofluid in the subsurface using traditional geophysical methods. This was evaluated by measuring the anomalies produced by model ferrofluid shapes using a three-axis fluxgate magnetometer. The magnitude of the anomalies was compared to model predictions. These laboratory-scale anomalies can be upcaled to predict detection depths for field-scale anomalies.

Results

In general, the flow experiments demonstrated that magnetic forces cause ferrofluid to flow over distances of about 0.25 m on timescales of hours to days.
tion depths of a 3 m³ spherical anomaly containing a 10% ferrofluid-water mixture is on the order of 5 to 10 m.

Significance of Findings

From our experiments on ferrofluid flow, we find the following: (1) permanent magnets create a predictable pressure gradient in a magnetic fluid that leads to fluid flow, (2) ferrofluid can be held in porous media in predictable final configurations which are controlled solely by the magnetic field and are unaffected by the flow pathway, initial injection shape or permeability of the porous medium, and (3) ferrofluid exhibits only limited filtration effects in the advancing front during flow through porous media.

The potential of controlling fluid motion in porous media without direct physical contact has potentially significant applications. These include controlled emplacement of subsurface barrier liquids or treatment chemicals, as well as emplacement of geophysically imageable liquids into particular zones for subsequent imaging. While the objective is the development of subsurface environmental remediation solutions, our results to date on the movement of ferrofluid have been limited to laboratory length scales up to approximately 0.25 m. As such, these results are particularly relevant to laboratory work where ferrofluids may find immediate application in any situation where it is desirable to control the motion or final configuration of fluid in an experimental flow apparatus.

From our experiments on ferrofluid detection, we find that the magnetite in the ferrofluid provides a signature sufficiently strong for conventional magnetic detection methods. The magnetic anomaly created by ferrofluids could be used as a novel subsurface tracer technique. In field-based application of ferrofluids as tracers, magnetometer grids could be established around the injection site and changes in the magnetic field during injection of the ferrofluid-laden injection liquid could be monitored. This would provide a sensitive and non-invasive method of detecting the injection plume, or determination of high-permeability pathways. Furthermore, since the ferrofluid consists of magnetite, water and a small amount of surfactant, the environmental impacts of its use would be minimal.

Possible applications of this technique include use as a subsurface barrier verification tool by either magnetizing the barrier and using the magnetic detectors to locate the extent of the barrier, or using magnetized liquid to detect leaks or fractures in existing non-magnetic barriers.

Limitations of ferrofluid-based tracer techniques include the effect of ambient magnetic noise, which can obscure small anomaly signals and significantly increase detection limits. This may become significant if large injection pumps are utilized in field sites. Other interferences could come from natural magnetic anomalies in the subsurface, which, however, can be minimized by background surveys of the area prior to injection.

Related Publications


Funding

This work has been supported by the Laboratory Directed Research and Development Program of Lawrence Berkeley National Laboratory under U.S. Department of Energy Contract No. DE-AC03-76SF00098.
Research Objectives

Several Department of Energy (DOE) sites contain volatile organic contaminants (VOCS) within deep fractured rock vadose zones, originating from improper handling and disposal of non-aqueous phase organic liquids (NAPLS). The nature of fast, channelized flow of liquids through rock fractures, ponding at lithological discontinuities and longer-term diffusion into less accessible matrix rock presents tremendous characterization and remediation challenges. Biological degradation of VOCS may be a significant factor in containing the spread of these plumes. Field evidence for biodegradation of chlorinated solvents in fractured rock vadose zone settings exists (Conrad et al., 1997), but major questions remain as to how to characterize the extent of naturally-occurring biological activity and how to stimulate and monitor it for site remediation. During our three-year investigation of the fate of NAPLS in fractured rock vadose zones, we have developed a suite of bench-scale experimental techniques to characterize multi-phase flow (water, NAPL and air) and biotransformation of contaminants in this environment, with a particular emphasis on the coupling of fluid flow dynamics and biotransformation processes (Geller et al., 1998). In this summary, we present the results of a "geocosm" experiment to assess biological activity on rock fractures as a function of environmental factors.

Approach

Geocosms are core-scale flow cells, designed to incorporate some aspects of natural conditions, using site samples, indigenous microorganisms (mixed culture) and maintaining near 100% relative humidity in the vapor phase. Biological activity is monitored by tracking changes in the abundance and stable carbon isotope ratios ($\delta^{13}C$) of carbon dioxide ($CO_2$) in the vapor phase. The value of $\delta^{13}C$ of $CO_2$ produced by biological activity reflects the isotope ratio of the carbon source utilized by the bacteria, allowing a distinction between biological and other $CO_2$ sources.

Vesicular basalt rock samples and indigenous microorganisms obtained from a drillcore from DOE's Idaho National Engineering and Environmental Laboratory (INEEL) were used for these experiments. The drillcore was from a site where VOCS contamination threatens the Snake River Aquifer. The basalt sample was broken into 1-to-2-cm-sized chips, sterilized and packed into a glass column. The experimental schematic is shown in Figure 1. Water-saturated $CO_2$-free air with 100 ppm toluene was delivered to the column at a rate of approximately one pore volume/hour. The abundance and $\delta^{13}C$ values of $CO_2$ in 1-ml gas samples extracted with a syringe from the septum port at the top of the column were analyzed using an automated pre-concentration system interfaced with a Micromass Isoprime isotope ratio mass spectrometer (Isoprime). The $\delta^{13}C$ values of the toluene in separate 1-ml gas samples were analyzed using a gas chromatography-combustion system interfaced to the Isoprime.

After monitoring the influent and effluent vapor phase for changes under abiotic conditions, the rock chips were inoculated with bacteria grown in a liquid medium made from basalt rock extract. Subsequent experiments monitored biological activity due to the basalt rock extract and toluene for both flow-through and recycle configurations.

The use of basalt chips ensures adequate surface area for bacteria coverage and access to flowing fluid to produce measurable changes of fluid phase constituents. This is a preliminary step to the use of naturally-fractured cores, where the accessible surface area will be much lower. The column experiments complement ongoing, micron-scale monitoring of biotransformations with IR spectroscopy on single basalt chips incubated with organic vapor in a closed system (Holman et al., 1998).

Results

Table 1 presents the $\delta^{13}C$ values for the various compounds of interest. Under abiotic conditions, the shift in $\delta^{13}C$ and in $CO_2$ concentrations between the column influent and effluent were insignificant, with $\delta^{13}C$ approximately equal to -15‰.

Following inoculation, humid
Laboratory Monitoring of VOC Biodegradation in Unsaturated Fractured Rock

CO₂-free air was again supplied to the column, without the addition of toluene, in order to monitor CO₂ changes due to utilization of the basalt rock extract. Six days following inoculation, δ¹³C of CO₂ dropped to a low of -35% (significantly lower than δ¹³C of toluene; see Table 1), then recovered to -16% (near pre-inoculation values) over the next 18 days. Thirteen days following inoculation, CO₂ concentrations reached a peak of 40 times pre-inoculation levels, then declined to several-times pre-inoculation levels over the next 13 days. The recovery in CO₂ values, as well as carbon mass balance, suggested that the organic substrate from the extract had been nearly exhausted.

For delivery of 100 ppm toluene for flow-through conditions, CO₂ concentrations in the effluent increased by a factor of 1.5, while δ¹³C shifted from -15% in the influent to -21% in the effluent. To increase the residence time of the vapor phase with the rock chips and CO₂ changes, the column was shut in for four days and the vapor phase circulated by means of the recycle line shown in Figure 1. Figure 2 is a plot of the relative abundance of CO₂ and the δ¹³C values during recirculation. CO₂ concentrations increased approximately six-fold, while δ¹³C values decreased by 4 to -9‰. On the day of the last measured value of CO₂, the concentration of toluene was 30% of its initial value. The sensitivity of δ¹³C values is indicated by the fact that drop in δ¹³C precedes the increase in CO₂ abundance due to the degradation of toluene.

**Significance of Findings**

For vapor-phase delivery of toluene at near 100% relative humidity, δ¹³C measurements of CO₂ indicated that the mixed culture utilized toluene without the presence of flowing water. While the numbers of indigenous bacteria in the fractured-rock vadose zone in arid regions are low, other experiments have indicated that their activity may be stimulated by the addition of water, nutrients and organic carbon.

The geocosms can be used to assess the various environmental factors that may limit biological activity in the vadose zone and to test hypotheses of contaminant transformation processes derived from field monitoring with stable isotope ratios. Given that contaminant "storage" in fractured basals (vesicular matrix) in the vadose zone may be away from accessible flow paths, our ultimate objective is to identify factors that can stimulate biological activity in the presence of contaminants and test methods of delivering limiting substrates. While this study focuses on fractured basalt, the approach can be applied to unconsolidated or partially consolidated porous media.

**Related Publications**


**Funding**

This work has been supported by the Office of Science, Office of Health and Environmental Sciences, Biological and Environmental Research Program, of the U.S. Department of Energy under Contract No. DE-AC03-76SF00098.
Removal of Uranium (VI) From Contaminated Sediments
By Surfactants

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Research Objectives

Given the significant health risks uranium poses, numerous Department of Energy and mine tailing sites require decontamination. Promising chemical treatments such as H₂SO₄ and carbonate/bicarbonate (CB) suffer from serious limitations: strong matrix dissolution with the acid and reduced desorption efficiency with CB due to the buffering capacity of soils. As an alternative to these chemical treatments, surface active agents (surfactants) might be used to remediate metal-contaminated acidic soils. Surfactant aggregates or micelles bind metal ions (e.g., Cd²⁺, Pb²⁺, UO₂²⁺) in aqueous solutions. However, studies conducted in simple aqueous solutions without the presence of contaminated soil are not directly amenable for evaluating the effectiveness of surfactants in removing strongly sorbing ions from soils. The objective of this research is to understand uranium sorption onto natural sediments and determine the efficiency of surfactants in desorbing U(VI) from contaminated soils.

Approach

The soil used in this study was collected at the midslope of the Melton Branch Watershed on the Oak Ridge Reservation (Tennessee). The watershed has a shallow soil profile underlain by fractured saprolite. The soil texture is 25% clay, 35% silt and 40% sand. The clay fraction is composed of illite (40%), mixed-layer illite and smectite (40%), kaolinite (20%) and traces of quartz. Carbonates have been completely weathered and a large quantity of amorphous Fe oxides (3%) is present as coating.

The experiments consisted of two steps: (1) sorption of U(VI) onto the Oak Ridge soil and (2) desorption from the soil. Here sorption is operationally equated with measured removal of U(VI) from the aqueous phase and may include influences from precipitation. Likewise, desorption may include influences from dissolution. In the sorption experiments, a known amount of sediment was combined with a background electrolyte (1 mM NaCl and 1 mM CaCl₂ in deionized water) in centrifuge tubes. Uranium was added to the mixture from a uranyl nitrate stock solution. Sorption of U(VI) was studied as functions of time and concentration of uranium (10⁻⁷ to 10⁻⁴ M). The pH of the soil solution was adjusted with HNO₃ and NaHCO₃, and calcium concentration varied from 0 to 100 mM.

In the desorption step, a selected treatment solution (10 mL) was added to the previously contaminated soil. Following the desorption period, the samples were centrifuged and the supernatant was collected, diluted with deionized water and acidified for determination of the amount of U(VI) removed from the soil. The treatments included salt solutions, NTA, bicarbonate, H₂SO₄, and surfactants. Desorption experiments with deionized water and artificial groundwater were used as controls. Desorption times varied from 5 to 120 hours. Treatment concentrations ranged from 25 to 200 mM. The concentration of sorbed U(VI) ranged from about 10⁻⁹ to 10⁻⁶ mol/g. U(VI) desorption was also investigated for soil-to-liquid ratios of 0.1, 0.2 and 0.5 g/mL. The effect of increasing Ca²⁺ concentration was also determined.

Uranium was analyzed with inductively coupled plasma mass spectrometry using Bi (25 ppb) as an internal standard. Iron was analyzed with inductively coupled plasma atomic emission spectroscopy.

Results

Uranium Sorption. The rate of sorption is initially very fast (96.5% of the added uranium is sorbed in less than one hour). This fast sorption step is followed by a slow reaction rate (i.e., sorption levels off after approximately 48 hours). The fast sorption rate is attributed to uranium sorption onto readily available external surface sites, while the slow reaction rate corresponds to sorption onto less accessible sites and is controlled by diffusion of uranium into the sorbing phase. U(VI) sorption onto the Oak Ridge soil is strongly influenced by the pH: one observes an adsorption edge at pH = 2.4, followed by a maximum sorption at pH = 4.8 < pH < 7.0. The pH dependence of the sorption process indicates that protons, H⁺, compete with U(VI) for sorption sites (i.e., surface hydroxyl groups, -OH); at

Figure 1. U(VI) and Fe release from the Oak Ridge soil as a function of chemical treatment. [U(VI)]₀ = 10⁻⁸ mol/L. [Treatment] = 60 mM except [NaCl] = 140 mM and [CaCl₂] = 100 mM.
low pH, H⁺ is the principal sorbing species, forming positively charged diprotonated sites (SOH₂⁺). As the pH increases, U(VI) ions displace H⁺ and bind to OH groups on the surface. U(VI) reaction with those surface hydroxyl groups is similar to the hydrolysis reaction observed in aqueous solution: 8. Sorption experiments with Ca²⁺ suggest that a relatively minor fraction of U(VI) might be sorbed onto fixed negative charge sites and that Ca²⁺ could compete with U(VI) for these sites.

The strong pH influence and the relatively minor effect of Ca²⁺ on sorption suggest that U(VI) is mostly sorbed onto amphoteric hydroxyl groups. The nature of the sorbed U(VI) species was not determined in this study. However, one would expect U(VI) to be strongly sorbed to the Oak Ridge soil, principally as inner-sphere complexes.

**Uranium Desorption.** As shown in Figure 1, mild chemical treatment solutions such as NaCl and CaCl₂ are ineffective at releasing U(VI) from the soil matrix. More aggressive treatment by H₂SO₄ can desorb U(VI) efficiently. However, the strong matrix dissolution by the acid prevents its application as a useful agent for in-situ removal of U(VI). Bicarbonate can also desorb U(VI); however, the desorption efficiency is severely reduced by the buffering capacity of the acidic soil and by the presence of calcium.

As an alternative to these treatment solutions, two anionic surfactants, AOK and T77, were found most suitable for U(VI) removal from the contaminated soil. AOK is a sodium C₁₄-₁₆ olefin sulfonate and T77 is sodium oleyl n-methyl taurate. The most likely mechanisms responsible for U(VI) desorption using the surfactant approach include cation exchange and, to a lesser extent, dissolution of the soil matrix. The ion-exchange reaction takes place in the electric double layer (diffuse and Stern layers) surrounding the micelles. During ion exchange, U(VI) cations replace the counterions Na⁺. Monovalent cations such as UO₂⁺(OH)⁺ are expected to be "loosely" bound to the micelles, while the divalent cation UO₂²⁺ is expected to attach strongly to the micellar surface and is specifically located in the Stern layer. Evidence of some matrix dissolution is illustrated by the amount of Fe released during the desorption experiments: 38 and 28 mg/L for AOK and T77, respectively. These surfactants are very efficient solubilizing agents at low uranium concentrations: about 100% U(VI) removal for [U(VI)]_0, sorbed = 10⁹ mol/g. At greater uranium concentrations, the desorption efficiency of the surfactant solutions increases with an increase in surfactant concentration and reaches a plateau of 75-80%. Limitations associated with the surfactant treatments were also identified. Surfactant sorption onto the soil and greater affinity between U(VI) and the soil matrix reduce the efficiency of the treatment solutions at large soil-to-liquid ratios. Due to the cation-exchange nature of the desorption process, competitive cations such as calcium reduce the amount of U(VI) removed from the soil.

**Significance of Findings**

Results obtained in this study suggest that the use of surfactants such as AOK and T77 to remove metals/radionuclides from contaminated soils can potentially be developed as an ex-situ or in-situ remediation method. Acidic soils with lower oxide and clay contents would be the preferred candidates for such an in-situ surfactant treatment. While competition with divalent cations such as Ca²⁺ would reduce the treatment efficiency, the non-specificity of the desorption process also suggests that these surfactants could be used to remove other hazardous or radioactive cations (e.g., Cd²⁺, Pb²⁺, Co²⁺, Sr²⁺, etc.) from contaminated soils.

**Related Publications**


**Funding**

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

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HTTP://WWW-ESD.LBL.GOV
Research Objectives

The objectives of this investigation are to introduce a new approach to the multi-scale characterization of flow and transport in the fractured basalt of the vadose zone and to develop physically based conceptual models on a hierarchy of scales.

Approach

We illustrate this new approach using results of field and laboratory investigations conducted in the fractured basalt near Idaho National Engineering and Environmental Laboratory (INEL). The results were obtained from field tests carried out at three different sites: (1) small-scale infiltration tests (ponded area 0.5 m²) conducted at the Hell’s Half Acre site near Shelley, Idaho, (2) intermediate-scale infiltration tests (ponded area 56 m²) conducted at the Box Canyon site near Arco, Idaho, and (3) a large-scale infiltration test conducted near the INEL Radioactive Waste Management Complex (RWMC; ponded area ~26,000 m²). In addition, laboratory investigations included measurements on fractured basalt cores and small-scale dripping experiments in fracture models.

Results

We find that, at each scale of investigation, different models for flow phenomena must be used to explain the observed behavior. These models can be used to describe the flow processes on different scales, with no apparent scaling principles evident. To characterize flow phenomena in fractured basalt, we recommend that investigations be carried out in the following hierarchy: elemental, small-scale, intermediate-scale and large-scale (Figure 1). An elemental component is a single fracture or a block of homogeneous porous medium. Small-scale components include one or a few fractures and the surrounding matrix. Intermediate-scale components include a fracture network and other parts (fracture zones, vesicular lenses, soil, massive basalt, rubble zone) of a single basalt flow finger. Large-scale components include multiple basalt flows and their surrounding network of rubble zones and sedimentary interbeds.

Several laboratory and field infiltration tests conducted in fractured basalt have shown that a typical feature of flow in fractured rocks is channeling that occurs at all scales, including individual fractures, the intra-basalt fracture network and the inter-basalt rubble-zone network. However, the instrumentation used in lab and small-scale field conditions (in particular, to record dripping phenomena) is not practical for use at larger scales. Field measurements of flow characteristics in fractured rocks using single probes (such as tensiometers) are uncertain, because the locations of the probes in relation to the flow paths are not precisely known and these probes average fracture and matrix hydraulic characteristics.

An important feature of flow in the basalt vadose zone is that the hydraulic system includes both unsaturated and saturated rocks. During flooding at the surface, the saturated zones have a limited and local extent within flow channels in the fractures and vesicular zones. Single probes crossing the saturated fractures also intersect the matrix; hence, the probes measure an averaged water pressure in the fracture-matrix system. However, it is difficult to separate the contribution of the fracture from that of the matrix. Using available monitoring techniques under field conditions, we cannot perfect our knowledge of initial conditions; we can only measure approximate values of different parameters (pressure, moisture content, temperature, concentrations) or determine the ranges of these parameters.

Fluid flow in fractured basalt of the vadose zone can be considered a nonlinear dynamic process in which the behavior, both temporally and spatially, may be chaotic. The chaotic nature of flow results from nonlinear processes and the strong spatial and temporal varia-

Figure 1. Hierarchy of scales of hydrogeological components in fractured basalts.
tions in moisture content, hydraulic conductivity and fracture connectivity. As a result, in fractured basalt (that is, a nonlinear system) small variations in flow parameters may lead to significant variations in predicted results. The dissipative nature of the system implies that its phase-space volume decreases with time, leading to the formation of strange attractors characterizing the range in which the flow parameters are expected to change. The dynamics of such systems are sensitive to the initial conditions. The response of such systems may include a stochastic component that it is not necessarily a dominant factor on the system behavior. If the stochastic component is not dominant, then a stochastic analysis will not provide useful information.

We also find that under field conditions with a limited number of single-probe measurements, we can detect neither the spatial nor temporal chaotic variations of the flow parameters. Therefore, we must use conventional (i.e., nonchaotic) stochastic or deterministic methods to describe flow and transport processes. If the stochastic component is not a dominant factor, then a stochastic analysis will provide incorrect answers and should be replaced by a chaotic analysis. If the stochastic component is significant (or if the phase-space dimension is so large that the dynamics look stochastic), then a stochastic analysis is the most appropriate tool to use. Because the system exhibits sensitivity to initial conditions, we can predict only the range in which the flow rate is expected to change, but not the exact flow rates. Where elemental and small-scale components are involved, the flow data can be analyzed using methods of nonlinear dynamics. Where intermediate and large-scale components are involved, a combination of deterministic and stochastic methods of flow analysis can be used.

**Significance of Findings**

It has become apparent that monitoring technologies, characterization methods and prediction procedures developed for porous media are not sufficient to treat fractured basalt. The results of studies on the elemental level can be used to better understand water dripping from a fracture under field conditions in boreholes, tunnels, caves and other underground openings. However, laboratory studies of fractured rocks have certain limitations, because we cannot determine how to combine the individual processes for characterizing the total system.

The most important practical application of small-scale investigations is the study of physics and models of flow taking into account the fracture-matrix interaction.

The practical application of the intermediate-scale investigation is understanding the flow processes underneath single tanks like those at the RWMC in Idaho and at Hanford. The practical application of the large-scale investigation is to understand the flow processes and develop models to study the distributed flow and contaminant transport problems that exist under the RWMC and elsewhere at INEEL or in the tank farms at Hanford.

**Related Publications**


**Funding**

This work has been supported by the Office of Environmental Management, Office of Science and Technology, Characterization, Monitoring and Sensor Technology Crosscutting Program, and the Environmental Management Science Program of the U.S. Department of Energy under Contract No. DE-AC03-76SF00098.
Research Objectives

The U.S. Department of Energy and the Polish Institute for Ecology of Industrial Areas have been cooperating in field studies of environmental remediation since 1995. One of the major focuses of this program has been the demonstration of bioremediation techniques to clean up soil and sediment associated with a waste lagoon at an operating petroleum refinery in southern Poland. After a thorough characterization and treatability and risk assessment studies, a remediation system was designed that took advantage of local materials to minimize costs and maximize treatment efficiency. Passive and active gas injection were compared and contrasted as a bioremediation technique for low pH soil contaminated with polycyclic aromatic hydrocarbons (PAHs).

Approach

Since 1995, DOE has worked with the Institute of Ecology of Industrial Areas (IETU) in Poland to develop and demonstrate mutually beneficial, cost-effective environmental remediation technologies. The Czechowice Oil Refinery (CZOR), our industrial partner for this project, was chosen because of their foresight and commitment to the use of new approaches for environmental restoration. This program is a precedent for Poland in which a portion of the funds necessary to complete the project were provided by the company responsible for the problem. The Czechowice Oil Refinery, located in southern Poland, was named by PIOS (State Environmental Protection Inspectorate of Poland) as one of the top 80 most polluted sites in Poland. Nearly a century of continuous use of a sulfuric acid-based oil refining method by CZOR has produced an estimated 120 thousand tons of acidic, highly weathered petroleum sludges. This waste has been deposited into three open, unlined process waste lagoons, 3 m deep, now covering 3.8 hectares. Initial analysis indicated that the sludges were composed mainly of high-molecular-weight paraffin and polycyclic aromatic hydrocarbons. The overall objective of this full-scale demonstration project is to test and evaluate a combination of U.S.- and Polish-developed remediation technologies and methodologies. Specifically, the goal of the demonstration is to reduce the environmental risk from PAH compounds in soil and to provide a green zone (grassy area) adjacent to the site boundary.

A 0.3 hectare site, the smallest of the waste lagoons, was selected for a modified aerobic biopile demonstration. Approximately 3,300 m$^3$ of contaminated soil (mean TPH concentration of 30,000 ppm) was targeted for treatment. The biopile was divided into two sections; an area of approximately 1,610 m$^2$ passively aerated using BaroBall(sm) and an area of approximately 1,390 m$^2$ actively aerated via direct air injection from the bottom of the pile. Use of both passive and active aeration methods allows for an accurate assessment of cost and efficiency, with the most appropriate design to be deployed for future lagoon remediation at the refinery.

Results

The innovative biopile design deployed used a combination of passive and active aeration and injection of nutrients to increase biodegradation of the very acidic soil containing high PAH concentrations. Simultaneous lab studies using soil columns were used to optimize treatment techniques and verify field observations under more controlled conditions. This full-
scale demonstration showed that with minimal cost the total mass of petroleum hydrocarbons could be reduced by more than 75% (82 metric tons) in only nine months. During this time the most toxic compounds were reduced to levels acceptable for multi-use resource activities. Though a variety of biodegradation monitoring methods were used, in-situ respiration and dehydrogenase activity were found to be best correlated with rates of biodegradation in the biopile. In addition, it was found that passive aeration alone could reach the same end point as the active aeration—it just took longer (Table 1). The rates of biodegradation were comparable to other prepared bed studies done using petroleum contaminated soil; i.e., about 60 mg/kg/day. However, given that this material was highly weathered and very acidic, these rates are quite high. Much of this increase can probably be attributed to the sawdust added as a bulking agent and the active aeration process.

**Significance of Findings**

The finding that in-situ respiration and dehydrogenase measurements more accurately reflect the biodegradation rate suggests that these direct measurements can be used to provide real-time control of biopile operation to maximize biodegradation rates under a variety of conditions. The cost savings from passive aeration may give it a significant advantage over active aeration when clean-up time is not a primary consideration.

The remediation strategies that have been applied at the CZOR waste lagoon were designed, managed and implemented under the direction of the Westinghouse Savannah River Company for DOE, the Institute for Ecology of Industrial Area (IETU) and Florida State University. This collaboration between IETU, DOE and its partners provides the basis for international technology transfer of innovative remediation technologies that can be applied to DOE sites as well as in Poland and other sites worldwide.

### Table 1. Biodegradation rate (mg Petroleum/kg soil/day).

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<thead>
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<th>Campaign</th>
<th>Average</th>
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**Related Publications**


**Funding**

LBNL work on this project has been supported by the Westinghouse Savannah River Company under U.S. Department of Energy Contract No. DE-AC09-89R180035. The Savannah River Technology Center, Florida State University, and the Polish Institute for Ecology of Industrial areas were all collaborators on this project. Funding was also provided in part from the Polish National Science Foundation, National EcoFund and the Czechowice Oil Refinery.
**Research Objectives**

The purpose of this aerobic landfill bioreactor pilot study was to demonstrate the use of air injection and leachate recirculation in promoting aerobic bioremediation within the waste mass and remediation of contaminated leachate in a solid waste landfill. The processes include (1) air injection into the waste mass, (2) recirculation of leachate and (3) addition of gaseous nutrients into the waste mass. These components are considered individually and in combination to determine their technical, economical and practical aspects of their use in the study. Technical support was provided to American Technologies, Inc., to test and implement this technology at a Georgia county landfill.

**Approach**

Conventional municipal solid waste (MSW) landfills worldwide operate under anaerobic (no oxygen) conditions in which slow stabilization of the waste mass occurs, producing methane gas and toxic leachate over long periods of time. The current designs of most modern landfills utilize clay caps, liners and collection systems to contain the waste ("dry tomb") and prevent the spread of toxic constituents that could find their way into a landfill. Older, unlined landfills pose a constant threat to the environment. Even with the newer landfill designs meeting the U.S. Environmental Protection Agency (EPA) requirements (RCRA Subtitle-D), the caps and liners ultimately fail, potentially releasing toxic constituents, typically found in aging landfill leachate, will reach local groundwater.

The EPA recognizes that "once the unit is closed, the bottom layer of the landfill will deteriorate over time and consequently, will not prevent leachate transport out of the unit" (40 CFR 258). As a result, leachate collection systems and impermeable caps do not decrease the risk that toxic constituents, typically found in aging landfill leachate, will reach local groundwater.

Over the past several years we have successfully demonstrated and treated groundwater in-situ at two unlined solid waste landfills at DOE's Savannah River Site. We used horizontal wells to inject air and gaseous nutrients (methane, nitrous oxide and tri-ethyl phosphate) into the groundwater to bioremediate chlorinated solvents and reduce metals leaching in both the groundwater and the vadose zone. For the past two years, American Technologies, Inc. (ATI), in cooperation with the author, now at LBNL, has demonstrated that it can safely and economically convert a conventional lined and capped landfill to aerobic conditions utilizing an aerobic landfill bioreactor (ALB). They have shown that aerobically degrading MSW within a landfill significantly increases the rate of waste decomposition and settlement, decreases the production of methane gas, reduces the level of toxic organics in the leachate and significantly reduces the volume of landfill leachate. The ALB eliminates the source of groundwater contamination caused by solid waste landfills, and combined with the pumping and treating of the groundwater as a supplemental source of landfill moisture addition, provides for the in-situ treatment of groundwater. A secondary effect of this strategy at most sites is to stabilize metals in the groundwater. This is due to increases in ambient redox potential and pH caused by the aerobic or microaerophilic environment created by air sparging and biodegradation of high-oxygen-demand organics and reducing agents.

At the Columbia County Baker Place Landfill, a 100-acre unlined Subtitle-D municipal landfill near Govetown, Ga., we connected blowers to the cleanout ports of the leachate collection system to provide air and recirculated leachate via drip tubes through the temporary cover. An initial pressure test was followed by the placement of vadose zone piezometers throughout the test cell to determine changes in soil gas composition. Soil gas and leachate were analyzed weekly for 24 months. See Figure 1 for the design plan.

**Results**

Initial air injection tests in the leachate collection system of the landfill showed that air penetrated the entire landfill via the gravel bed in the bottom of the landfill. Indeed pressure and flow rate measurements around the landfill showed that even
A single blower could provide substantial air flow more than 1,000 ft from the injection point, the farthest point in the landfill. Measurements of soil gas showed that initially oxygen increased and then declined to low levels once the microbial population had adapted to aerobic conditions (Figure 2). Both $\text{CO}_2$ and $\text{CH}_4$ declined immediately to low or undetectable levels, further indicating that aerobic conditions within the waste were attained. After aerobic biodegradation became active the temperature and $\text{CO}_2$ increased; however, $\text{CH}_4$ never appeared again except transiently when the air was shut off. Since methane can only be produced by methanogens under completely anaerobic conditions, the production of methane was stopped by the air injection.

Laboratory analyses of biochemical oxygen demand (BOD) and volatile organic compound (VOC) concentrations in the leachate indicated significant reduction by the aerobic process. BOD in the "Sump One" leachate samples were reduced by at least 70%. Organics such as methyl-ethyl ketone (MEK) and acetone were reduced significantly, and fecal coliform was eliminated from the leachate. Total VOC concentrations in many of the vapor samples collected were less than 1 ppm. No leachate was treated during the entire study. Prior to this, the landfill was treating 150,000 gal of leachate each month.

Significance of Findings

This study demonstrated that air injection and leachate recirculation can be used to greatly increase biodegradation of municipal solid waste using a standard subtitle-D configuration, thereby converting the dry tomb to an active bioreactor typical of composting. Operating data collected from the ALB at the Baker Place Road landfill in Grovetown, Ga., since late-January 1997 provides representative cost-benefits that could be realized by any comparable solid waste landfill. Short-term benefits include: (1) increased rate of waste mass stabilization and settlement, (2) much improved leachate chemistry, (3) significant reduction in leachate treatment, (4) significant reduction in noxous odors, and (5) significant reduction in methane generation. Long-term benefits resulting from waste mass stabilization in less than five years include the following savings: (1) post-closure monitoring reduced from 30 to five years ($6,000,000); (2) impermeable closure cap reduced to reduced permeable cap or alternative cover ($2,000,000); (3) Clean Air Act emission control of methane gas (plus cost of gas controls, $240,000); (4) leachate collection and treatment ($1,000,000); and (5) elimination of groundwater treatment costs ($1,500,000).

Related Publications


Funding

This work has been supported by American Technologies, Inc., and the U.S. Department of Energy under Contract No. DE-AC02-76SF00098 and DE-AC09-89R180035. Funding was also provided by Columbia County, Appleton, GA.
New Software Tool
For Visualizing Fracture Data
From Oriented Cores

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Figure 1. Visualization of fracture data from oriented core. (a) Fractures colored by type of filling. (b) Only fractures with an angle of dip between 10° and 40° have been included. Fractures are colored by angle of strike.

Project Objectives

Geological characterization of fractured sites relies on analysis of cores and surface fracture mapping. Fracture data from cores usually consists of fracture location, staining and filling. In some cases, "oriented" cores are collected; i.e., not only is the location of a fracture known, but also its orientation in space. This report describes the development of a software tool for visualizing oriented fracture data in a 3-D context. The fractures are visualized as oriented disks. The software tool includes the capability to select subsets of fractures based on angle of dip, angle of strike, fracture filling and fracture staining; it is described in more detail in Jacobsen (in preparation).

The oriented core fracture data used to develop the software tool was supplied by the California Environmental Protection Agency's Department of Toxic Substances Control (DTSC), which funded and provided technical guidance for the development of the visualization tool.

Approach

The software tool was developed using the general-purpose visualization software package AVS/Express, from Advanced Visual Systems Inc. AVS/Express is widely used for research, engineering and financial applications. It provides a visual programming environment in which the user builds a data flow network consisting of software modules that provide various techniques and capabilities for visualizing field data or simulation output. AVS/Express was chosen not only because of its wide range of visualization capabilities, but also because it is extensible; that is, user-developed computer programs can be incorporated as modules into a network of AVS/Express modules.

A contractor to DTSC collected cores from 29 wells in a contaminated, fractured site. The fracture data consist of the following information:

- depth down the borehole to the fracture
- fracture dip: specified as angle from horizontal and direction, either north or south
- fracture strike: specified as angle with respect to north and direction, either east or west
- fracture staining: specified as contaminant stained, iron stained, not stained, or "other" (not specified)
- fracture filling: specified as clay filled, sand filled, no filled or "other" (not specified)

Altogether, the data set contains data for 1,962 fractures. In addition, DTSC provided coordinates (in easting and northing) of the wells from which the cores were taken, ground surface elevations of the wells, and text well identifiers. The well coordinates, depths and elevations were all specified in feet; the dip and strike angles were specified in degrees.

As described above, the fracture data from oriented cores consist of strike and dip, which together specify the orientation in space of a plane containing the fracture. In the visualizations, disks rather than planes represent the fractures. A C++ computer program was written to convert strike and dip data into the geometric information required by AVS/Express to visually represent the fractures as disks. The computer program also includes the logic needed to select a subset of fractures according to the following criteria:

- range of dip angles
- range of strike angles
New Software Tool for Visualizing Fracture Data from Oriented Cores

- type of fracture filling (clay, sand, none, or “other”)
- type of fracture staining (contaminant, iron, none, or “other”).

When selecting a subset of fractures, the user may choose one or more criteria. For example, the user could choose to limit the range of dip angles to 0° to 10°, the range of strike angles to N30°W to N30°E, the type of fracture filling to clay and sand and the type of fracture staining to contaminant and iron. Each fracture would then be checked against all of these criteria before including it in the set of fractures to be visualized.

A user interface (UI) was developed to facilitate specifying visualization parameters and selection criteria. When the visualization application is loaded into AVS/Express, the user is presented with a menu giving the following options:
- name of input file of strike and dip data
- radius to use when displaying the fractures as disks
- how to color the fracture disks (by angle of dip, angle of strike, type of fracture filling or type of fracture staining)
- whether to include all fractures or only a subset of fractures in the visualization.

If the user chooses to specify subgroups of fractures to include, then a second menu pops up. The second menu first gives the user the option to specify which criteria (angle of dip, angle of strike, type of fracture filling, type of fracture staining) to use to select fractures. Once the user has toggled on one or more of these criteria, the parts of the UI menu corresponding to the selected options become active and the user may specify range of dip and/or strike and type of fracture filling and/or staining. As discussed above, the user may combine different criteria to specify the characteristics of a subset of fractures.

**Results**

This project resulted in the development of a software tool for visualizing fracture data from oriented cores. The tool consists of a visualization network and user interface developed from AVS/Express modules and a C++ computer program developed to convert strike and dip data into the geometric information required by AVS/Express to visually represent the fractures as disks. The software tool includes the capability to select subsets of fractures, based on angle of dip, angle of strike, fracture filling and fracture staining. This capability has been implemented by incorporating the necessary logic in the computer program and also by developing a user interface to facilitate specifying visualization parameters and selection criteria.

Figures 1a and 1b provide examples of how the software tool can be used. Figure 1a shows all of the fractures in the data set color coded by type of fracture filling. The visualization in Figure 1b includes only fractures with an angle of dip between 10° and 40°. In this figure, the angle of dip of the fractures is clear, so color has been used to indicate the angle of strike angle in order to show the distribution of strike for the subset of fractures.

**Significance of Findings**

The software tool developed by this project provides the user with the capability to:
- include all oriented fracture data from a site in a single view
- look for trends in or correlations among the fractures
- select subsets of fractures to include in the visualization, thereby reducing the density of fractures and the complexity of the visualization
- include in the visualization other types of data (e.g., seismic, water sample, lithology, etc.).

Visualization of oriented core fracture data is a powerful analysis tool because it provides practically the only way to include all fracture data from a site in a single view. Unlike other analysis techniques (e.g., Rose diagrams), other types of data also can be included in the visualization.

**Related Publication**


**Funding**

This work has been supported by the California Environmental Protection Agency through its Department of Toxic Substance Control, which also collaborated in the research through Integrated Contract Order B347960.
Research Objectives

The Vadose Zone Monitoring System (VZMS) installed at McClellan Air Force Base has been collecting data on pressure, temperature, gas, and liquid-phase VOC concentrations and moisture content over a 100-ft vertical section of alluvial sands and silts for the last two years. Thirteen levels of instrument clusters were installed over the vadose zone in each of the two boreholes (VZMS-A and VZMS-B), spaced 10 ft apart at site S-7 in Investigative Cluster-34 (IC-34). A third VZMS (VZMS-C) was constructed in 1998 in between VZMS-A and VZMS-B to collect matric potential data to a depth of 25 ft. The instruments are connected to a data acquisition system installed in a portable building at the site. Two nearby boreholes for neutron logging were also constructed to monitor moisture content. Gas and liquid samples are brought to the LBNL Environmental Measurements Laboratory for chemical analysis. The primary contaminants are trichloroethylene (TCE) and cis-1,2-DCE. Most of the contamination is concentrated in the top 6 m (20 ft) of the section, with some additional contamination near the water table. The main issue to be addressed concerns the rate of downward transport of TCE from the shallow vadose zone to the water table. Through modeling, we estimate values of sediment permeability, effective thermal conductivity and moisture content as a function of depth, comparing estimates to laboratory and site-measured values. By matching various types of data from the site, we are building a defensible conceptual model for modeling contaminant transport.

Approach

A considerable data analysis effort is required to use VZMS data to infer contaminant transport. Our approach is to use all relevant data including VZMS temporal data to build a plausible conceptual model and then to use forward and inverse modeling to analyze the data and continue to improve the model. We refer to this process as “enhanced data analysis.” We have taken data from drilling logs, laboratory measurements of core samples, and the VZMS, and constructed a one-dimensional conceptual model of the vadose zone at the site. The 100 ft of vadose zone are discretized with 0.5-ft gridblocks to represent the many different layers of silts, sands and clay present. We use T2VOC, the multiphase and multicomponent model for the flow and transport of water, volatile organic compounds and air for forward simulations, and the inverse modeling code ITOUGH2 for sensitivity, uncertainty and inverse modeling. These modeling tools allow us to carry out numerical experiments and inverse modeling to determine key parameters controlling movement of gas and liquid phases in the subsurface. The goals of enhanced data analysis are to (1) increase the value of the VZMS data by constructing models that can be used in a predictive mode and (2) validate the models such that defensible remediation decisions at other similar sites are possible.
Enhanced Data Analysis for the Vadose Zone Monitoring System

![Figure 2. Observed formation volumetric moisture content and simulated 1-D moisture profiles using recharge rates of 1, 10 and 50 cm/yr.](image)

...can be made based on the understanding gained at the S-7 site.

**Results**

Using a one-dimensional conceptual model that contains a site-averaged hydrostratigraphy (at resolution of 0.5 ft) defined by lithologic logs and laboratory analysis of core, we estimated values of permeability by simulating gas-phase pressure response at depth in the subsurface to a time-varying barometric signal. Permeabilities were estimated by matching observed and simulated gas-phase pressure at the four shallowest instrument cluster depths (6, 11, 18 and 30 ft), where the response to atmospheric variation was strongest, and where, at site S-7, the shallow VOC contamination has persisted over 25 years or so.

Figure 1a illustrates the pressure response (simulated and observed) at 30 feet. Results indicate that the inversion is most sensitive to the permeability of the overlying concrete layer. A similar inversion was performed to evaluate effective thermal diffusivities of sediments by comparing observed and simulated formation temperature (Figure 1b). Simulations matched the observed temperature fluctuations at depths of 11, 18 and 30 ft, below which the effects of surface temperature are not discernible. Inclusion in the simulation of an annual recharge of 10 cm/yr provided a better fit to the observed moisture content profile relative to 1 cm/yr and 50 cm/yr (Figure 2). These parameters of permeability, thermal diffusivity and annual recharge are three key features in the conceptual model to be used to model contaminant transport.

**Significance of Findings**

The enhanced data analysis has reproduced multiple types of site data and allowed the estimation of sediment properties critical to the transport of contaminants at the S-7 site. The estimated values of permeability, thermal diffusivity and recharge will be incorporated into the conceptual model used to assess TCE transport in the gas- and liquid-phases.

**Related Publication**


**Funding**

This work has been supported by the U.S. Department of Defense under Military Interdepartmental Purchase Request FD2040-96-T-40206M to the Ernest Orlando Lawrence Berkeley National Laboratory under U.S. Department of Energy Contract No. DE-AC03-76SF00098.
## Research Objectives

Ferrofluids are stable colloidal suspensions of magnetic particles in carrier liquids. Due to their ability to be held in place by magnetic fields, ferrofluids currently find application in a variety of industrial processes and engineered devices, as well as limited use in the biomedical field. We have conceived of many potential applications for ferrofluids in the field of subsurface environmental restoration. These applications fall broadly into two main areas: (1) guiding liquids and holding liquids in place in the subsurface through application of magnetic fields; and (2) using ferrofluids as subsurface flow tracers that can be imaged by standard electromagnetic and geophysical methods. In order to facilitate the design and experimentation of porous media ferrofluid applications, as well as to carry out numerical experiments of ferrofluid flow phenomena, we have developed simulation capabilities for ferrofluids. The simulation capabilities are built upon the reservoir simulator TOUGH2.

## Approach

In the presence of an external magnetic field, the single-domain colloidal magnetite particles suspended in ferrofluid align, causing the ferrofluid to become magnetized. The magnetization of the fluid interacts with the magnetic field to produce attractive magnetic forces analogous to the body force on a liquid due to gravity. The attractive force on ferrofluid per unit volume is given by \( F_{\text{mag}} = \mu_0 M V H \) \([=] \text{Tesla Ampere-turn m/m}^3 \) \([=] \text{N/m}^3 \), where \( \mu_0 \) is magnetic permeability of free space in units of \( \text{T m/A} \), \( M \) is the magnetization in \( \text{A/m} \) and \( H \) is the magnetic field strength in \( \text{A/m} \). As the magnetic field strength increases, the ferrofluid reaches a maximum magnetization, or saturation magnetization. Thus, the magnetization is a function of \( H \) and can be approximated by simple arctangent functions.

In our development of simulation capabilities, we built upon the T2VOC module of TOUGH2 by (1) substituting ferrofluid for the non-aqueous phase liquid organic compound, (2) adding calculations for external magnetic field strength around a permanent magnet, (3) adding arctangent function approximations for the magnetization of ferrofluid, and (4) adding the ferromagnetic force term. We calculate the external magnetic field \( H \) for permanent rectangular magnets using analytical expressions that neglect the presence of ferrofluid, an approach considered reasonable for the applications we consider. The gradient of \( H \) is calculated by simple first-order differencing in each of the coordinate directions. At any value of \( H \), we assume that magnetization increases linearly with ferrofluid saturation. While we neglect the coupling between \( H \) and the ferrofluid distribution, we consider explicitly the full coupling between flow and transport driven by both the magnetic force (arising from the \( M \) and \( VH \) terms) and the buoyancy force (when gravity is present), which combine to make this a strongly coupled flow problem. Once the magnetic field strength \( H \) and its gradient are calculated, we calculate magnetization and the magnetic force at the interface between each gridblock. This term is added to the pressure gradient and gravitational body force terms. A diagram showing the calculation procedure is presented in Figure 1.

## Results

The demonstration problem models a laboratory experiment designed to show one potential application of ferrofluids in subsurface environmental engineering, that of pulling fluid underground by application of a permanent magnet. In the experiment, a small volume of ferrofluid (EMG 805TM) is injected through a catheter into the left-hand corner of a fluid-filled gap between one plate of smooth glass and one plate of rough glass with a magnet on the right-hand side. The narrow gap between the plates creates an analog porous medium similar to a Hele-Shaw cell. The domain is modeled as a porous medium with porosity set to 0.999. The ferrofluid flow experiment is carried out with the cell in a horizontal position and filled with a colloidal silica fluid that closely matches ferrofluid in density. The gradient in the magnetic field produces the attractive force that pulls ferrofluid toward the magnet, while viscous forces resist the motion.

Shown in Figure 2 are snapshots at four times in the simulation: (a) initial state; (b) \( t = 6 \) min; (c) \( t = 9 \) min; and (d) \( t = 13 \) min. Results as shown in Figure 2 agree qualitatively with the experiment in terms of the direction and geometry of ferrofluid movement in the system. Note in particular the tendency for the ferrofluid to elongate in the direction of the magnet just as we observed in the experiment.
Numerical Simulation of Ferrofluid Flow

Figure 2 Ferrofluid saturation and flow in Hele-Shaw cell simulation at t = 0 min, t = 6 min, t = 9 min and t = 13 min.

ment. This occurs because the force on ferrofluid is proportional to both the magnetic field strength (prior to saturation) and to the magnetic field gradient. Thus, ferrofluid that is already closer to the magnet is more strongly magnetized and pulled more strongly toward the magnet than ferrofluid that is farther away. Note also the accumulation of ferrofluid around the magnet. The good general agreement between experiment and simulation serves to qualitatively demonstrate the validity of the new simulation capabilities.

Significance of Findings

We developed and demonstrated simulation capabilities for ferrofluid flow in porous media. A number of the physical processes of ferrofluid flow shown in the sample problem are rather uncommon. First, we observe the tendency of the ferrofluid to elongate in the direction of the magnet due to the larger forces on the fluid at smaller distances from the magnet. Second, ferrofluid starts out at nearly full saturation and then in the course of traversing the domain becomes a two-phase ferrofluid–water mixture. Near the magnet, it segregates and becomes pure ferrofluid ($S_{ff} = 1.0$). Such segregation effects are not particularly common in flow and transport where diffusion and dispersion usually lead to smoothing and mixing of constituents. Third, near the magnet, water must be expelled as ferrofluid is pulled strongly toward the magnet. During this evolution, there is a minimum in phase saturation between the initial ferrofluid injection point and the magnet where it segregates out. This phase saturation minimum tends to be close to the edge of the segregating volume near the magnet. Finally, the forces on the ferrofluid become very large near the magnet where the magnetization is strong and there is a high field strength gradient. This problem is an example of an overstable problem, where fluid is pulled strongly toward an impenetrable boundary and tends to stagnate. An example application simulation we carried out involving barrier verification shows that the effective distances over which a single magnet can pull ferrofluid are on the order of 1 m.

Related Publications


Funding

This work has been supported by the Laboratory Directed Research and Development Program of Lawrence Berkeley National Laboratory under U.S. Department of Energy Contract No. DE-AC03-76SF00098.
Research Objectives

Organochlorines (OCs) and polycyclic aromatic hydrocarbons (PAHs) are ubiquitous environmental contaminants that are toxic and suspected human carcinogens. Traditional assessment of human exposures to these organic toxins and the subsequent biological responses relies primarily on high-dose and short-term animal experiments. A major uncertainty inherent to this approach is the extrapolation from the high-dose animal experiments to the low-dose and long-term human exposures. To overcome this uncertainty, we recently have directed our research effort towards exploring the use of synchrotron radiation-based (SR) Fourier transform infrared (FTIR) spectromicroscopy for identifying chemical changes in cellular nucleic acids and proteins as a result of OC and PAH exposures.

To date, the primary research objective has been to identify SR FTIR spectroscopic signals of human cell culture systems that are indicative of low-dose exposures to OCs and PAHs and could be used as biomarkers. SR FTIR spectromicroscopy is used because our earlier work has demonstrated that this is a sensitive and nondestructive technique capable of providing direct biochemical information at molecular levels in a biological system. The fine spatial resolution of 5-10 microns and strong signal to noise levels of SR FTIR spectromicroscopy allow one to detect the subtle changes in intracellular biochemical processes as the cells are exposed to environmental stimuli.

Approach

The biomarker considered for OC and PAH exposures is the induction of the cytochrome P4501A1 CYP1A1 gene expression and the increase in the associated enzyme activity. It is well established that CYP1A1 transcript levels increase in response to exposure to OCs and PAHs through their binding to the Ah receptors (Figure 1).

HepG2 (human hepatoma-derived) cells were used as model human epithelial cells that can metabolize PAHs; 2,3,7,8-tetrachlorodibenzo-p-dioxin (TCDD) modeled OCs; BaP modeled PAHs and coal tars modeled mixtures of PAHs. HepG2 cells were maintained in Eagle's Minimum Essential Medium with non-essential amino acids and Earle's BSS supplemented with 10% fetal calf serum, 1 mM L-glutamine, 10 mM Hepes and antibiotics. Cells were sub-cultured, and then treated for 2 - 20 hours with TCDD, BaP and coal tars at environmentally relevant concentrations.

The effect of TCDD was monitored and mapped by the SR FTIR spectromicroscopy technique in the mid-IR region (4000-4000 cm⁻¹). SR FTIR signals (from individual cells) that are specific to the intracellular response after their exposure to these organic toxins were identified. To validate the SR FTIR spectromicroscopy technique, results from the TCDD experiments were compared with the CYP1A1 transcript levels measured by the widely accepted yet more time-consuming reverse transcription-polymerase chain reaction (RT-PCR).

Results

Dimensionless SR FTIR spectra were recorded at the proximity of a cell nucleus of HepG2 cells that were exposed to TCDD of different concentrations (0, 0.01, 0.1, 0.5, and 1.0 nM) for 20 hours. There are considerable differences in the SR FTIR spectra associated with the CYP1A1 gene expression and the increase in the associated enzyme activity, with one difference being the increased absorption of the vibration band 1180-1160 cm⁻¹, centered at ~1170 cm⁻¹. Here, the normalized absorbance intensity for individual cells increased from 0.007 to 0.21 when the TCDD concentration increased from 10⁻¹¹ to 10⁻⁹ M (Figure 2a). The normalized absorbance intensity at ~1170 cm⁻¹ for individual control cells was 0.005. This is a 42-fold increase in the absorbance intensity. This systematic spectral change might be related to the alteration in the DNA base structure and will be the subject of future investigation.

A comparison of the dose response described above with that obtained using the RT-PCR technique is shown in Figure 2b. The solid line was the least-squares fit to the data. The excellent agreement (with r² = 0.99) for measurements from the two methods indicated that the fast and direct...
SR FTIR spectromicroscopy technique was indeed comparable to the more time-consuming and widely accepted RT-PCR technique that specifically measures increases in the CYPIA1 transcript levels.

The SR FTIR spectra recorded at the proximity of a cell nucleus of HepG2 cells that have been exposed to BaP and coal tars at environmentally relevant concentrations showed similar spectral characteristics at \(-1170\) cm\(^{-1}\). The recorded dose-response behavior was also similar to those reported in the literature.

**Significance of Findings**

The agreement between the SR FTIR spectromicroscopic data for dioxin exposures and the RT-PCR results, and the agreement between the PAH measurements and those reported in the literature indicate that the intracellular biological responses to low-dose exposures to these organic toxins are well represented by our specific spectral changes. These changes are associated with CYPIA1 gene expression and the increase in the associated enzyme activity with different types of damage. The capabilities of SR FTIR spectromicroscopy for the direct detection of intracellular biochemical responses to exposures to dilute concentrations of OCS and PAHs will have significant impacts in future research methodology of environmental toxicology.

**Related Publications**


**Funding**

This work has been supported by the Office of Science, Office of National Petroleum Technology Program, Offices of Health and Environmental Sciences, Biological and Environmental Research Program and Basic Energy Sciences, Materials Science Division, of the U.S. Department of Energy under Contract No. DE-AC03-76SF00098.

![Figure 2. Development of a micro-fabricated device for detecting human exposure to environmental organic toxins. (a) Dose response of individual living HepG2 cells after 20 hour exposure to 2, 3, 7, 8-tetrachlorodibenzo-p-dioxin, as measured by the new IR technique (after hours of work). (b) New IR technique versus RT-PCR assay.](HTTP://WWW-ESD.LBL.GOV)
An Algal-Bacterial Treatment System for Drainage Selenium Removal

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Research Objectives

Selenium drainage water treatment has been an active area of research for more than a decade since the discovery of selenium toxicosis at Kesterson Reservoir in the western San Joaquin Valley of California. The Grassland Bypass Project established monthly and annual selenium load targets for tile drainage from agricultural water districts within the Grassland Basin—exceeding these could lead to fines of up to $500,000 per year. This has proved a powerful incentive for investment in irrigation scale, up to 20,000 gallons per day. University of California, Berkeley, are well suited for this application. These have been an active area of research for more than a decade since the discovery of selenium toxicosis at Kesterson Reservoir in the western San Joaquin Valley of California. The Grassland Bypass Project established monthly and annual selenium load targets for tile drainage from agricultural water districts within the Grassland Basin—exceeding these could lead to fines of up to $500,000 per year. This has proved a powerful incentive for investment in irrigation scale, up to 20,000 gallons per day. Hence, technologies such as the Algal-Bacterial Selenium Removal System (ABSR), developed by Professor Oswald and his co-workers at the Applied Algae Research Group (AARG) at the University of California, Berkeley, are well suited for this application. The primary goal of this project is to demonstrate the technical and economic feasibility of the ABSR system at a larger scale, up to 20,000 gallons per day.

Approach

The current collaborative demonstration project involves scientists in LBNL's Earth Sciences Division, the AARG and the departments of Cell Biology and Plant Biology at UC Berkeley. The ABSR system was constructed in July 1996 and consists of two parallel systems, each having a reduction pond (RP), a paddle-wheel mixed algal high rate pond (HRP) and an algae settling pond (ASP); see Figure 1. By operating two systems simultaneously, the operational parameters of one system can be varied while the other system is operated as a control.

The basic concept of the ABSR system is to grow microalgae on drainage water and to utilize the algal biomass as a carbon source for native bacteria such as Acinetobacter and Pseudomonas, which reduce nitrate to nitrogen gas and selenate to selenite. Selenite combines with metal ions and precipitates or is further reduced to insoluble elemental selenium. The insoluble forms of selenium are then separated from the effluent by sedimentation in the ponds followed by dissolved air flotation and sand filtration. Past and current studies show a clear need to reduce dissolved oxygen and nitrate to low levels before selenite can be reduced to selenite. Oxygen is eliminated from the drainage water by the respiration of microorganisms. Nitrate is removed by reduction to nitrogen gas during denitrification, or in another flow scheme, by assimilation into algal biomass in addition to denitrification. Selenium removed from the water column accumulates in the algal-bacterial biomass and inert materials in the bottom of the RPs. Because the biomass is continuously decomposing, the volume of solid residues increases very slowly. Removal and disposal of the solids in a landfill should be required only after many years of accumulation.

The 0.1-acre RPs were designed to promote the growth of nitrate- and selenate-reducing bacteria. Floating covers on the RPs were installed to reduce wind-induced mixing. The 0.1-acre paddle-wheel mixed HRP s were designed to cultivate microalgae in high concentrations and at high productivities. The low speed mixing of HRPs enhances the selection of algal species that bioflocculate and settle in quiescent algae settling ponds.

Carbon dioxide supplementation to the algae is provided by sparging the gas into a carbonation sump near the paddle wheel in each HRP. A baffle in the carbonation sump forces the flow of water downward. Against this downward current, the carbon dioxide bubbles are held in suspension as they dissolve into the water. ASPs provide a quiescent zone for the algae grown in the high rate ponds to settle. The launders in the ASPs improve algae sedimentation by removing supernatant from the surface of the pond at a very low overflow velocity. A sloped floor and internal sump in each ASP enables the harvesting of the algal biomass using a diaphragm pump.

Two flow modes are possible in the ABSR facility in the Panoche Drainage District, each having its advantages in terms of the economics of the system. In Mode 1 (South ABSR system), drainage water is brought into a HRP where 15 to 30 mg/L of nitrate-nitrogen can be removed through assimilation by algal cells. The remaining nitrate is removed in the RP via heterotrophic denitrification to nitrogen gas. By removing some nitrate through assimilation, less algal biomass is required as a carbon source for the denitrifying bacteria. The disadvantage of this mode is that car-

Figure 1. The Algal-Bacterial Selenium Removal System (ABSR).
bon dioxide and phosphate must be added to the drainage water to increase algal growth in the HRP.

In Mode 2 (North ABSR system), the drainage water passes through the RP first, where most of the nitrate is removed by denitrification followed by soluble selenium removal. The RP effluent containing algal decomposition products such as ammonia, phosphate, and dissolved carbon dioxide passes to the HRP. Algae grow utilizing the decomposition products, thereby reducing the need for supplemental carbon dioxide and phosphate.

Results

For start-up, the RPs were fed algae collected over six months from the AIWPS Facility at the UC Berkeley Richmond Field Station. These algae were pretreated with heat, steam or by drying and milling. Subsequent laboratory experiments have shown that algae harvested directly from the Panoche and Richmond HRPs and used as substrate directly without pretreatment are two to 10 times more effective for nitrate and selenium reduction than the algae collected over months in the Richmond ASRs. The "fresh" algae reduced at least 0.2 g NO₃-N per gram volatile solids introduced. Steam pretreatment of the "fresh" algae did not significantly improve nitrate reduction. Molasses was also evaluated as a substrate and found to reduce 0.22 g NO₃-N per gram volatile solids. Acting on the laboratory results, animal-feed-grade molasses has been used to supplement the algal substrate in the North ABSR system, and freshly harvested algae have been exclusively the substrate in the South ABSR system.

From April to October 1997, the molasses-fed (North ABSR) system has consistently reduced nitrate nitrogen to less than 10 mg/L NO₃-N and total soluble selenium 70 to 80% from a mean of 413 ug/L in the influent down to a mean of 87 ug/L (Figure 2). The flow to each system was 3,500 gallons per day during this period, giving a hydraulic residence time of 58 days. A shorter residence time of 25 days gave similar removal rates when internal baffles were installed in the RPs to prevent flow short circuiting of influent and the flow was increased to approximately 7,000 gals/day.

In October 1998 some breakthrough of selenium was evident as selenium removal kinetics decreased with colder winter temperatures. Figure 2 shows the impact that variations in molasses feeding had on soluble selenium removal; the thinner lines in the graphs with the (T-4) suffix represent total selenium.

The South ABSR system has been fed "fresh" algae, harvested by dissolved air flotation from wastewater treatment ponds since April 14, 1997. The mean influent nitrate concentration has been 82 mg/L NO₃-N. Nitrate removal by the system has improved, reaching less than 1 mg/L in the RP effluent by September 1997, when the South ABSR was switched to Mode-1 configuration. With the gradual reduction in nitrate concentration in the South RP, selenium removal has increased. The total soluble selenium removal has averaged 25%, from an influent concentration of 413 ug/L to a concentration of 308 ug/L in the South RP effluent. Selenium removal decreased dramatically during the winter months (starting in October 1998), when algal assimilation of selenium is at its lowest and the selenium-reducing bacteria in the reduction pond are least active and limited in their supply of carbon.

Significance of Findings

The molasses-fed North ABSR pilot system performed well with an average removal of 70-80% of influent selenium. Although the current pilot plant removes less than 10% of the total selenium mass load generated by the field drainage sump, a full-scale facility, sized to treat the total drainage flow, would likely be 10 times as large, occupying a land area of between five and 10 acres.

The project goal over the next six months is to adjust operational parameters to achieve the greatest selenium mass reduction at the lowest operational cost. Selenium removal is greatest for the Mode-2 process, but the cost of adding molasses, an external carbon source, detracts from the cost-effectiveness of the system. Real-time telemetered sensors and a SCADA system for remote operation and control of the plant will be installed by summer 1999 in order to optimize plant operation and minimize chemical additions.

Related Publications


Funding

This project, which was funded initially by a Challenge Grant from the U.S. Bureau of Reclamation, is now supported by a three-year grant from the CALFED Bay-Delta Program.
Research Objectives

Designing strategies for using intrinsic microorganisms to successfully biodegrade and detoxify VOCs (volatile organic contaminants) requires a thorough characterization of key reactions at a molecular level on mineral surfaces occupied with microorganisms. This study shows that synchrotron radiation-based (SR) Fourier transform infrared (FTIR) spectromicroscopy — with a spatial resolution of 5-10 microns and strong signal to noise levels — can readily be applied to imaging characterization of the complex progress of VOC biodegradation on basaltic rock surfaces, especially the progress of the initial biodegradation.

Approach

Vesicular basalt rock samples and intrinsic microorganisms were taken from a site where VOC contamination has threatened the Snake River Aquifer near the Department of Energy’s Idaho National Engineering and Environmental Laboratory (INEEL). Toluene vapor was used as a model VOC that can be directly metabolized by intrinsic microorganisms. The SR FTIR spectra for films of microorganisms, toluene and possible toluene metabolites were measured and validated by comparison with those in the spectral literature. Basalt specimens were incubated in a closed system in the dark for a number of days. The biodegradation of toluene on specimen surfaces was monitored using SR FTIR spectromicroscopy.

Results

Global features of SR FTIR spectra for the intrinsic microorganisms, toluene and toluene metabolites were consistent with those reported in the literature. Detailed comparative analysis of spectra recorded on microbial surfaces of the coated-gold mirrors and on the cleaved basalt samples indicates the existence of distinct SR FTIR absorption bands as markers indicative of the presence of biomolecule markers (biomarkers) and of toluene and toluene metabolites.

Figure 1 shows the spatial distribution of IR absorption biomarkers associated with protein Amide I of intrinsic microorganisms (1687 cm⁻¹). The mapping was recorded on one of the basalt specimens after it was exposed to 100-ppm toluene vapor at 100% relative humidity for five days. The high intensity of the IR absorption band at 1687 cm⁻¹ implies that the intrinsic microorganisms in the basalt rock from INEEL could grow extremely quickly and form biofilms under our experimental conditions within five days. The striking similarities between the IR absorption and the optical images of the biofilms on the surface of the rock chip confirmed that SR FTIR spectromicroscopy is adequate for detecting the presence of biofilms on rock surfaces.

The spatial distributions of IR absorption associated with toluene (1029 cm⁻¹), and metabolites benzyl alcohol (1022 cm⁻
Characterization of VOC Biodegradation on Rock Surfaces by SR FTIR Imaging

Figure 2 SR FTIR mapping of microbial transformation of toluene vesicular basalt surfaces.

1) and catechol (1096 cm⁻¹) were mapped and are presented in Figure 2. The presence of these metabolites implies that intrinsic microorganisms probably degraded toluene via the pathway described in Figure 3. The absence of benzyl aldehyde and benzoic acid in our sample implies that the bottlenecks in the degradation process were the breakdown of benzyl alcohol and benzoic acid.

One-way analysis of variance was conducted to reveal the link between spatial distribution of the intrinsic microorganisms (1687 cm⁻¹), toluene (1029 cm⁻¹) and its metabolites. Results show that the link is significant for the intrinsic microorganisms (1687 cm⁻¹) and toluene (1029 cm⁻¹), with P<0.03. Similarly, the link is significant for the intrinsic microorganisms (1687 cm⁻¹) and the first metabolite benzyl alcohol (1022 cm⁻¹). However, the link is less significant as the degradation proceeds further down the degradation pathway. This lack of significant link will be the subject of a future study.

Significance of Findings

The results revealed that SR FTIR spectromicroscopy is a powerful nondestructive microprobe for direct characterization of toluene biotransformation on the surfaces of geologic materials. This novel surface analytical technique will have significant impacts in future research methodology in the field of environmental research and management.

Related Publication


Funding

This work has been supported by the Office of Science, Office of Health and Environmental Sciences, Biological and Environmental Research Program and Materials Science Division of the U.S. Department of Energy under Contract No. DE-AC03-76SF00098.
Research Objectives

Methyl tert-butyl ether (MTBE) is an "oxygenate" that is added to gasoline to promote cleaner combustion. The use of MTBE has become widespread as a result of U.S. Environmental Protection Agency programs targeted at reducing carbon monoxide and ozone air pollution. An unintended consequence of using oxygenates to control air pollution has been that service stations, fuel transfer terminals, farms and other places where gasoline is used or stored are now sources for the release of MTBE into the environment. Not surprisingly, there are many instances where gasoline spills and leaks have resulted in the contamination of groundwater with MTBE. This problem is particularly acute in California, where MTBE-containing fuels have been used since the early 1990s and groundwater resources are highly valued.

There is currently no well-established technology for treating MTBE-contaminated groundwater. The objective of this research is to develop a biological treatment technology. It has been shown that MTBE is biodegradable, therefore, biological treatment is a promising technology; however, the mechanism by which microorganisms degrade MTBE is unknown. Without an understanding of the physiology of MTBE biodegradation, the operation of MTBE biodegrading treatment systems remains hazardous and unreliable.

The objective of this ongoing research is to increase the efficiency of MTBE biodegradation in a "fluidized-bed" bioreactor. Research is being conducted to develop methods for rapid reactor start-ups and for lowering MTBE effluent concentrations from the reactor. A typical reactor start-up can take more than 100 days before MTBE removal is achieved. Furthermore, once MTBE is being removed, the removal will only be 99% efficient, whereas new regulations will require removals of 99.9% or greater.

In order to increase reactor treatment efficiency, it is necessary to understand the fundamental processes responsible for MTBE biodegradation. The hypothesis for this research is that MTBE is driven by a co-metabolic process; i.e., a process in which enzymes produced for an unrelated purpose (such as energy metabolism) can also transform MTBE by "accident." It is further hypothesized that if the proper co-metabolic additive can be found, the co-metabolite can be used to stimulate MTBE degrading microorganisms; thus, reactor start-up time can be shortened and removal efficiency can be improved.

Approach

The approach taken was to conduct field and laboratory research in parallel. Laboratory studies consisted of batch reactions in sealed vials where MTBE removal under different conditions was measured over time. Samples of full-scale, up-flow, MTBE-degrading biological reactors containing bacteria grown as a biofilm on activated carbon were transported to the laboratory and tested for stimulation of MTBE-degrading activity. Compounds tested for stimulation included gasoline components (such as toluene), suspected MTBE biodegradation products (such as tert-butyl alcohol) and contaminants commonly found in industrial grade MTBE (such as methanol). It was observed that the reactor had "iron-bacteria" in the biofilm, so conditions conducive to iron-bacteria were also tested for stimulation of MTBE degradation activity.

When a potential co-substrate was identified, field studies were conducted at the Sparks Solvent Fuel Site (SSFS) in Sparks, Nevada. MTBE-contaminated groundwater at SSFS is now being treated by a pair of six-ft-diameter Envirex/U.S. Filter up-flow, aerobic, fixed-film bioreactors. Controlled studies can be conducted in the field because the reactors are operated in parallel, allowing one reactor to be treated and the other to serve as a control. In the field tests, compounds found to be stimulants were added to one of the two reactors and the effect on the added compound on MTBE treatment was evaluated.

Results

Laboratory studies were used to evaluate the potential of more than two dozen compounds as potential co-metabolic stimulants of MTBE biodegradation (Figure 1). Organic compounds (fatty acids) known to support the growth of iron-bacteria stimulated
Stimulation of Methyl Tert-butyl Ether Biodegradation Using a Co-substrate Approach

MTBE biodegradation, whereas alcohols and gasoline components were found to have no effect on MTBE degradation when compared to controls. However, compounds used as growth substrates for iron-bacteria are also substrates for other bacteria, and the mechanism by which these compounds are effecting MTBE degradation is not well understood. Studies are currently underway to define the role of iron-bacteria, if any, in MTBE biodegradation. In addition, co-metabolic compounds are being used to enrich bacteria and fungi from the MTBE degrading reactor biofilm, and these isolates are being screened for MTBE biodegradation. Isolation of MTBE-degrading pure cultures is desirable if the fundamental mechanisms of MTBE bio-degradation are to be understood.

Field experiments were conducted to test the hypothesis that the addition of co-metabolites would stimulate MTBE biodegradation in a full-scale reactor. A review of reactor operations data demonstrated that the reactors behaved in a reproducible manner and that MTBE effluent data between the two reactors for the three months prior to testing were not statistically different. One of the two parallel reactors at SSFS was selected for treatment while the other served as a control. The treated reactor was conditioned with a high concentration of fatty acids for approximately 12 hours and then given continuous feed of a fatty acid solution over the next two days. MTBE effluent concentration was compared between the two reactors. It was found that the treated reactor out-performed the control reactor (Figure 2). The response was dose-dependent (data not shown). Based on these tests, longer term studies at multiple sites are now underway to more fully evaluate the efficacy of this co-metabolic approach for stimulating MTBE biodegradation.

**Significance of Findings**

This research is being conducted in an effort to provide innovative technology for the treatment of MTBE-contaminated groundwater. It is particularly important that the technology be applicable to the treatment of contaminated water in California and other western states, which have increasingly strict MTBE discharge limitations. We have found a co-metabolite stimulant that may allow the improved treatment of MTBE to lower levels than has been previously achievable. In addition, the discovery of this co-metabolite has given us a key with which to unlock the secrets of MTBE biodegradation. Only through a better and more complete understanding of how microorganisms degrade MTBE will we be able to develop a more efficient and robust, yet economical, treatment technology.

**Related Publication**


**Funding**

This work has been supported by Kinder Morgan Energy Partners, L.P., Vista Canyon Group, L.L.C., Envirex/U.S. Filter Co. and Varian Analytical Co.
Climate variability and carbon management research is a new addition to the Earth Sciences Division. Over the past two years we have added new staff with expertise in global and regional scale climate modeling, marine geochemistry and soil carbon cycling 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, 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 newly formed Center for Atmospheric Sciences at UC Berkeley.

In addition to recruiting the core staff for this effort and getting our research program under way, we have been successful in establishing a number of major new initiatives.

Our regional climate research group competed successfully to establish the NASA-sponsored California Water Resources Regional Atmospheric Sciences Application Center (RESAC). This Center will provide state-of-the-art real-time and forecast information (observation and simulation) on hydroclimate, water quantity and quality, and runoff-related hazards to water resources managers. It will also provide support for the ongoing regional and national assessment process by improving our understanding of specific regional features of the climate system and its impacts.

We have also been successful in establishing DOCS, the DOE Ocean Carbon Sequestration Center, in partnership with Lawrence Livermore National Laboratory, Scripps Institute of Oceanography, Massachusetts Institute of Technology, Rutgers University, Moss Landing Marine Laboratories and the Pacific International Center for High Technology Research (PICHTR). The purpose of DOCS is to conduct, focus and advance the research needed to evaluate and improve the feasibility, effectiveness and environmental acceptability of ocean carbon sequestration.

This has been a very exciting two years and we believe that this area will be a growing part of our research activities in the years and decades to come.

**Funding**

Climate Variability and Carbon Management research is funded by the U.S. Department of Energy’s Office of Science, Office of Basic Energy Sciences, Department of Engineering and Geosciences; and Office of Biological and Environmental Research; and the National Aeronautics and Space Administration.
Regional Climate Simulation
For the Western United States
Using the RCSM

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The main objectives of this regional climate simulation are to evaluate the Regional Climate System Model (RCSM) and to investigate the hydroclimate and its variability within the western United States. Results from this study will be used to compute the effects of future global climate variation in the western United States. In addition, evaluation of this multi-year simulation (also known as a hindcast) will be used to identify the strengths and weaknesses of the RCSM for future improvements. In parallel with the simulation experiment, development of a high performance version of the RCSM (RCSM.hp) is underway in collaboration with the National Energy Research and Scientific Computing Center (NERSC) at LBNL.

The focus of this hydroclimate simulation experiment is to study precipitation, snow budget and soil moisture variations that significantly affect human activities and natural environment in the western United States.

Approach

To generate the western U.S. hydroclimate, we downscaled the global analysis data from the National Center for Environmental Prediction (NCEP) at 2.5° x 2.5° resolution to a 36 x 36 km² resolution (Figure 1). This intermediate-resolution climate data will be further downsampled to a 12 x 12 km² resolution for a California-Nevada domain when the RCSM.hp is completed. The NCEP global analysis data, together with the global analysis data from the European Center for Medium-Range Weather Forecasts (ECMWF), is regarded as the most accurate large-scale data available. However, spatial resolution of both analysis data is too coarse for detailed regional impact assessments.

The Mesoscale Atmospheric Simulation (MAS) model is the limited-area atmospheric model of the RCSM. The MAS has an accurate advection scheme and comprehensive physics including short- and longwave radiation, convection, cloud microphysics and cloud-radiation interaction. The MAS is being used to simulate regional hydroclimates of the western United States and eastern Asia. It is continuously improved for better physics and numerical features.

The Soil-Plant-Snow (SPS) model calculates land-surface processes in the RCSM. The RCSM predicts soil moisture content, soil temperature, water-equivalent snow cover and canopy water content. It also calculates skin temperature and surface wetness, and drainage of soil water into deep ground. It needs data for soil texture, vegetation characteristics and initial guesses for soil moisture and temperature. The initial guesses for soil moisture and temperature were obtained from the NCEP global analysis data. The land-surface and vegetation characteristics were obtained from satellite-based monthly-mean data for leaf area index and green-leaf fraction data. This recent monthly vegetation data from the NCEP/NASA has eliminated much uncertainty and resulted in a significant improvement in the RCSM-simulated surface energy and water budget.

Precipitation and atmospheric forcing simulated by the MAS and SPS are processed to compute the area-averaged forcing data for the RCSM hydrologic models (spatially-distributed TOPMODEL and the spatially-lumped Sacramento model) using an area-matching method. This method preserves the total water/energy between the MAS model and hydrologic models in a way consistent with the basic assumptions of the models. Accurate area-matching is important for quantitative precipitation simulations in the western United States, where steep terrain generates a large spatial gradient in precipitation.

The western U.S. climate simulation starts in 1979 and covers the next 10-15 year period to capture several wet/dry periods in recent years. Due to an extensive requirement for computational resources, the actual period of this simulation will be determined by the available computational resources.

This preliminary study examined the atmospheric physics formulations for a long-term climate simulation. Different schemes for atmospheric physics, most importantly for cumulus convection, in the MAS can cause a significant difference in the simulated regional climate. The MAS is equipped with two convection schemes: the simple Anthes scheme and the Simplified Arakawa-Schubert Scheme (SAS). The SAS scheme, even though it is more physically based than the Anthes scheme, includes many tuning parameters. Most of these parameters are empiri-
Regional Climate Hindcast for the Western United States Using the RCSM

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Regional Climate Hindcast for the Western United States Using the RCSM and were obtained from observational studies taken in the Great Plains. As the storm environment and the resulting storm structure widely vary according to location, existing parameters may not be suitable for the western United States. Hence, rigorous evaluation of model results and sensitivity tests are important for a successful simulation of long-term regional climate simulation.

A preliminary evaluation of the RCSM is presented below.

Results

We have completed an initial evaluation of the RCSM for a long-term climate simulation. In this study, we used the SAS scheme with the parameter values currently employed by the NCEP for medium-range global forecasts.

Figure 2 illustrates a comparison between the observed and simulated daily-mean precipitation within California during the first 150 days of 1979. The observational data was from the co-op stations within California. For each month, 400-500 stations were available for comparison. We interpolated the simulated precipitation to match the location of each station, as precipitation varies rapidly over a mountainous terrain.

The MAS has well-simulated the daily precipitation events in California. Figure 2 shows that every observed precipitation event is present in the simulated precipitation, except the last event where the MAS has underestimated precipitation. This indicates that the dynamic framework of the MAS is capable of accurately handling the tendency of the large-scale flows imposed through time-dependent lateral boundary conditions.

The amount of precipitation is also generally well-simulated. The agreement between the observed and simulated values are especially good for January and February (Julian days 1-60). Precipitation was underestimated during the spring time from late March to May. This underestimation was partially corrected in the experiment using the Anthes scheme instead of the SAS scheme (not shown).

The simulated snow budget was also consistent with the observations. The simulated maximum snowfall occurred in January and February while the maximum snowmelt was in April and early May. The simulated snowcover was totally depleted at the end of June. Such variation of the snowcover is consistent with the observation in which snow remains only at high elevations after June.

Significance of Findings

The agreement between the observed and simulated climate features in this preliminary experiment indicates that the RCSM is capable of long-term climate simulation. Observed precipitation events and the amount of precipitation is well-simulated by the MAS. The surface snow budget by the SPS is also consistent with the observation. Underestimation of spring precipitation could be partially corrected by using the Anthes convection scheme instead of the SAS scheme. However, it needs more investigation to select a convection scheme most suitable for the western United States region. Long-term climate and streamflow simulation and development of a high-performance version of the MAS are currently underway.

Related Publications


Funding

This work has been supported by the Laboratory Directed Research and Development Program of Lawrence Berkeley National Laboratory under U.S. Department of Energy Contract No. DE-AC03-76SF00098.
The Regional Climate Center

Research Objectives

The objectives of the Berkeley Lab Regional Climate Center (RCC) are to provide downscaled climate research and applications to a specialized and general user community. Understanding climate variability and change at the scale of impacts requires analyzed simulations at a range of scales and comparison to past climate observations.

Approach

The core capability of the RCC is the Regional Climate System Model (RCSM). The RCSM (Figure 1) consists of pre- and post-processors that nest a suite of process models capable of producing hydroclimate products at short-term (two-three day), seasonal and long-term (downscaled 2 x CO2 scenarios) time scales. RCSM output is used for research, climate and weather forecasts, sensitivity analyses and impact assessments. We have a growing group of collaborators (regional, national and international) researching topics related to hydroclimate. The Regional Climate Center is currently working toward the advancement of mesoscale atmospheric simulations, distributed hydrologic simulations, landslide initiation, water quality, and sediment transport. Established partnered RCC collaborations include:

- Southwestern streamflow simulations with the National Weather Service's California Nevada River Forecast Center
- Identification of flooded central California valley and other sensitive regions via remotely sensed data from the National Aeronautics and Space Administration and the National Oceanic and Atmospheric Administration.
- Development of a shared information distribution system with DOE/ACPI collaborators.
- Annual Southwestern Significant Results Conference with the University of Arizona at Tucson's Institute for the Study of Planet Earth.

Figure 1. The Regional Climate System Model (RCSM) consists of a pre-processor (input data), process models and post processors (output data and analysis, visualizations and assessments).
Results

During 1998 we have reported on hydroclimate studies in the southwestern United States and eastern Asia (Kim et al., 1998). In 1999, results from ongoing climate research, a new deep groundwater flux parameterization and our northeastern Australian collaboration have been submitted for publication. We simulated California precipitation and streamflow during the 1997-1998 El Nino winter with good model skill for 48-hour forecasts. The experimental seasonal forecasts still require further refinement. The new deep groundwater flux parameter has improved the hydrologic model calibration and verification. Downscaled hindcast (control) and projected double-CO₂ simulations have started as part of the U.S. National Assessment Report.

Significance of Findings

The establishment of the Berkeley Lab Regional Climate Center represents an important advancement for the Berkeley community of climate researchers, as well as the California and southwestern region of climate information users. Our results are part of the U.S. National Assessment Report, the California Assessment Report, and the Southwestern Assessment Report of the U.S. Global Climate Change Research Program, and the Climate Change and California Ecosystems report of the Union of Concerned Scientists and the Ecological Society of America. Through our Eastern Asian project, we are representing hydroclimate issues related to sustainability in China at the U.S./China Water Workshop and the Third International Conference on the Global Energy and Water Cycle. Components of the Berkeley Lab RCSM have been implemented at the Korean Meteorological Administration and the Australian Department of Natural Resources. We view these activities as part of a growing climate research and applications collaborative initiative at Berkeley Lab with UC Berkeley, other UC institutions, Department of Energy labs and other government, university and private groups.

Related Publications


Funding

This work has been supported by the Laboratory Directed Research and Development Program of Lawrence Berkeley National Laboratory under U.S. Department of Energy Contract No. DE-AC03-76SF00098; by the Administrator of the National Aeronautics and Space Administration, NASA Earth Science Enterprise; and by the University of California Campus-Laboratory Collaboration Hydrology Project.
Climate Change and Wildfire Severity in California

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Research Objectives

Insurers are acutely aware that 85 percent of catastrophe-related payouts are due to natural disasters, with claims averaging about $10 billion per year worldwide over the past decade (Mills, 1998). A recent study by the Insurance Services Office (ISO), entitled "The Wildland/Urban Fire Hazard," concluded that wildfires are a pervasive insurance risk, consuming an average of five million acres per year across the United States at an average insured cost of about $300 million per year. Insurers feel the effects of wildfire in several ways. Insured property is at risk, and in some cases, the costs of fire-fighting or lost timber are underwritten. Wildfire-related injuries or loss of life also exact a cost from insurers. Moreover, in the aftermath of wildfire, secondary events, such as landslides, flooding and water quality impairment can all impose additional costs. The insured damages are only a component of the total economic loss and do not reflect the full human hardship that wildfires can cause.

The powerful impact that climatic anomalies can have on wildfire was demonstrated last year after droughts, linked to El Niño, were followed by widespread, devastating fires in Florida, Indonesia and elsewhere. The latest predictions suggest that global warming may also create conditions that intensify wildfire danger by warming and drying out vegetation and by increasing windspeed. This project asks the question: what effect will climate change—as predicted by climate simulation studies performed by general circulation models (GCMs)—have on the magnitude of wildfires in northern California?

Approach

To explore this question, we combined California weather and fire data and validated fire and fire suppression models and state-of-the-art general circulation models. The analysis produced a geographically-specific estimate of the potential effect of climate change on wildfires, including the effectiveness of fire-fighting infrastructure.

To capture some of the complexity of California's landscape, this study examined three climatically-distinct and geographically-separated areas of northern California: Santa Clara, near San Francisco Bay; Amador-El Dorado, in the Sierra foothills; and Humboldt (on the northern coast (Figure 1)). The regions studied contain substantial areas of wildland/urban interface conditions on the margins of the San Francisco Bay area, the Sacramento metropolitan area and the redwood region's urban center of Eureka. El Dorado is the fastest growing county in California and Amador is the sixth-fastest growing county in the state.

The analysis was accomplished with an innovative coupling of California Department of Forestry wildfire models with the Goddard Institute for Space Sciences GCM, plus site-specific data on actual fire-starts over a six-year historical period. The number, location and timing of fire starts was not changed in the analysis; rather fire behavior and fire suppression were simulated with present climate (1 X CO2) and future climate (2 X CO2) GCM scenarios.

Results

According to our analyses, climatic change would cause fires to spread faster and burn more intensely in two of the three regions. The biggest impacts were seen in grassland, where the fastest spread rates already occur. In forests, where fires move much more slowly, modeled impacts were less severe. The response of chaparral brush and oak woodlands fell between that of grass and forest. The reason that faster fuels respond more is that fire behavior in these fuels is more sensitive to wind speed, and elevated wind speed during fire season was a striking feature of the...
Climate Change and Wildfire Severity in California

changed climate weather data. Summarizing over all vegetation types, predicted global warming results in a greater number of fast fires and fewer slow fires.

Future changes in fuel moisture and wind speeds also cause modeled fires to burn with greater intensity, triggering more intensive suppression efforts. The utilization of extra fire suppression resources at high dispatch level, such as air tankers and bulldozers, can lead to large increases in suppression costs. In addition, even increased dispatch of the available fire-fighting equipment and personnel could not always compensate for the effect of warming on the number of acres burned and the number of "escape" fires (those that exceed size or time limits, such as those that burn more than 300 acres in grasslands; Figure 2).

The faster, hotter fires caused by climatic change outran fire suppression and many more acres were burned than in the current climate scenario in two out of three regions. In the Santa Clara region, for example, contained fires in grass and brush burned 41% and 34% more area, respectively, under climate change than they did in the present climate. The number of escaped wildfires increased by 53% and 21% in grass and brush.

In the Sierra foothills, the effect of climatic change was even more severe. Here, the number of potentially catastrophic (escaped) fires predicted went up dramatically—143% more each year in grassland and 121% more in brush. With the number of escaped wildfires more than doubling, climatic change could lead to a serious jump in fire damage in this region.

Climate change had little impact in California's Humboldt redwood region, thanks to predictions of a wetter, less windy climate.

Significance of Findings

This report describes a geographically specific estimate of the potential effect of climate change on wildfires and the effectiveness of fire-fighting infrastructure in California. The regions studied contain substantial areas of wildland/urban interface near the San Francisco Bay area and the Sacramento metropolitan area as well as forest resources in Humboldt and Del Norte counties. Our results showed that global warming predictions lead to a greater risk of wildfire damage in California, by causing more flammable fuel conditions and faster fire spread rates. As indicated by the models, in most cases climate change would lead to dramatic increases in both the land area burned by California wildfires and the number of potentially catastrophic fires—more than doubling these losses in some regions. Several important climate-wildfire interactions not currently captured by these models would amplify the expected growth in wildfires. The growth in wildfire damages would occur despite deployment of fire suppression resources at the highest current level, suggesting that climatic change could cause an increase in both fire suppression costs and economic losses due to wildfires.

Related Publications


Funding

This work has been supported by the U.S. Environmental Protection Agency, Atmospheric Pollution Prevention Division, via the Assistant Secretary for Energy Efficiency and Renewable Energy, Office of Building Technologies and State Community Programs, of the U.S. Department of Energy under Contract No. DE-AC03-76SF00098.
A Simple Physical Model
Of the Global Hydrologic Cycle: Implications for Paleothermometry

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Research Objectives
Significant environmental policy decisions rest on our ability to predict future climate conditions. Because water vapor is one of the most important greenhouse gases it is important that we understand the global hydrologic cycle and its connection to the earth’s climate. Ice cores contain long records of the hydrologic cycle through oxygen and hydrogen isotopic ratios (normally expressed as $\delta^{18}O$ and $\delta^D$). Most climate reconstructions assume that isotopic ratios are a unique proxy for temperature and use the relationship observed between $\delta^{18}O$ of snow and mean annual temperature in the present climate to extrapolate to temperatures throughout the ice core record. However, isotopic ratios may be dependent on climatic parameters other than temperature, in which case, the present temperature-isotope correlation may not apply to past climates. The objective of this research is to (1) develop a relatively simple model of latitudinal moisture transport and use it to evaluate the physical mechanisms that play dominant roles in determining $\delta^{18}O$ and $\delta^D$ of precipitation, and (2) reevaluate the isotopic data from polar ice cores in terms of paleotemperature and other climatic parameters.

The heavy isotopes, $^{18}O$ and $^2H$ (D), systematically decrease in abundance in precipitation falling in regions of decreasing mean annual surface temperature because of isotopic fractionation that occurs at every evaporation and condensation step in the hydrologic cycle. Heavy isotopes are most depleted in Antarctic precipitation, in which there is also a nearly linear relationship between $\delta^{18}O$ and surface temperature, $T$. The linear relationship is typically attributed to Rayleigh distillation, which is a simple conceptual model that neglects all complexities of atmospheric water vapor transport. Simple Rayleigh models over-predict the depletion of heavy isotopes with decreasing temperature. By contrast, general circulation models (GCMs) produce reasonably good fits to the modern $\delta^{18}O$ -temperature relationship, but are too complex to clearly elucidate the controlling mechanisms. Our model expands on Rayleigh models by including the physical processes of evaporative recharge during water vapor transport and variations in the transport mechanism. However, this model is still significantly less complex than GCMs allowing simple and direct tests of climate parameters.

Approach
We start with a relatively simple conservation statement describing the essential transport processes that affect isotopic fractionation. The concentration of water in the atmosphere, $w$, is described by:

$$\frac{\partial w}{\partial t} = \nabla \cdot (D \nabla w) - \nu \nabla w + E - P \quad (1)$$

The first term on the right hand side is transport due to eddy (diffusive) processes, and the second term is transport due to advection. The third and fourth are source/sink terms: evaporation from the ocean and land surfaces ($E$) and precipitation ($P$), respectively. By treating isotopes as different species, analogous equations for the isotopic ratios are derived.

Isotopic fractionation ultimately is caused by the fact that cold air holds much less water than warm air. As moisture is transported from warm to cold areas, precipitation must exceed evaporation and the net “rainout” of atmospheric moisture causes isotopic fractionation. Isotopic gradients in precipitation follow temperature gradients, which are primarily a function of latitude. Consequently, the $\delta^{18}O$ values of precipitation are high near the equator and very low at the poles. The simplest description of the earth, therefore, is a one-dimensional version of Equation 1 in spherical polar coordinates, with the single spatial variable being latitude. This is valid for the Southern Hemisphere because Antarctica is a large landmass centered approximately at the South Pole. Since we are examining long-term averages, we also use the steady state approximation ($\partial w/\partial t = 0$). Equation 1 therefore implies that three processes control fluxes and isotopic ratios in precipitation: evaporation from the ocean surface, eddy-diffusive transport, and advective transport.

Results
In the Southern Hemisphere, at latitudes poleward of $45^\circ$S (average annual surface temperatures less
than 10°C, evaporation rates drop significantly and δ18O and δD of precipitation decrease quickly as air loses moisture due to decreasing temperature. Because evaporation rates are low, the relative amount of diffusive versus advective transport determines the rate of decrease in δ18O and δD since transport by eddy-fluxes induces less fractionation than transport by advection (Figure 1). δ18O of Antarctic surface snow generally falls between the predicted results for transport by eddy-fluxes only and the results for transport by advection, indicating that isotopic ratios in precipitation might be useful for determining transport mechanisms in Southern high latitudes.

Results of sensitivity tests reveal that isotopic composition of precipitation in polar regions is very dependent on the amount of water vapor over the continent and on the surface temperature. Other climatically driven changes in the variables that affect the hydrologic cycle, such as changes in the location of the evaporation source, decreases in sea surface temperature or variations in the total annual precipitation, do not have a large effect on the values of δ18O and δD, but do affect the relationship between δ18O and δD in precipitation, which is very accurately known from observations.

**Significance of Findings**

Using this model, we estimate changes in δ18O and δD for changes in global temperature, including temperature changes that are thought to be representative of the transition from the last glacial maximum to the Holocene. As expected, the model shows that significant changes in δ18O and δD have occurred in response to changes in the annual average surface temperature and in response to changes in the temperature gradient between the equator and the South Pole. Model trials with linear changes in the equator-to-Vostok temperature gradient were used to estimate likely ranges of temporal δ8O-Τ relationships at three locations: 70°S in Western Antarctica near the coast, the South Pole and Vostok (the coldest, most remote location in Antarctica (Figure 2). The resulting ranges in δ18O are bounded by pure eddy-diffusive transport for the smallest slope and by advective transport for the largest slope, demonstrating again the importance of including the transport mode in atmospheric models.

Two important general results are represented in Figure 2. The first is the difference in temporal relationship between δ18O and local surface temperature for the three locations. This implies that a universal relationship between isotopic composition and local surface temperature does not exist and that the present-day spatial relationship is not generally applicable to paleotemperature estimates. The second is the increased sensitivity to temperature changes with distance from the coast. In general, the isotopic ratio is most sensitive to temperature at locations far inland, such as the South Pole and Vostok, and is very weakly dependent on temperature at coastal locations, such as the Antarctic Peninsula. Our results suggest that, at locations other than Vostok, temperatures during the last glacial maximum were substantially lower than has been previously estimated based on δ18O data and the modern spatial relationships.

**Related Publications**


**Funding**

This work has been supported by the Laboratory Directed Research and Development Program of Lawrence Berkeley National Laboratory under U.S. Department of Energy Contract No. DEAC03-76SF00098.


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