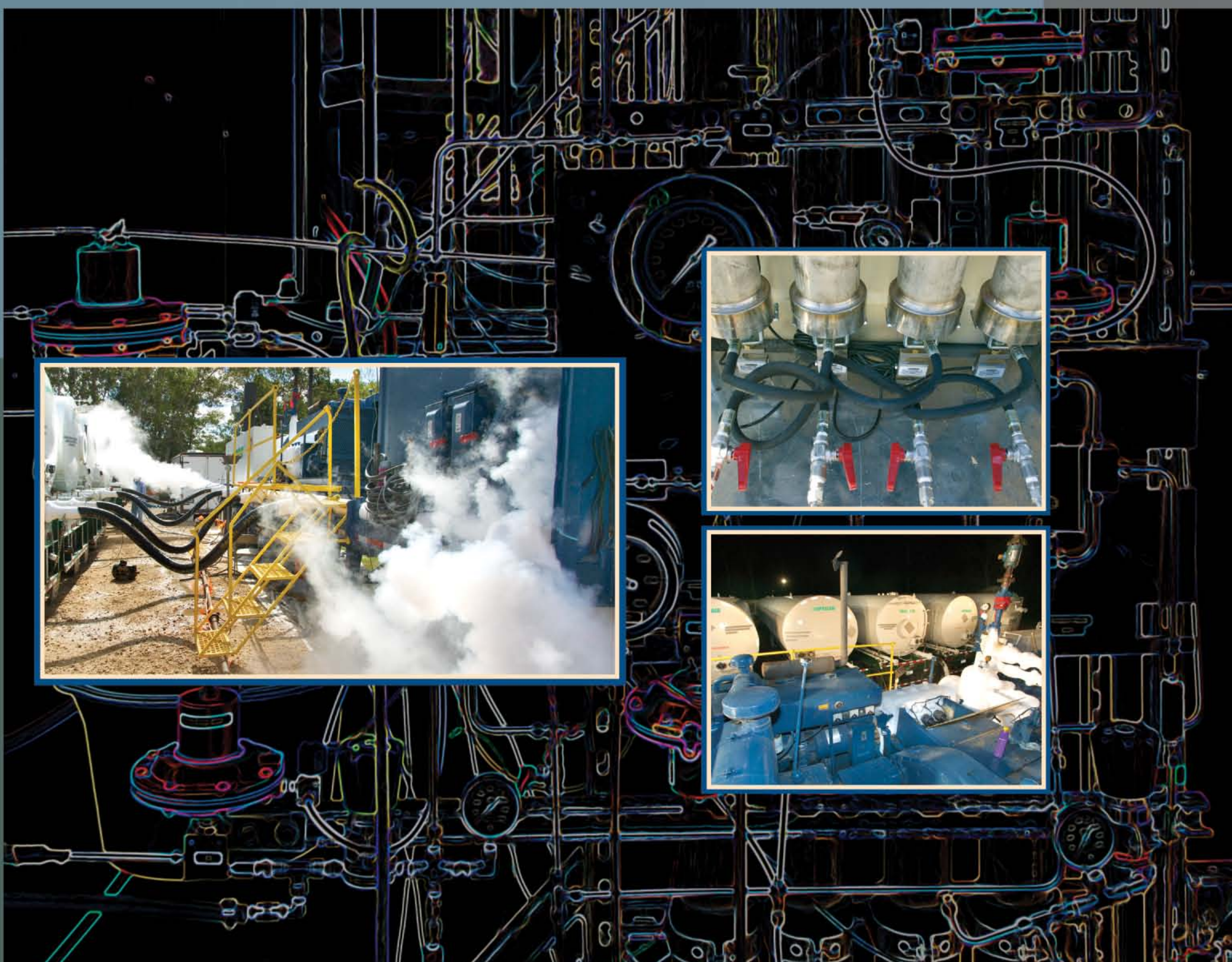
LBNL-59633

EARTH SCIENCES DIVISION
RESEARCH SUMMARIES
2004-2005



ERNEST ORLANDO LAWRENCE
BERKELEY NATIONAL LABORATORY

LBNL-59633

Earth Sciences Division

Research Summaries

2004–2005

Berkeley Lab
http://www-esd.lbl.gov/

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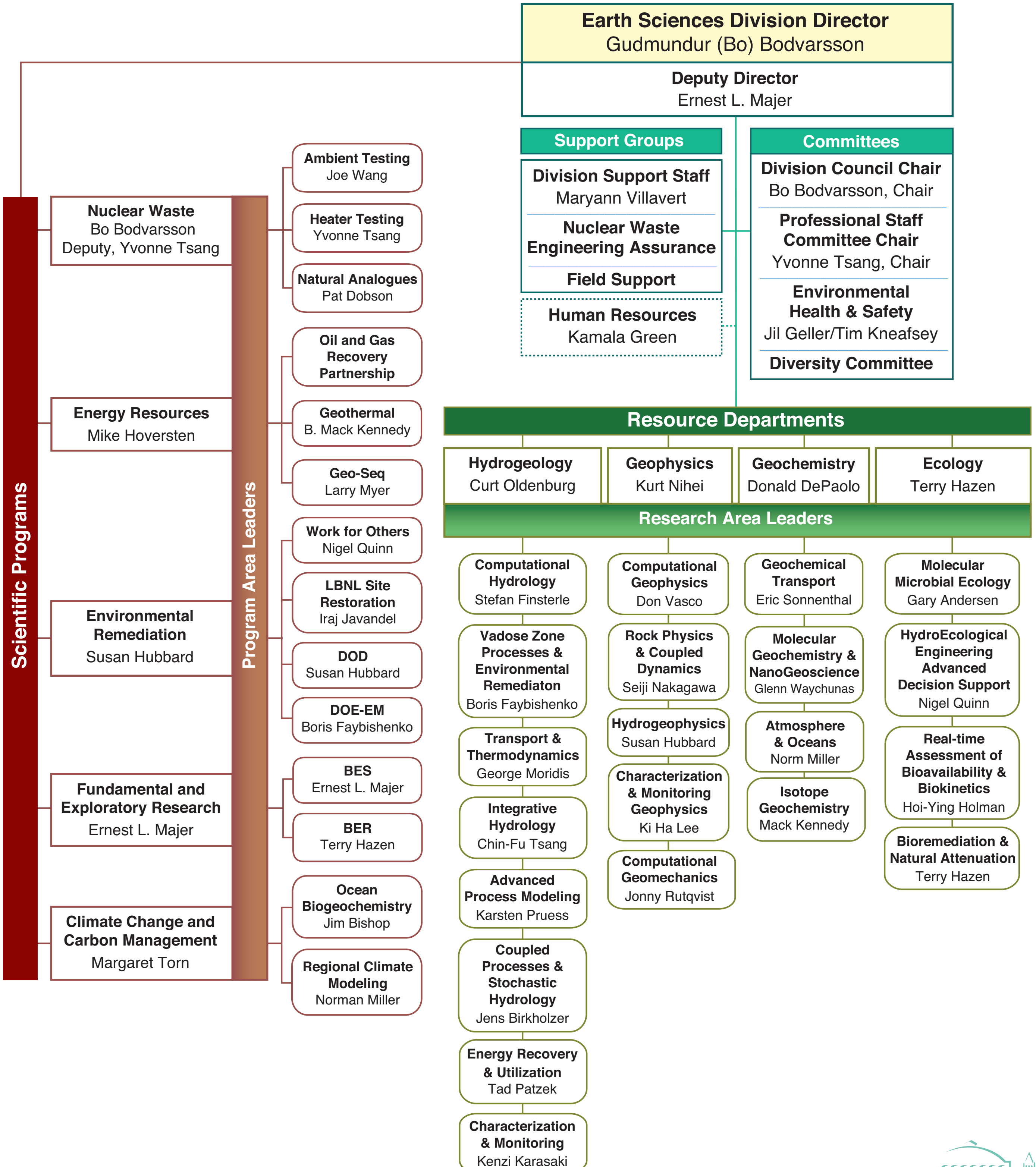
Earth Sciences Division Organization Chart



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Ernest Orlando Lawrence Berkeley National Laboratory

Earth Sciences Division Research Summaries 2004-2005

A Perspective from the Division Director

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Research in earth and atmospheric sciences is becoming increasingly important in light of the energy, climate change, and environmental issues facing the United States and the world. The development of new energy resources other than hydrocarbons and the safe disposal of nuclear waste and greenhouse gases (such as carbon dioxide and methane) are critical to the future energy needs and environmental safety of this planet. In addition, the cleanup of many contaminated sites in the U.S., along with the preservation and management of our water supply, remain key challenges for us as well as future generations. In order to address future energy and environmental issues, we think that it is critical to integrate the earth sciences and disciplines in a timely fashion. This will involve focusing on fundamental, crosscutting science common to many energy and environmental issues. A primary focus will be the characterization, imaging, and manipulation of fluids in the earth. This addresses many DOE applications, from environmental restoration to energy extraction and optimization.

The Earth Sciences Division (ESD) of the Ernest Orlando Lawrence Berkeley National Laboratory (Berkeley Lab) is currently addressing many of the key technical issues described above. Our total staff of over 200 scientists, UC Berkeley faculty, support staff and guests—performing world-acclaimed fundamental research in hydrogeology and reservoir engineering, geophysics and geomechanics, geochemistry, microbial ecology, and environmental engineering—provide the foundation for all of our programs. Building on this scientific foundation, we perform applied earth science research and technology development to support the Department of Energy in a number of its program areas, namely:

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

In this document, we present summaries of many of our current research projects. While it is not a complete accounting, it is representative of the nature and breadth of our research effort. We are proud of our scientific efforts, and we hope that you will find our research useful and exciting. Note that sound health and safety practices are critical to all our research.

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

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

These programs draw from each of ESD's disciplinary departments: Ecology, Geophysics, Geochemistry, and Hydrogeology. Short descriptions of these departments are provided as introductory material. A list of publications for the period from January 2004 to September 2005, along with a listing of our personnel, are appended to the end of this report.

ACKNOWLEDGMENTS

We gratefully acknowledge the support of our major sponsors in the Department of Energy, which include the Office of Science, the Office of Fossil Energy, the Office of Energy Efficiency and Renewable Energy, the Office of Civilian Radioactive Waste Management, and the Office of Environmental Management. We also appreciate the support received from other federal agencies such as the Bureau of Reclamation, the Department of Defense, the Environmental Protection Agency, and NASA. Lastly, we must also acknowledge and thank our industrial collaborators, who provide both financial and in-kind support through various partnership projects, and who bring additional ideas, data, and experience to ESD.

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Earth Sciences Division Operations and Facilities

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OUR ORGANIZATION

Management (and Name) Changes

In 2001, the Earth Sciences Division (ESD) Director G.S. (Bo) Bodvarsson developed a strategic succession plan that rotates on an approximately three-year term for department head appointments. This plan, an important priority for ESD, will prepare our current and future leaders (who make up our Division Council) for management responsibilities. The program head appointments are indefinite.

During the 1st quarter of 2004, Susan Hubbard was appointed Environmental Remediation Program Head (formerly held by Terry Hazen). By the 4th quarter of 2005, Kurt Nihei, the Geophysics Department Head, completed his appointment and additionally, Mike Hoversten stepped down as the Energy Resources Program Head. Ernie Majer is currently acting in both positions, and a search is currently under way for candidates to assume these roles.

Additionally, in early 2004, Bo tasked the Division Council to come up with new department names that were short, to the point, and easy to remember. They are as they appear now on the Organizational Chart (refer to p. ii).

New Laboratory Leadership

In August 2004, the new Berkeley Lab Director, Dr. Steven Chu (Nobel Laureate in Physics), took office. By early 2005, the Earth Sciences Division moved organizationally into a new Associate Laboratory Directorate (ALD) called “Life and Environmental Sciences,” which includes the Life Sciences and the Genomics Divisions. Regardless of how we are organized, we continue to collaborate with the other divisions outside of this new ALD assignment. These include Physical Biosciences, Environmental and Energy Technologies, Engineering, and Physics Divisions. For more information on Berkeley Lab’s organization, please visit http://www.lbl.gov.

OUR SAFETY-CONSCIOUS WORK ENVIRONMENT

The ESD approach to safety includes Berkeley Lab’s Integrated Safety Management model. This model identifies the individual employee as the first person accountable for his or her own health and safety, augmented with a Division Safety Coordinator who in turn works with a Berkeley Lab Environmental Health and Safety Liaison, to maintain an open line of communication with Berkeley Lab's Environmental Health and Safety Division. Because ESD has a matrix structure, the employee works with both supervisors and principal investigators to identify, manage, and elevate issues to the ESD Safety Coordinator, Department Head, and Division Director. Additionally, the ESD Safety Committee meets regularly to discuss ESD and Berkeley Lab issues.

In August 2004, Jil Geller was appointed the new ESD Safety Coordinator. Tim Kneafsey was assigned as the new ESD Safety Committee Chair. Since this time, ESD’s safety program has continued to grow with increased visibility, awareness, and proactive communication. We also revamped our Health and Safety website (at http://www-esd.lbl.gov/ESDEHS/index.html), giving it a new look and easy access to forms, reports, and other key documents developed by our staff.

Safety will always be a top priority for ESD. We attribute the success of our safety program to all our staff, which has been very cooperative and pro-active in resolving safety issues, providing suggestions on improvements to safety practices, and implementing changes that result in a safer work environment.

TRAINING AND DEVELOPMENT

EHS26 for Managers & Supervisors is a safety training class that was initially developed for Berkeley Lab’s Operations Department (known as EHS20). ESD participated in a successful pilot program for EHS26 to refocus ESH concepts to scientific divisions. This class provided a forum to discuss real-life case studies and emphasize ESD’s Integrated Safety Management.

ESD Mentoring & Supervising was a class developed by Chin-Fu Tsang and Susan Hubbard. Bodvarsson and the Division Council feel that mentorship is an important role for supervisors and senior staff scientists, to ensure succession planning and maintain the livelihood of ESD’s scientific mission for Berkeley Lab. This course covered all aspects of mentoring and supervising, from hiring a new employee, helping the employee develop into capable and independent scientists, and mentoring employees to help find their place in ESD and identify professional opportunities.

TECHNOLOGY TRANSFER

In recent years, the ESD has successfully licensed several of its software codes, such as Tough-Fx and Tough-Fx / Hydrate Software and EM2D_INV. These codes and others are available for purchase through Berkeley Lab's Technology Transfer Department. ESD is continuing to identify and develop more technologies that can be licensed. To learn more about Earth Sciences and Berkeley Lab's available licensed technology, go to http://www.lbl.gov/Tech-Transfer/

The LBNL Award for Excellence in Technology Transfer is given by Berkeley Lab's Technology Transfer Department and recognizes inventors whose technologies, by virtue of being licensed to the private sector, bring significant benefit to society.

Inventors/ Developers/ Contributors	Technology	ESD Department (unless in parenthesis)
2005 LBNL Award for Excellence in Technology Transfer		
Greg Newman	EM2D_INV	Geophysics
Hoi-Ying Holman	A Reflectance-Absorption Spectroscopy Device To Evaluate Abnormal Tissue	Ecology
George Moridis, Stefan Finsterle, Michael Kowalsky, Karsten Pruess	Tough-Fx and Tough-Fx / Hydrate Software	Hydrogeology
2004 LBNL Award for Excellence in Technology Transfer		
Chris Doughty, Frank Hale (NERSC), Chin-Fu Tsang	Bore II Software	Hydrogeology (National Energy Research Scientific Computing Center--NERSC)

A DIVERSE WORKFORCE

One of ESD's primary goals is to create a supportive environment to attract, nurture, and retain the most qualified and diverse workforce, including under-represented group members. Working closely with Berkeley Lab's Workforce Diversity Office and the Center for Science and Engineering Education (CSEE), we have created a working Diversity Plan, within which we continually evaluate and identify the necessary tools to support and enrich our workforce.

As mentioned in the Training and Development Section, we recently provided our staff with a Mentoring and Training course. This is a great step in creating an avenue for ways to retain staff through the career development process. Additionally, a Verbal Communications course was developed to nurture our staff whose native language is not English. This course is currently in development to include other Berkeley Lab divisions that have recently expressed interest in participating.

ESD FACILITIES /CENTERS

Center for Computational Seismology

The Center for Computational Seismology (CCS), which focuses on geophysical computing research, maintains a state-of-the-art computing environment in support of various seismological and geophysical research programs, in particular the development of new methods for imaging the subsurface and its processes, and methods for visualizing results. A wide variety of modern software and hardware is developed and maintained to support this high-level research. In addition to the many "in-house"-developed codes (3-D modeling, forward and inverse codes, etc.), we use a wide variety of commercially supported packages, including CogniSeis Focus (interactive 3-D seismic processing), Baker-Atlas SEISLINK (VSP and crosswell imaging), GeoQuest GXII (interactive raytrace modeling for surface and borehole data), Lynx (geologic modeling), Earthvision (Dynamic Graphics) AVS (3-D visualization), and the complete Promax/Landmark processing and modeling software.These packages provide a powerful modeling base upon which we build our specialized codes.

Our facilities support research focused on subsurface imaging, using active and passive sources at scales ranging from meters to whole-Earth dimensions. Research activities include the processing and interpretation of vertical seismic profiles (VSP) for fracture detection and fault delineation, induced seismicity associated with energy resources, seismic reflection imaging, single well and crosshole seismic profiling for 2- and 3-D imaging, fracture detection between wells, and processing/analysis of micro-earthquake data for imaging of geothermal fields. The hardware facilities include multiple Exabyte tape drives, over 8000 Gbytes of hard drive storage, a 24-inch color Versatec plotter, a 36-inch HP color plotter, and multiple X-terminals and workstations. We have recently upgraded our computer system to the new SUN series 4-CPU server, with10 GByte of memory and 4 Tera bytes of disk. We also recently acquired a "pc cluster" with 128 nodes (2 cpu per node) at 3.6 GHz and 4 Gbyte memory per node. In addition, the CCS facility is linked to the National Energy Research Supercomputing Center at Berkeley Lab, which hosts a variety of supercomputers available for use.

Geophysical Measurements Facility

Our field work is supported by the Geophysical Measurements Facility (GMF), a DOE-supported facility designed to develop and maintain a variety of geophysical and geoscience instrumentation and measurement equipment. For example, research on piezoelectric sources and borehole sensor arrays, as well as high-frequency seismic recording, has been supported by GMF for over 10 years. GMF is the focal point for an extensive inventory of complex scientific equipment used for Berkeley Lab projects, with responsibility for the maintenance, upgrading, training, and field operations of this hardware. GMF will allow for management of the full complement of sophisticated field instrumentation and associated support vehicles necessary to test and develop a piezoelectric multi-source phased array. GMF maintains a state-of-the-art multidisciplinary field instrumentation facility in support of various environmental, geophysical, and hydrogeological research programs at Berkeley Lab. This facility also assists in development of new instrumentation and field methods for investigating the subsurface and its processes by providing professional in-field technical support for scientific staff and management of the complex and varied field studies required in scientific research programs. The GMF includes electronic and mechanical technicians and shop facilities, field support vehicles, (including wireline and recording trucks), and a three borehole test facility.

Soil and Rock Properties Laboratory

At Berkeley Lab's Soil and Rock Properties Lab, electrical resistivity, ultrasonic wave propagation, and hydraulic conductivity can be measured in a triaxial cell equipped to measure all these parameters simultaneously. Confining and axial stresses are set independently to represent in situ states of stress. The cell is designed to handle samples from 3-inch-diameter Shelby tubes, using sample transfer techniques developed from geotechnical practice. The sample is jacketed with a flexible membrane, either latex, viton or teflon, depending on the sample texture and fluid composition. Sample length is determined by considerations of ultrasonic wave attenuation and the extent of stratification of the core. Typically, samples of approximately 5 cm lengths are used, although different lengths can be accommodated. The advantage of making these measurements simultaneously on the same sample is that disturbance from sample transfer between test cells, a particular concern for unconsolidated samples, is avoided. The endcaps of the test cell contain 1 MHz piezo-electric crystals for P- and S-wave transmission and receiving, flow ports, and pressure ports. Porous aluminum plates between the sample and the end-caps provide even flow distribution over the sample cross section.

Electrical resistivity is measured by the four-electrode technique. Both faces of the aluminum plates are gold coated. Electrical current is driven through the outside faces, and voltage drop is measured from the inside faces; a GenRad 1692 RLC Digibridge supplies current and measures voltage drops at five test frequencies varying from 100 Hz to 100 kHz. P-wave and S-wave propagation (velocity and attenuation) is measured by the pulse-transmission technique.

Voltage pulses are generated by Cober Model 605P High Power Pulse Generator (Cober Electronics, Stamford, Connecticut), and data are acquired via a 40 MHz Gagescope data acquisition board (Gage Applied Sciences Inc., Montreal, Quebec) installed in a PC. Hydraulic conductivity is measured either by the constant head method for more permeable samples, or by the falling head method for tighter samples. Differential pressure across the column is measured with variable reluctance transducers (Validyne, Northridge, CA). When possible, site water is used for the hydraulic conductivity measurements to avoid dispersion of clays. Otherwise, test water is generated based upon a chemical analysis of the site water.

In addition to the above facilities, a high resolution x-ray facility (linear x-ray and CAT scan) and NMR imaging facility was added in 2000 for detailed core studies and simultaneous flow and transport studies. In 2003, further capability was added by linking these studies with ultra-high-resolution tomographic work at Berkeley Lab's Advanced Light Source.

For more information on CCS, GMF, or the Rock Lab, please contact Ernest L. Majer, phone: 510-486-6709, elmajer@lbl.gov

Berkeley Lab Center for Environmental Biotechnology Core Facility

The core microbiology facility of Berkeley Lab is in the Center for Environmental Biotechnology, located in Building 70 and 70A. The 11-laboratory unit, which occupies a total area of 6,000 ft^2, is set up for Class II, Type A/B3 molecular, microbiology, and tissue culture work. Level 1 quality and safety assurance procedures are in place. The following work-specific equipment and instruments are available in this facility:

- Omnilog Phenotypic Microarray System with Computer
- Lietz Laser Con Focal Microscope with digital imaging
- Affymetrix Gene Microarray Processor 3000
- 6 SterilGARD II 6-foot vertical laminar-flow, biological-safety cabinet (Baker)

- 2 Avanti J-25 high performance centrifuge (Beckman)
- 6 Extremophile Fermentors (3 L capacity)
- 2 Coy Anaerobic Chambers double wide with microscope and incubators
- 2 Fermentor BioFlow III (New Brunswick)
- DU 640 UV/VIS scanning spectrophotometer (Beckman)
- Ultra-low temperature freezer (Revco)
- 2 Axioskop RLF for DIC, phase contrast, and epifluorescence with microphotography (Zeiss)
- 2 Integrated SpeedVac (Savant)
- GeneAmp PCR system 9600 (Perkin-Elmer)
- Expedite 8909 DNA synthesizer (PerSeptive Biosystems)
- Model 377 ABI Prism automated DNA sequencer (Perkin Elmer)
- CHEF DRII pulsed field electrophoresis equipment (Bio-Rad)
- MIDI identification system (Hewlett Packard)
- High sensitivity MSD mainframe for the HP 6890 GC (Hewlett Packard)
- BIOLOG microbial identification system (BIOLOG)
- Environmental shakers with photosynthetic light banks (New Brunswick)
- Alliance HPLC system with a 996-photodiode array detector and a 474 scanning fluorescence detector (Waters)

Other support equipment and installations are also available—such as autoclave, DI-water, refrigerators, freezers for low temperature storage of temperature-sensitive materials, balance, ice-maker, shakers, incubators, magnetic stirrer, hotplates, microcentrifuges, computers, different electrophoresis boxes and power supplies, and fume hoods. The core facility also has access to the Environmental Measurement Laboratory at Berkeley Lab.

The core microbiology facility preserves and maintains laboratory strains and wild-type strains isolated from environmental samples, microbial genomic DNA, plasmids, and cloned genetic material. We also have three glove boxes and several incubators that allow us to work with anaerobic microorganisms and microaerophiles.

For more information concerning the Center for Environmental Biotechnology Core Facility, please contact Terry Hazen, phone: 510-486-6223, e-mail: TCHazen@lbl.gov

Center for Isotope Geochemistry

The Center for Isotope Geochemistry (CIG), Lawrence Berkeley National Laboratory, and Department of Geology and Geophysics, University of California, Berkeley, is directed by Donald J. DePaolo. The Center has fully equipped radiogenic, noble gas, light stable isotope, cosmogenic radionuclide laboratories and an adjunct environmental measurements laboratory for organic and inorganic chemistry.

Ash deposits formed during the climactic eruption of the Long Valley volcanic system near Mammoth Lakes, California. This ash was deposited about 750,000 years ago by an enormous eruption that formed the Long Valley depression. The area is still volcanically active, and researchers at CIG are studying the volcanic formations of Long Valley to try to determine whether there can be another catastrophic eruption. Researchers are also monitoring the helium isotope ratios in carbon dioxide-rich volcanic gas that is presently escaping from the ground near Mammoth Mountain; the escaping gas is coming from magma deep in the ground.

The analytical facilities of CIG are designed to provide the capabilities for measuring isotopic and trace element concentrations of rocks, minerals, and groundwater. These measurements can be used to deduce the age of groundwater, the flow directions, the rate at which the groundwater chemistry changes by reaction with surrounding rocks, and also the age and origin of the rock units themselves.

Current effort is concentrated on Sr, Ca, O, C, He, Ne, Ar, Xe, Pb, and Nd isotopic ratios, and on problems of mass transport in fluid-rock systems, interpretation of past global climatic change, crustal magmatic and tectonic processes, and Quaternary geochronological methods. A mathematical basis for the application of isotopic measurements of fluids and rocks to the field-scale parameterization of hydrological systems is a major effort of CIG. Modeling is accompanied by systematic measurements of relatively simple natural systems, and by improved sampling and measuring techniques. Emphasis in development is on microsampling of geological materials, on high-precision measurement of the small amounts of recovered material, and on rapid, automated low-blank chemical separation of trace elements. Other efforts of the Center are aimed at geochemical techniques for dating and correlation of sedimentary and volcanic rocks, and for understanding the time scales and mechanisms of crustal processes such as extensional faulting, mountain building, and volcanism. All efforts are aimed at improved characterization of natural rock and fluid systems.

For more information concerning the Center for Isotope Geochemistry, please contact: B. Mack Kennedy, Center for Isotope Geochemistry, phone: 510-486-6451, e-mail: bmkennedy@lbl.gov

Earth Sciences Division Research Summaries 2004-2005

SECURE EARTH

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Over the past two years, ESD has focused efforts on an initiative called "Scientific Environmental/Energy Crosscutting Underground Research" (SECURE Earth, or SE), initially developed in partnership with Idaho National Laboratory and since expanded to a multilaboratory university and industry initiative at Pacific Northwest National Laboratory (PNNL), Oak Ridge National Laboratory (ORNL), Los Alamos National Laboratory (LANL), Sandia National Laboratories (SNL), and Lawrence Livermore National Laboratory (LLNL). The overall goal of SE is to achieve timely solutions to critical national problems associated with the earth's subsurface, to accelerate subsurface science research, and ultimately, identify how research leads to improvements in understanding and prediction (as well as ultimately reducing risk). Crosscutting scientific thrust areas have been identified as follows: energy, CO_2 sequestration, environmental cleanup, water, geothermal energy, and nuclear waste disposal.

Efforts prior to and during 2004 focused on briefing the U.S. Department of Energy, Office of Basic Energy Sciences (BES)/Biological and Environmental Research (BER) at the director level. A number of major milestones were also reached in 2004: (1) the formation and meetings of a multidisciplinary/multi-institutional advisory panel; (2) the expansion of the initiative development by including Pacific Northwest National Laboratory and Oak Ridge National Laboratory; (3) the organization of a two-day meeting at the National Academy of Sciences to "roll out" the initiative to many federal agencies and industry; and (4) the presentation of the SE initiative to a variety of research groups and possible sponsors.

The primary conclusions of the National Academy were that this is a worthwhile initiative, and that the DOE/OS, National Science Foundation, National Aeronautics and Space Administration, and U. S. Geological Survey are initiating a process to carryout a "decadal study" in the earth sciences, similar in scale, which justified and identified the need for such projects as the Superconductor Super Collider. This is a very significant achievement, in that never before has such a study been carried out for the geosciences.

Efforts in 2005 focused on preparing for and holding a national workshop in September to define the crosscutting scientific thrust areas of the initiative. Colorado School of Mines hosted this workshop in Golden, Colorado, September 12–13, 2005, with attendance by scientists from around the country (and supported by the various national laboratories). Also conducted were briefings and talks about SE at several national conferences (American Geophysical Union, Geological Society of America, International Society for Subsurface Microbiology) to inform the geoscience community, as well as, gaining grassroots support within the community. The outcome of the September workshop was a detailed listing of the crosscutting scientific thrust areas, which included facilities and technologies needed to accomplish the goals of SE. This list is not meant to be a list of scientific needs, but rather are the nucleus of an overall science plan that is needed to meet the goals of SE.

It is now clear that the fundamental concept of SE has become widely accepted. Notably, Berkeley Lab Director Dr. Steven Chu, in his comments to an ESD-wide meeting, stated that "addressing critical energy and environmental problems will probably have a larger societal impact than curing cancer. Now we just have to convince Congress of that."

The official SECURE Earth web site (http://wwwesd.lbl.gov/SECUREarth/ index.html) is located at Berkeley Lab and contains current information about the initiative.

Resource Departments

Hydrogeology

Geophysics

Geochemistry

Ecology

Resource Department

HYDROGEOLOGY

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The Hydrogeology Department (HD) consists of more than 50 scientists, postdocs, research associates, and graduate students carrying out a broad range of cutting-edge research in fundamental and applied hydrology. HD has expertise in theoretical, experimental, field, and modeling approaches in a variety of research areas, among which are unsaturated zone hydrology (including fracture flow and transport), reservoir engineering (including pore-level modeling and gas hydrate studies), contaminant hydrology (including reactive and colloid-assisted transport), and coupled nonisothermal, geochemical, and geomechanical processes. The HD addresses national needs in the areas of subsurface energy resource recovery, subsurface remediation, geologic CO_2 storage, and nuclear waste disposal. Highlights of research efforts in these areas over the last two years include the following:

SUBSURFACE ENERGY RESOURCE RECOVERY

Researchers in HD are studying ways to enhance production of energy from subsurface reservoirs containing methane gas hydrates, geothermal energy, and traditional oil and gas resources. In the area of methane hydrates, HD scientists are carrying out a sustained laboratory campaign to uncover fundamental properties of methane hydrates, such as dissociation kinetics and constitutive models, that can be incorporated into the world's leading methane hydrate simulator, TOUGH-Fx/Hydrate. This simulation code, developed by HD scientists, is now in public release, and several licenses have been purchased by international energy companies. A similarity solution for methane hydrate production has been developed for verifying the simulation capabilities in TOUGH-Fx/Hydrate. Continuing the long tradition of geothermal research in the ESD, staff members in HD are investigating reactive geochemistry in geothermal reservoirs to devise ways to avoid mineral scaling and maintain injectivity without inducing short-circuiting flow paths. This effort is undertaken using TOUGH-REACT, the reactive geochemical simulator developed by HD researchers. HD staff also developed a version of TOUGH2 called T2CA to study the feasibility of detecting hidden geothermal systems through monitoring of CO_2 emissions in the shallow subsurface environment. In collaboration with researchers in the Geophysics Department, HD staff confirmed that viscous fluid flow creates anomalies at low seismic frequencies that can be used to image oil reservoirs. By this method, re-analysis of 3-D seismic data using frequency-dependent approaches has revealed hydrocarbon-rich layers where none were detected by standard analysis.

SUBSURFACE REMEDIATION

HD researchers address national and international needs for subsurface contaminant characterization and remediation across the spectrum of approaches. In the lab, HD researchers are investigating some of the nation's most critical subsurface contamination issues, including the chemical evolution of highly alkaline Hanford tank waste, reduction, re-oxidation, and diffusion of Uranium VI in sediments, hydraulic properties of unsaturated gravels, and the natural production of transport-enhancing mobile nanoparticles in the subsurface. In the field, HD investigators lead the Berkeley Lab site restoration effort to remediate groundwater plumes containing dissolved chlorinated solvent and fuel contaminants. The remediation plan developed over the last several years, on time and under budget estimates, has been approved by DOE, placing the LBNL site in position for an efficient and cost-effective remediation phase. Additional field studies include work at a nearby closed army base to analyze contaminant plume evolution and measure groundwater flow velocities using heat-based flow sensors. Advances in subsurface characterization are expected to follow from HD's work on joint hydrologic and geophysical inversion that exploits the iTOUGH2 inverse modeling code. Continued collaboration with scientists in other ESD departments and Berkeley Lab divisions is currently under way, with a focus on the coupled water-energy system in California. Finally, HD maintains an international program to develop and test advanced technologies at sites worldwide, which can then be used domestically to help with our nation's most difficult contamination problems.

GEOLOGIC CO_2 STORAGE

HD researchers are involved in a wide range of efforts involving field pilot tests, laboratory work, simulation and modeling of coupled CO_2 flow and transport processes, and risk assessment. HD staff carry out experiment design, instrumentation, and field monitoring of geologic CO_2 storage pilot tests, as well as laboratory experiments of CO_2 flow behavior. In the area of field tests, HD staff performed exhaustive simulations in advance of the Frio CO_2 pilot injection to predict the resulting CO_2 migration. In a parallel effort for the Frio CO_2 injection pilot project, HD staff successfully developed, deployed, and operated a novel U-tube sampler for monitoring CO_2 and other fluids at the observation well. As for more general research in the modeling area, TOUGH-REACT has been used to study coupled flow and reactive geochemistry to evaluate the impacts of impurities in the injected CO_2 stream on mineral trapping of CO_2. New TOUGH2 modules are being used to evaluate complex phase-change and phase interference behavior that could arise during severe leakage events. HD scientists showed by simulation that even small CO_2 leakage fluxes can produce high CO_2 concentrations in the shallow subsurface environment. A screening and ranking framework was developed to prioritize candidate storage sites on the basis of CO_2 leakage risk. HD researchers will continue to be at the forefront in all aspects of this growing field.

NUCLEAR WASTE DISPOSAL IN THE UNSATURATED ZONE

The motivation for HD's extensive effort in unsaturated zone hydrology and coupled processes is stimulated by the need to understand flow and transport in the unsaturated zone at Yucca Mountain, Nevada, the site of the proposed nuclear waste repository. Research by HD scientists in this prominent area includes infiltration and seepage, coupled nonisothermal and geomechanical effects, and transport of radionuclides. Starting with research underground, HD scientists have found evidence for significant water vapor transport in closed-off tunnels at Yucca Mountain, with implications for natural-fracture vapor transport as the source of the water vapor. Field investigations at a natural analogue site in Mexico suggest that radionuclide transport is primarily in unsaturated fractures, just as predicted for Yucca Mountain. Field experiments have ranged from the large multi-year drift-scale heater test to smaller-scale liquid releases in boreholes. The practical difficulties of running tests underground at a remote site have motivated the development of sophisticated remote monitoring and operation capabilities, whereby instrument adjustments, liquid releases, and data collection can be controlled remotely by scientists on site at Berkeley Lab. The coupled approach of field experiment and modeling analysis has served to advance understanding of the coupled flow and transport properties of Yucca Mountain. Field data are used to constrain and calibrate numerical models of flow and transport using the inverse modeling version of TOUGH2 called iTOUGH2, also developed by HD personnel. On the mountain scale, a large three-dimensional TOUGH2 model has been developed to evaluate mountain-scale thermal effects on multiphase flow. The details of seepage into drifts, flow diversion, and flow focusing are modeled on appropriate scales, as are processes of water-rock interaction and geomechanical effects. Work in the nuclear waste area also extends to saturated systems in Japan, where transient pressure data have been used to constrain a flow model in fractured granite.

A considerable amount of general unsaturated zone hydrology knowledge and understanding is generated by HD researchers. For example, new broadly applicable conceptualizations of fracture-matrix interaction and scale dependence of matrix diffusion have been investigated. Often models developed in one area find application in other areas. The large effort in HD on a broad range of hydrologic processes related to nuclear waste disposal typifies the strong integration of field, laboratory, and modeling analyses characteristic of ESD scientific investigations.

FUNDING

Funding for HD comes primarily from the U.S. Department of Energy, including: the Director, Office of Science, Office of Basic Energy Sciences, Division of Chemical Sciences, Geosciences, and Biosciences; the Director, Office of Science, Office of Biological and Environmental Research; the Assistant Secretary for Energy Efficiency and Renewable Energy, Office of Technology Development, Office of Geothermal Technologies; the Assistant Secretary for Fossil Energy, Office of Coal and Power Systems and Office of Natural Gas and Petroleum Technology, through the National Energy Technology Laboratory; the Director, Office of Civilian Radioactive Waste Management; and the Assistant Secretary of the Office of Environmental Management, Office of Science and Technology, Environmental Management Science Program. The department also receives funding support from the U.S. Environmental Protection Agency. Other funding is provided through the Laboratory Directed Research and Development Program at Berkeley Lab.

Resource Department

GEOPHYSICS

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The primary focus of the Geophysics Department is to advance the development of new methodologies for extracting subsurface properties, including fluid properties, saturation, porosity, pore pressure, permeability, and *in situ* stress. These new methodologies incorporate a variety of data, including geophysical (seismic, electromagnetic, electrical, seismo-electric, gravity, ground-penetrating radar), geomechanical (tilt, deformation), and fluid flow (pressure). Fundamental and applied research carried out in support of this objective include laboratory rock physics and pore-scale imaging studies, field geophysical-imaging hardware development, theory development, computational geophysics and geomechanics modeling, and imaging and inversion (deterministic and stochastic) algorithm development. The driver for this research is the increasing need to directly image fluid saturations, pore pressures, and permeability in the subsurface for energy production, environmental remediation, carbon management, and nuclear waste disposal purposes, and to do so in the presence of anisotropy and multiscale heterogeneities.

SCIENTIFIC RESEARCH AREAS

The department is organized into five scientific research areas:

- Computational Geophysics
- Rock Physics and Coupled Dynamics
- Hydrogeophysics
- Characterization and Monitoring Geophysics
- Computational Geomechanics

The primary purpose of these research areas is to advance the science supporting high-resolution methods for extracting subsurface properties and process information from geophysical, geomechanical, and fluid flow data.

Computational Geophysics

The focus of this research area is to develop efficient, 3-D numerical codes for modeling seismic wave propagation and electromagnetic wave propagation and diffusion. The challenge is to develop accurate and efficient computer codes capable of modeling the seismic and electromagnetic response of complex geologic structures (i.e., structures that may contain anisotropy or multiscale heterogeneities in the form of fractures, faults, or patchy saturation). A variety of methods, including boundary integral equation, global matrix, finite difference, spectral element, discrete element, and asymptotic ray methods, are in the process of being developed for high-performance parallel computing frameworks. These codes will serve as the *computational engines* for the next generation of modeling-based deterministic and stochastic inversion algorithms. This research is performed using the supercomputers at the National Energy Research Scientific Computing Center (NERSC) at Berkeley Lab, and the PC cluster maintained by the Center for Computational Seismology (CCS), within Berkeley Lab's Earth Sciences Division.

Rock Physics and Coupled Dynamics

The connections between a geophysical observable, such as seismic velocities and attenuation, electrical conductivity, and dielectric constant; and rock properties, such as porosity, permeability, and fluid saturation, are provided by rock-physics measurements and/or theories. Rock-properties measurement efforts are carried out at our Rock and Soil Physics Lab. This facility has the electronic instrumentation and mechanical equipment to perform a variety of geophysical measurements, including seismic, electrical, electromagnetic, and fluid flow, under low to moderate confining pressures. Experiments that require detailed information about the porous microstructure and fluid saturations at the pore level are carried out by using the x-ray computed tomography (CT) scanner in the Rock Imaging Lab, or by using the focused ion beam (fib) located at Berkeley Lab's National Center for Electron Microscopy. In addition, facilities at the Berkeley Lab Advanced Light Source are also used for microtomography of geologic materials.

The primary focus of our laboratory efforts is towards the understanding of the geophysical properties of rock and sediments that are either not well described by conventional rock physics theories (e.g., poorly consolidated sands and clays, gas hydrates, fractured rock) or that have yet to be fully exploited (e.g., seismic attenuation, seismo-electric response). Complimentary theoretical efforts are also under way to explore the dynamics of poroelastic and seismoelectric response of rocks that contain multiple fluid phases.

Hydrogeophysics

Research in the area of hydrogeophysics combines the disciplines of geophysics and hydrogeology to develop new approaches for characterizing the shallow subsurface over a range of scales for subsurface properties (such as hydraulic conductivity, geochemical heterogeneity, lithology, and moisture movement over time). This interdisciplinary field is unique in the level of fusion between hydrogeological and geophysical data sets, the incorporation of complex petrophysical models, and the application of emerging stochastic inversion techniques. In this area, new research is also being carried out to investigate the role of biogeochemical changes associated with bioremediation in the hydrological and geophysical responses resulting from processes such as dissolution/precipitation of minerals, gas evolution, and biofilm generation.

Characterization and Monitoring Geophysics

The focus of this research area is the development of innovative geophysical hardware and methodologies for subsurface imaging and monitoring. Efforts that are currently under way include the development of passive and active seismic systems for utilizing microhole technology, an optimum electromagnetic system for detecting and identifying unexploded ordnance, a novel electromagnetic imaging system (for environmental applications) that operates in the frequency band between electromagnetic diffusion and wave propagation, a miniature rotary shear source for crosswell and single-well seismic imaging applications, high-resolution tomographic (radar and seismic) tools, and micro-earthquake monitoring systems.

Computational Geomechanics

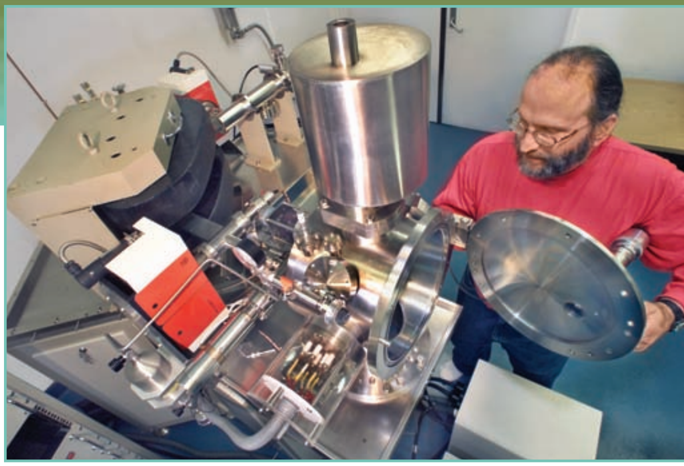
This research area is concerned with the development of new computational tools for predicting stress-induced changes in transport properties, fracturing, and fault slip resulting from fluid injection, fluid withdrawal, and thermal loading. Of particular interest is the development of new computational geomechanics-based inverse methods for estimating subsurface fracturing and fluid movement, and for predicting the seismic response resulting from fluid injection into fractured rock.

FUNDING

The Geophysics and Geomechanics Department derives its funding from a variety of U.S. Department of Energy (DOE) and non-DOE sources. The primary sources of DOE funding are the Director, Office of Science (Basic Energy Sciences and Biological and Environmental Research), Office of Environmental Management, Fossil Energy, Office of Geothermal Technologies, Office of Civilian Radioactive Waste Management, the Environmental Protection Agency, and the Berkeley Lab Laboratory Directed Research and Development Program. Non-DOE funding sources include the U.S. Department of Defense (SERDP), Shell Oil Company, and ChevronTexaco Energy Research and Technology.

Resource Department

GEOCHEMISTRY



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ESD's Geochemistry Department has expertise in isotopic geochemistry, reactive transport modeling, experimental mineral-water kinetics, molecular geochemistry and nanogeoscience, soil geochemistry, marine geochemistry, global and regional climate modeling, and mineralogy. The department has four major thrust areas, as described below.

MOLECULAR GEOCHEMISTRY AND NANOGEOSCIENCE

This effort involves fundamental studies on the nature of the aqueous solution/mineral interface, the structure of solvated ions and colloids down to the nanometer scale, and the properties and aggregation behavior of nanoparticles. Current work includes: molecular-dynamics modeling of the interlayer-solvated cations in clays, the aggregation dynamics of nanoparticle iron oxides, and the structure of mineral interface water; studies of the solvation environment of contaminant and nutrient molecules in aqueous solution; determination of the molecular identity and kinetics of formation of iron oxide precipitates on quartz surfaces; and characterization of the surface chemistry and structure of environmentally important minerals using simulation, x-ray scattering, and x-ray spectroscopy. Many of the studies employ newly developed capabilities such as synchrotron x-ray grazing-incidence methods, and laser-based phase-sensitive nonlinear optical spectroscopy. Studies of the aqueous behavior of organic species on mineral surfaces and in solution, and on nanoparticle structure, are carried out at Berkeley Lab's Advanced Light Source as well as other synchrotron sites. The group also does extensive collaborative research using the National Center for Electron Microscopy (NCEM) at Berkeley Lab and takes advantage of the National Energy Research Scientific Computing (NERSC) facility (also at Berkeley Lab) as well as other computational sources for large-scale molecular dynamics and *ab initio* simulations. Kinetics studies, mainly focusing on heterogeneous precipitation reactions, are also conducted collaboratively with the National Science Foundation Environmental Molecular Science Institute (NSF EMSI) at Pennsylvania State University.

ISOTOPE GEOCHEMISTRY

The Center for Isotope Geochemistry (CIG) includes stable isotope and noble gas isotope laboratories; a soil carbon laboratory; an analytical chemistry laboratory; the Inductively Coupled Plasma Multi-Collector Magnetic Sector mass spectrometry laboratory; and a thermal-ionization mass spectrometry laboratory located on the UC Berkeley campus. There is also an affiliation with the cosmogenic isotope laboratory in UC Berkeley's Space Sciences Laboratory. The CIG facilities enable state-of-the-art characterization of all types of earth materials. The instrumentation and laboratories are an integral part of the Center's focus on new ways to use isotopic ratio methods to study fundamental earth processes, and environmental and energy problems of national interest.

Examples of current research programs are: (1) development of models that use isotopic composition data from element pairs in fluids to constrain fluid flow rates, water-mineral reaction rates, and the geometry and spacing of fractures in rock matrices; (2) development and application of noble gas isotopes as natural tracers for fluid source and movement in hydrocarbon and geothermal systems, and as induced phase-partitioning tracers for monitoring geologic sequestration of CO_2; (3) development of techniques for dating Quaternary geological events using U-Th-He; (4) use of U, N, and O isotopes to understand subsurface contamination sources; (5) geochemical monitoring and analysis of large-scale experiments simulating the effects of nuclear-waste heat generation within the proposed repository in Yucca Mountain, Nevada; (6) the use of C, N, and O isotopes to quantify *in situ* bioremediation and monitor remediation; (7) the use of carbon isotopes to quantify rates of organic carbon cycling and storage efficiency in soils, the impact of climate change on carbon cycling, and linkages between carbon, water, and nitrogen cycles; and (8) applications of hydrogen and oxygen isotopes to issues concerning the water cycle.

CLIMATE CHANGE: ATMOSPHERIC, OCEANIC, AND TERRESTRIAL BIOGEOCHEMISTRY

The focus of this group is on the characterization of processes in the atmosphere, oceans, and terrestrial biosphere, and the development of models to understand and predict climate change, carbon cycles, and water resources.

The California Water Resources Research and Applications Center maintains a suite of research and operational tools for weather forecasts, climate prediction, and basic research. Ongoing collaborations include: streamflow simulations with the National Oceanic & Atmospheric Administration's California Nevada River Forecast Center; runoff contaminant monitoring and management with the U.S. Bureau of Reclamation; development of landslide-hazard prediction models with faculty at UC Berkeley; development of snow-cover and snow-water equivalent maps for California with UC Santa Barbara; and development of a shared information distribution system with the U.S. Department of Energy's Accelerated Climate Prediction Initiative (DOE/ACPI) collaborators. A new water-energy model with surface water, groundwater, and dynamic vegetation is being applied to a multidecade drought study of California. Additional recent activities include a regional climate model intercomparison that evaluated California land-use change between pre-industrial and present time, multidecadal high-resolution simulation of land-surface processes with scaling relationships for soil moisture, an analysis of the impact of China's Three Gorges Dam on the local climate, an analysis of the relationship between atmospheric circulation and snowpack in the western U.S., heat island effects in California's Central Valley, climate change water allocation sensitivities, and new ensemble simulations for the initialization of soil moisture and plant functional types.

The central motivation for ocean science research is to better understand the biological and physical processes governing carbon in the ocean, how these processes affect the balance of CO_2 between atmosphere and ocean, and the efficacy of using the oceans to sequester carbon. The issues are technologically challenging because of the rapidity of ocean biological processes—the entire carbon biomass in the ocean is replaced every one or two weeks. The Berkeley Lab team collaborates with other scientists to deploy Carbon Explorers—robotic floats with telemetry capability and special sensors that can measure the distribution and fate of ocean carbon, as well as temperature, salinity, and pressure. In the laboratory, work is directed at expanding the sensor suite carried by Carbon Explorers. The latest innovation is an imaging optical sensor designed to simultaneously quantify the sedimentation of both inorganic and organic particulate carbon. A large volume *in situ* filtration system is also used to collect size-fractionated particulate samples from surface to kilometer depths in the oceans. Recent projects include (1) continuous observations of particulate organic carbon variability in remote and biologically dynamic ocean regions, (2) examination of the spatial variability of particulate organic and inorganic carbon, (3) linkages between the oceanic iron and carbon cycles, (4) sources of iron in the ocean, including observations and Ocean Global Circulation Model simulations of the transport to the open ocean of iron released from shallow-water sediments.

A major concern about future climate forcing is how the current terrestrial and marine carbon sinks will respond as fossil fuel emissions increase and climate changes. ESD scientists have added interactive land and ocean carbon cycles to the global Community Climate Simulation Model (CCSM) to study how diverse features of the environment—including plants, soil, precipitation, microbes, oceans, phytoplankton, clouds, and carbon dioxide emissions—interact to affect the strength of carbon sinks. Other projects include a coordinated suite of carbon concentration, isotope, and flux measurements in the Southern Great Plains as part of the DOE Atmospheric Radiation Measurement (ARM) Program, and ecosystem experiments and isotopic analysis to study the rates of carbon cycling and storage in soils. A new effort explores the impact of climate change on ecosystems. This work tests whether we can improve predictions of ecosystem response to future climate change by incorporating genomic, transcriptomic, and bioinformatics analysis with traditional biogeochemical and physiological approaches.

GEOCHEMICAL TRANSPORT

This effort involves simulation and study of coupled mineral-water-gas reactive transport in unsaturated porous media. The work covers infiltration/evaporation processes in the soil zone, reaction-transport processes in fractured rock under boiling conditions, injection of CO_2 in deep aquifers, hydrothermal alteration in geothermal systems, the controls on the rates of chemical weathering, and biogeochemical reaction networks in low-temperature environments. Although reaction-transport modeling and code development are the predominant activities, the group is also active in planning the analysis and drilling activities for underground thermal experiments, laboratory experiments focusing on the rates of water-mineral interaction, and field studies of geothermal systems and natural analogues for nuclear waste isolation. A new effort in this regard applies Lattice-Boltzmann models to reaction-transport processes at the microscopic scale. Efforts are also under way to understand the scale dependence of mineral-water reaction kinetics using pore network models. These new modeling efforts are being combined with the world's first experimental studies using engineered microfluidic reactors to determine mineral-water reaction rates directly at the pore (mm) scale.

Much of the geochemical transport work is focused on predicting thermally driven processes accompanying the proposed emplacement of high-level nuclear waste at Yucca Mountain, Nevada, and on the understanding of the evolution of the natural hydrogeochemical system. One focus of this work is on integrating the thermal-hydrologic-chemical environment in the near field of the proposed Yucca Mountain repository with THC processes occurring inside emplacement drifts, including on the surface of the waste package (where corrosion is the main issue) and inside the waste packages (where dissolution of spent fuel is the main issue). Another focus is on understanding the controls on chemical weathering. One such effort involves integration of uranium-series isotopic disequilibria with major element profiles to determine *in situ* reaction rates in deep-sea marine sediments. Another involves understanding the controls on, and rates of, formation of weathering rinds; this work has demonstrated the key role of reaction-induced porosity change in controlling the weathering rate. Collaboration with other departments in ESD brings together essential pieces of the problem, including hydrological processes in the unsaturated zone, thermodynamics and kinetics of geochemical processes, and isotopic effects.

Current projects include:

(1) Analysis of geochemical and isotopic data from Yucca Mountain to constrain models of flow and transport in the unsaturated zone
(2) Development of models for reactive-transport in unsaturated systems and co-development of the reactive-transport code TOUGHREACT
(3) Improved thermodynamic and kinetic databases for water-rock interaction modeling
(4) Research on natural analogue sites, including the Yellowstone geothermal system, Peña Blanca, Mexico, and the Idaho National Engineering and Environmental Laboratory subsurface conditions
(5) Modeling of CO_2 sequestration in saline aquifers
(6) Modeling hydrothermal alteration in geothermal systems
(7) Development of a Pitzer-type geochemical reactive transport model and simulation of high-ionic-strength groundwater contamination
(8) Prediction of the rate of strontium migration at the Hanford site
(9) Experimental and modeling studies on the scale dependence of mineral reaction kinetics
(10) Modeling of bioremediation field tests at the Hanford site
(11) Study of long-term benthic biogeochemical dynamics of heavy metal cycling and benthic fluxes in lake sediments at Lake Coeur d'Alene, Idaho, including the development of a dynamic numerical biogeochemical model of heavy metal fate and transport in benthic sediments.

FUNDING

Funding for the Geochemistry Department comes from the U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences, Chemical Sciences, Geosciences and Biosciences Division; DOE Office of Biological and Environmental Research; DOE Office of Environmental Management, Office of Science and Technology; DOE Office of Energy Efficiency and Renewable Energy, Office of Utility Technologies and Office of Geothermal Technologies; DOE Office of Civilian Radioactive Waste Management; U.S. Environmental Protection Agency; U.S. Navy; NASA Space and Earth Sciences Program; National Science Foundation, Office of Polar Programs; U.S. Department of Agriculture; the University of California Campus-Laboratory Collaboration Hydrology Project; National Oceanographic Partnership Program (administered by the Office of Naval Research); National Oceanic and Atmospheric Administration, Office of Global Programs of the U.S. Department of Commerce, California Environmental Protection Agency, the California Energy Commission, National Institutes of Health, National Institute of Environmental Health Sciences program, the Hanford Science and Technology Program, and the Berkeley Lab Laboratory-Directed Research and Development Program.

Resource Department

Ecology

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SCIENTIFIC FOCUS AREAS

The Ecology Department (ED) intends to maintain the highest quality and highest visibility for its research and development in four areas:

- Hydroecological engineering advanced decision support
- Molecular microbial ecology
- Real-time assessment of bioavailability and biokinetics
- Bioremediation and natural attenuation

These four R&D areas are largely integrated, but contain some domains that are not inclusive. These four areas are considered ED's core competencies.

HYDROECOLOGICAL ENGINEERING ADVANCED DECISION SUPPORT (HEADS)

The HEADS research focus area has established a strong track record in the rapidly growing, new subject area of Ecological Engineering. The term "hydroecological engineering" signifies the group's concentration on water resources and wastewater engineering. Recognizing the growth in the field of environmental informatics and the application of computer-based models in the development of decision support systems, the group is active in this niche area. Interest in decision support interfaces well with the group's expertise in the deployment of real-time flow and water quality sensors, rapid laboratory assessment techniques, and mathematical models to develop an early warning system for contaminant management and containment.

MOLECULAR MICROBIAL ECOLOGY (MME)

Understanding microbial interactions is key to the study of global warming, biodegradation of harmful compounds, and the exploration of complex microbial communities in their natural environment. The DOE has placed an increased emphasis on the role microbes play in modifying their environment and their impact on energy security. The MME group has responded to these needs by aggressively seeking out new projects and expanding its staff to develop new core capabilities. One of the key challenges has been to harness the explosion of microbial DNA sequence information to accurately measure the microbial dynamics in extreme environments. Since less than one percent of the microbial species can be cultured from these environments, our knowledge of what these organisms may be doing is limited to where they are observed and the similarity of their genomes to studied organisms. By understanding the ecological structure of microbial communities and the fine-scale dynamics resulting from subtle perturbations, it may be possible to identify novel functional pathways and use the diverse microbial capabilities to assist in key DOE missions. The molecular tools being developed in the ESD's Center for Environmental Biotechnology will position us to be leaders in this area.

REAL-TIME ASSESSMENT OF BIOAVAILABILITY AND BIOKINETICS (RABB)

Interactions between environmental pollutants and ecological receptors begin when the pollutants become available to the target sites of a live ecological receptor. The ability to characterize the dynamics of the bioavailability of pollutants, their transformation kinetics, and the subsequent ecological response is a keystone to advancing the science in relevant DOE areas, including biogeochemistry, bioremediation, and exposure and risk assessment. Since 1999, the RABB research group at ED has pioneered the development and application of several cutting-edge technologies, such as synchrotron radiation-based spectromicroscopy, *in vitro* human gastrointestinal mimetic reactors, and *in vivo* mouse protocols that allow for the real-time assessment of bioavailability and biokinetics of environmental pollutants. The RABB group intends to establish this capability further by seeking out new projects and new collaborators, as well as expanding our staff, to position us as leaders in the areas of biological and environmental sciences.

BIOREMEDIATION AND NATURAL ATTENUATION

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

ED scientists and engineers are recognized leaders in the field of bioremediation and natural attenuation. The Center for Environmental Biotechnology provides the primary facilities used by ED, including state-of-the-art equipment for microbiology and environmental engineering. ED investigators have extensive experience in both water treatment and bioremediation, especially co-metabolic biodegradation and the treatment of inhibitory compounds. In addition to basic research, ED investigators have been involved in various aspects of more than 100 field demonstrations and deployments, and have five patents in this area that are licensed to more than 30 companies. The types of contaminants in which ED investigators have expertise include chlorinated solvents, petroleum hydrocarbons, polynuclear aromatic hydrocarbons, ketones, methyl tert-butyl ether (MTBE), TNT, inorganic nitrogen (NO_3, NH_4), tritium, plutonium, neptunium, chromium, and uranium. The Bioremediation and Natural Attenuation area has both basic research and field application foci for the ED. The basic research foci are co-metabolism, biotreatability, biotransformation kinetics, and modeling of biogeochemical processes. Field-application foci are co-metabolic techniques, biogeochemical assessment techniques, and modeling of attenuation and environmental fate.

FUNDING

ED personnel are funded by DOE Programs in (1) the Office of Science, Office of Biological and Environmental Research (OBER) (Natural and Accelerated Bioremediation Research Program, Genomics:GTL, and Medical Sciences); (2) the Office of Environmental Management, Environmental Restoration Programs; (3) the Office of Fossil Research, the Petroleum Environmental Research Forum; and (4) the National Nuclear Security Administration, Office of Nonproliferation Research and Engineering (NN20). In addition, support is provided by the U.S. Department of Homeland Security, the Department of Agriculture; the Department of the Interior, Bureau of Land Management, and Bureau of Reclamation under the CALFED program, NASA Astrobiology Instititutes, as well as several projects with remediation companies using DOE-patented technologies for *in situ* bioremediation. ED personnel are also funded by Berkeley Lab's Laboratory Directed Research and Development (LDRD) Program in the area of microbial fuel cells, fungal rDNA arrays, and FTIR biokinetic analaysis.

Earth Sciences Division Research Summaries 2004-2005

Research Programs

Fundamental and Exploratory Research

Nuclear Waste

Energy Resources

Environmental Remediation Technology

Climate Change and Carbon Management

Research Program

Fundamental and Exploratory Research

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

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

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

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

CHEMICAL AND MASS TRANSPORT INVESTIGATIONS

Current research in this area is focused on nanoparticle and colloid transport in unsaturated porous media and rock fractures, chemical transport in structured porous media, unsaturated fast flow in fractured rock, and production and evaluation of coupled processes for CO_2 in aquifers. The nanoparticle research focuses on the mobile fractions and natural abundance in soils. Also studied is the rate of infiltration in the unsaturated zone, an important issue in studying and defining the driving forces and boundary conditions in the containment and cleanup of contaminants in the subsurface. Also being researched are interfacial reactions such as at quartz/water interfaces and the intergranular diffusion in uranium and in sand. Another study has focused on the use of x-ray absorption and diffraction methods to study sorption processes.

ISOTOPE GEOCHEMISTRY

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

One of the major problems being studied at CIG is how to estimate fluid-solid reaction rates in natural-groundwater higher-temperature geothermal conditions, particularly as these rates affect mineral dissolution and secondary mineral precipitation. ESD researchers are developing novel ways of estimating reaction rates by using isotopic tracers (primarily strontium, but also uranium and neodymium) to determine solid-fluid exchange rates in various natural situations. Scientists are able to derive the "reaction length," a parameter that depends on the ratio of isotope transport by diffusion and advection to the reaction rate. The ultimate objective is to understand the microscopic (as well as pore-scale and mesoscale) characteristics of natural systems that have been characterized in terms of "field scale" reaction-rate measures. An intermediate goal is to establish empirically the natural range of fluid-solid reaction rates. Examples are the U-Th/He geochronology of young volcanic rock, understanding and predicting the microbial degradation of chlorinated solvents with carbon isotopes, and using Xenon isotopes to study buried wastes.

ADVANCED COMPUTATION FOR EARTH IMAGING

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

ROCK PHYSICS

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

FUNDING

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

U-Th/He Geochronology of Young Volcanic Rocks

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RESEARCH OBJECTIVES

Constraining time scales for Quaternary (<1.8 my) events remains a challenge. Despite considerable progress in C-14 and Ar-Ar dating, no single method with wide applicability has emerged. This project investigates the use of the U-Th/He system for dating young volcanic rocks, which is based on the accumulation and retention of ^{4}He from decay of U and Th in mineral grains.

APPROACH

The first step was to assess technique viability by analyzing young samples of known age: garnets from the 79 AD eruption of Mt Vesuvius. The second was application to a system that could benefit from direct age measurements, but for which only cursory knowledge of age is known: olivine phenocrysts from a suite of Hawaiian basalts.

Inherent in the application of the U-Th/He technique are several sources of error that must be addressed. First, typical minerals (garnet, olivine) have low and heterogeneous U,Th concentrations, making measurement of U,Th, and He concentrations difficult and necessitating measurement on the same aliquot. A furnace was designed capable of melting 1–2 g samples in platinum containers from which the melted sample can be retrieved for U,Th determination. Second, basalt matrix often has more U and Th than the embedded phenocrysts, leading to additional helium accumulation in the phenocryts by alpha recoil implantation. Modeling indicates that for a given matrix/phenocrysts (U,Th) concentration ratio, the magnitude of the age correction is strongly dependent on grain size (Figure 1). Furthermore, the correction assumes perfect extraction of unbroken phenocrysts from the matrix. The range of recoiled alpha particles is on the order of 10's of microns. Therefore, to overcome alpha recoil effects, we abrade samples, removing the exterior portions that are most effected. Since the matrix/phenocryst U,Th concentration ratio in the Vesuvian garnets is close to one, the correction is negligible. However, the high ratio in Hawaiian lavas is more problematic. To assess our abrasion technique, we analyzed abraded and nonabraded olivine aliquots to compare alpha recoil model ages with those determined directly from the abraded samples.

ACCOMPLISHMENTS

We successfully determined the age of the 79 AD eruption of Mt Vesuvius within analytical error. Analyses of abraded and nonabraded samples indicated that the alpha recoil model overcorrects for injection of radiogenic helium. Detailed analysis of the accuracy of abrasion is still required, but this initial investigation indicates that it is possible to date young olivine samples with low U,Th concentrations, despite high concentrations in the matrix. For two Hawaiian samples, the calculated ages of 329 kyr and 189 kyr fall within the age range constrained by previous methods.

SIGNIFICANCE OF FINDINGS

We have demonstrated the ability to date Quaternary volcanic samples, indicating that the U-Th/He method can be used as a reliable geochronological tool. Extension of the technique will vastly improve constraints on time scales for Quaternary events.

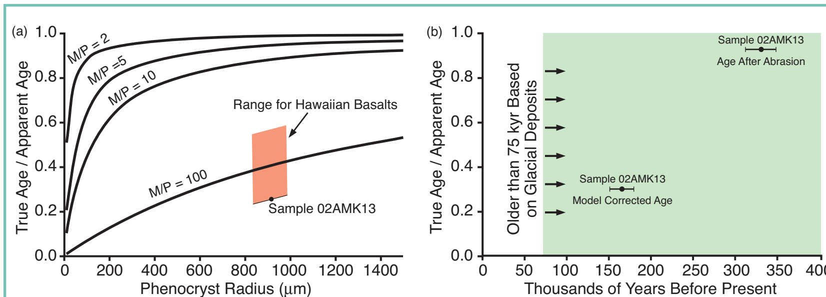

Figure 1. (a) Contours of age correction factors as a function of grain size, using varying matrix/phenocryst (M/P) concentrations of U and Th. Also plotted are the range of correction factors for Hawaiian samples using measured [U,Th] and U-series isotopes. Sample 02AMK13 has a M/P ratio of 145 and a 800–1,000 µm grain size, which corresponds to a correction factor of 0.32. (b) Comparison of ages for sample 02AMK13 constrained by glacial deposits—shown are calculated ages plotted against the correction for alpha recoil; the unabraided sample has a model correction factor of 0.32, while the abraded sample requires no alpha recoil correction and thus has a correction factor of 1.

RELATED PUBLICATION

Aciego, S.M., B.M. Kennedy, D.J. DePaolo, J.N. Christensen, and I. Hutcheon, U-Th/He age of phenocrystic garnet from the 79 AD eruption of Mt. Vesuvius. Earth and Planetary Science Letters, 216, 209–219, 2003. Berkeley Lab Report LBNL-53622.

ACKNOWLEDGMENTS

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

Monitoring Microbial Degradation of Chlorinated Solvents with Carbon Isotopes

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RESEARCH OBJECTIVES

Chlorinated solvents are common groundwater contaminants. Because of their high density (greater than water) and low solubility, they are extremely difficult to remove from groundwater using standard remedial techniques such as pump-and-treat. *In situ* bacterial degradation of these compounds represents one alternative solution to this problem. However, it is very difficult to verify that these processes are actually occurring. One promising technique for monitoring subsurface microbial activity is to measure the carbon isotopic compositions of the contaminants and their degradation byproducts. Because microbial degradation of organic compounds favors breaking bonds with ^{12}C rather than ^{13}C, the isotopic ratio of the substrates tends to become enriched in ^{13}C. As a result, with a good understanding of the magnitude of the shift in the carbon isotope ratios caused by a specific process, we can determine the degree of degradation that has occurred. The purpose of this research is to quantify the carbon isotopic fractionation caused by different biologic processes known to degrade chlorinated solvents.

APPROACH

We have concentrated our studies on bioremediation of chlorinated ethenes that include some of the most toxic and recalcitrant chlorinated solvents, including perchloroethylene (PCE), trichloroethylene (TCE), isomers of dichloroethylene (DCE), and vinyl chloride (VC). These compounds can be anaerobically degraded by reductive dechlorination (whereby chloride ions are stripped from the molecules, progressively converting the contaminants from PCE to TCE to DCE to VC to ethene). Some organisms are only capable of completing one of these steps, whereas others can do more than one. Under aerobic conditions, chlorinated ethenes can also be oxidized to nontoxic end products (chloride ions and carbon dioxide) by several different oxygenase-expressing cultures. Some of the oxygenase-catalyzed degradations are metabolic (yielding energy and carbon for cell growth), while others are co-metabolic (providing no energy to the cells). Most prior studies of carbon isotope fractionation during biodegradation of chlorinated ethenes have used mixed cultures enriched from field sites where degradation is suspected. However, the results of these studies are variable. We are performing a series of experiments with pure cultures to determine how organisms using different mechanisms fractionate carbon isotopes.

ACCOMPLISHMENTS

We have completed and published a study of carbon isotope fractionation during aerobic degradation of chlorinated ethenes. The observed shifts were small (<1‰) for degradation of all of our experiments except those with VC, which were as high as 6‰. A series of anaerobic experiments with pure cultures are currently in progress. The carbon isotopic fractionation effects we have observed for these experiments are much larger (15 to 33‰, depending on the organism and the substrate) than for aerobic processes.

SIGNIFICANCE OF FINDINGS

The results of our work demonstrate that there can be significant differences in the magnitude of carbon isotope fractionation during biodegradation of chlorinated ethylenes, depending on the organisms involved and the metabolic process utilized. These differences can be used to determine which organisms are present and active in the field. When coupled with microbial genetic studies, this will lead to a comprehensive understanding of intrinsic bioremediation processes occurring at field sites. This understanding can be used to guide efforts to enhance biodegradation of the chlorinated solvents, by adding nutrients or bacteria to the system, and to monitor the success of these efforts.

RELATED PUBLICATIONS

Chu, K.-H., S. Mahendra, D.L. Song, M.E. Conrad, and L. Alvarez-Cohen, Stable carbon isotope fractionation during aerobic biodegradation of chlorinated ethenes. Environ. Sci. Technol., 38, 3126–3130, 2004. Berkeley Lab Report LBNL-55658.

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ACKNOWLEDGMENTS

Funding for this study was provided by National Institute of Environmental Health Sciences Grant P42-ES04705 and by the Assistant Secretary for Environmental Management, Office of Science and Technology, under the Environmental Management Science Program of the U.S. Department of Energy under Contract DE-AC03-76SF00098.

Uranium Isotope Comminution Ages: A New Way to Study Sedimentation Processes

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RESEARCH OBJECTIVES

Erosion is a fundamental Earth process, in which rocks are broken down by mechanical and chemical means into small fragments and transported by streams, glaciers, winds, and ocean currents, ultimately to accumulate as sediment on the ocean floor, or in lakes, or river floodplains. The time that it takes for individual particles to travel from the their source to the site of deposition can be roughly estimated using material balance calculations, but there has not been a means to measure it. In the course of research using uranium (U) isotopes to measure weathering rates of soils and sediments, we have discovered a means to measure the transport times of sedimentary particles. This method now allows us to evaluate how transport time changes with climate, tectonic activity, and other factors, and may also be useful for dating nonmarine sediments and atmospheric dust.

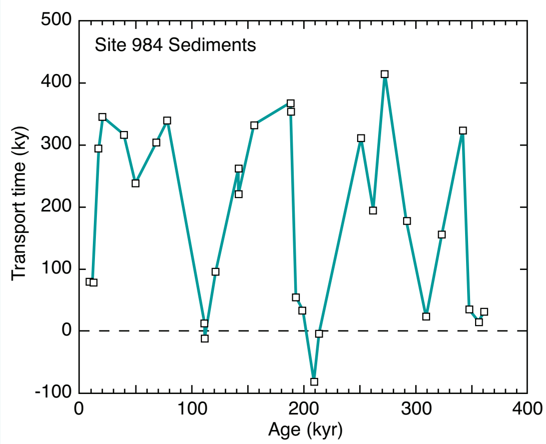

Figure 1. Calculated transport time (from sediment source to site of deposition) for fine-grained silicate fraction of sediment from ODP Site 984 in the North Atlantic. During interglacial periods, transport is rapid; during glacial times, it is much slower. The relationship between glaciation and transport time is less simple for age greater than 250 thousand years. Measured $^{234}U/^{238}U$ activity ratios vary from 0.83 to 0.97.

APPROACH

The basis for the method is that the $^{234}U/^{238}U$ ratio of sedimentary particulates of diameter less than about 50 μm measures the age of the particle. The "clock" is provided by the disruption of the normal ^{238}U decay series resulting from the loss of the ^{238}U decay product, ^{234}Th, by recoil during alpha decay of ^{238}U. When a small mineral grain is produced by erosion, it begins to leak ^{234}Th to its surroundings, and its $^{234}U/^{238}U$ ratio starts to decrease. To reach the steady-state $^{234}U/^{238}U$ ratio appropriate to its size requires about 1 million years, during which time the $^{234}U/^{238}U$ is measuring the time since the small grain was produced, which we refer to as the "comminution age." If the time between production of the small grains and deposition on the sea floor is relatively short (10,000 years or less), then the particles will still have $^{234}U/^{238}U$ activity ratios that are close to 1.0. If the time scale for transport to the ultimate site of deposition is much longer (≥100,000 years), then the grains will be deposited with a $^{234}U/^{238}U$ activity ratio significantly less than 1.0. Typical depletions in ^{234}U in fine-grained sediments are 5% to 30%, and this depletion can be measured to ±0.1% using multicollector inductively coupled plasma mass spectroscopy (ICPMS).

ACCOMPLISHMENTS

Data have been collected for a clastic deep sea sedimentary sequence from Ocean Drilling Program (ODP) Site 984A in the North Atlantic. The sediments contain primary marine carbonate and authigenic components, and hence were first leached with hydrochloric acid. The data show cyclic variations in the measured $^{234}U/^{238}U$ activity ratio, indicating that transport time for sediment to this site has varied considerably with time (Figure 1). Comparison with O isotope records and Nd and Sr isotopes shows that the transport time variations correlate with glacial cycles, and that the source of the sediment also shifts as the transport time changes. During interglacials, the sediment is dominated by material derived from Iceland and transported rapidly to the site of deposition. During glacials, the sediment is from a continental source and has a long transport time, probably because Iceland is surrounded by sea ice and the deposition is either aeolian or redistributed from exposed continental shelves.

SIGNIFICANCE OF FINDINGS

The U isotope comminution age model may open up new ways of understanding the movement of sediment and dust on the Earth. The method may be useful for dating glacial moraine, loess, lake and river sediments, and for determining the sources of atmospheric mineral dust.

RELATED PUBLICATION

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ACKNOWLEDGMENTS

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

Flowing-Fluid Electric-Conductivity Logging for Hydrologic Characterization of Fractured Rock

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RESEARCH OBJECTIVES

For the study of flow and transport in the subsurface, knowledge of flow zones and their hydraulic properties is essential. Boreholes drilled deep into the rock are often employed to determine this information. Coring and geophysical methods may be able to identify the fractures themselves, but they are unlikely to provide information on fracture flow properties. Straddle-packer pump testing yields fracture flow properties, but is very time-consuming and expensive. Flow-logging techniques are an attractive alternative—they are sensitive to fracture flow and are efficient to deploy in the field. The objective of the present work is to develop the theory for the multi-rate flowing fluid-electric-conductivity (FEC) logging method and demonstrate its application to field data.

APPROACH

The flowing FEC logging method involves the replacement of wellbore water by de-ionized or constant-salinity water, followed by constant pumping with rate Q, during which a series of FEC logs are taken. The logs can be analyzed to identify depth locations of inflow, as well as evaluate the transmissivity and electric conductivity (salinity) of the fluid at each inflow point. When the method is repeated with two or more pumping rates, a combined analysis of the multi-rate data allows an efficient means of determining transmissivity and salinity values of all inflow points—as well as their inherent (so-called far-field) pressure heads.

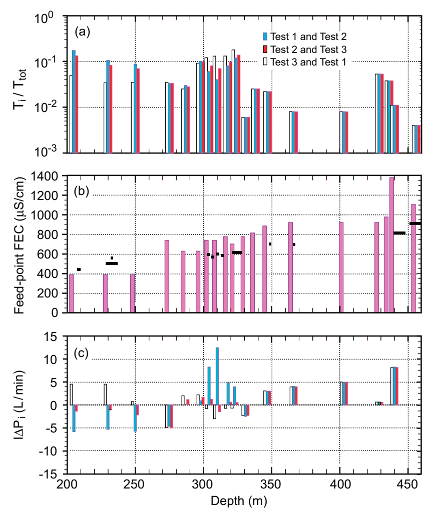

Figure 1. Results of multi-rate flowing FEC logging: (a) feed-point transmissivity normalized by total transmissivity of the borehole; (b) feed-point salinity (the black segments show independent salinity information, which was not used in the present analysis); (c) normalized inherent pressure head of feed-points (IDPi = 0 corresponds to the pressure head of the wellbore as a whole under zero pumping conditions).

ACCOMPLISHMENTS

Flowing FEC logging was performed in Well DH-2, very close to the Japan Nuclear Cycle Development Institute's MIU (Mizunami Underground Research Laboratory) site in the Tono area of Gifu Prefecture, Japan. Well DH-2 is about 500 m deep; the upper 167 m penetrates tertiary sedimentary rocks, which unconformably overlie a medium-grained biotite granite of Cretaceous age that is weathered and highly fractured. Flowing FEC logging was repeated three times, using pumping rates of 10 L/min, 20 L/min, and 5 L/min. The suite of FEC logs for each pumping rate were matched (through trial and error) by varying feed-point strength and salinity. Feed-point salinity is constrained to remain the same for each pumping rate, whereas the variation in feed-point strength with pumping rate provides the basis for determining feed-point transmissivity and inherent pressure head.

Performing the flowing FEC logging method at different pumping rates has enabled us not only to estimate inflow strengths and salinities of hydraulically conductive fractures intersecting Well DH-2, but also to compare their transmissivities and inherent pressure heads (Figure 1). Moreover, using three pumping rates provides a consistency check on the analysis, supplying a measure of the uncertainty within the results. Comparisons against static FEC profiles and independent chemical, geological, and hydrogeological data provide further checks on the validity of the multi-rate flowing FEC logging-method results.

SIGNIFICANCE OF FINDINGS

Flowing FEC logging provides an efficient, affordable means of characterizing the hydraulically conductive features intersecting a borehole with high vertical resolution. Such information is invaluable for characterization of regional groundwater flow, design of nuclear waste storage facilities, remediation of subsurface contamination, and a host of other issues. Moreover, it can be very useful in conjunction with other subsurface site characterization activities, such as providing high-resolution monitoring during a tracer test, or providing ground truth at boreholes for crosshole geophysical imaging methods.

RELATED PUBLICATIONS

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ACKNOWLEDGMENTS

This work was jointly supported by the Director, Office of Science, Office of Basic Energy Sciences, Division of Chemical Sciences, Geosciences, and Biosciences of the U.S. Department of Energy, and by the Japanese Nuclear Cycle Development Institute (JNC) under the binational research cooperative program between JNC and U.S. Department of Energy, Office of Environmental Management, Office of Science and Technology (EM-50), under Contract No. DE-AC03-76SF00098.

Xenon Isotopes Released from Buried Transuranic Wastes

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RESEARCH OBJECTIVES

This project addresses the Department of Energy need to characterize and assess the location, type, and mobility of wastes in the subsurface. The specific objective is to evaluate the use of xenon isotopes in soil gases to detect the presence of radioactive transuranic wastes, characterize the waste, and model the transport of fission xenon through the unsaturated soil gas environment.

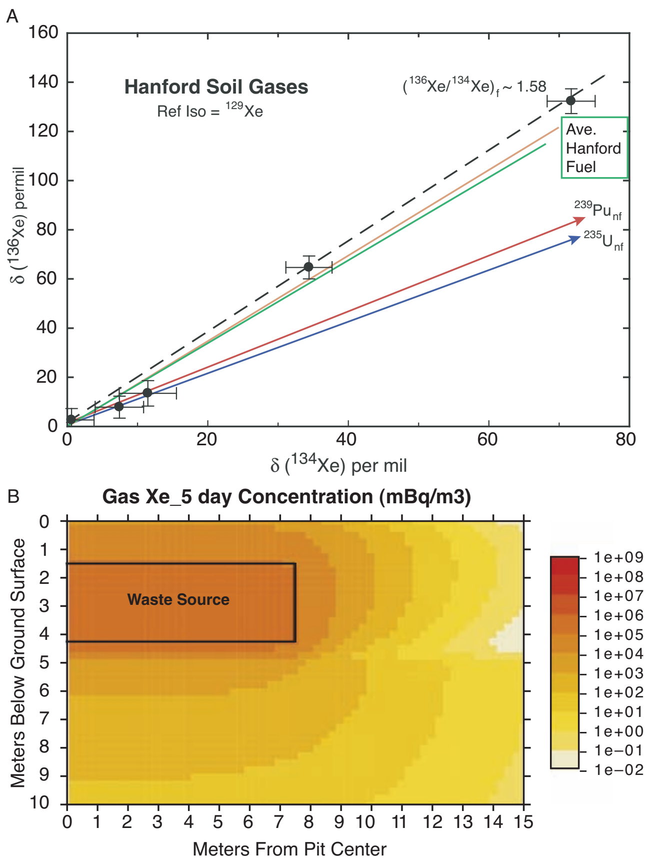

Figure 1. A: Isotopic composition of xenon in Hanford soil gases. Dashed line is a least squares fit to the data. Solid lines represent the composition of various fission sources, including the composition expected for Hanford fuel rods (orange and green lines). B: Modeled distribution of ^{133}Xe in the vadose zone relative to a waste source and constrained by the the values measured in the soil gases.

APPROACH

Xenon is a chemically inert noble gas and therefore a conservative tracer under most geologic conditions. Several stable and short-lived radioactive xenon isotopes are produced as fission products in nuclear reactors and through spontaneous fission. The isotopic composition of fission-produced xenon will have a characteristic yield pattern that can be used (1) to detect fission xenon in soil gases saturated with ambient atmospheric xenon, and (2) as a diagnostic tool for characterizing the fission source(s). Presence of short-lived fission xenon isotopes (^{133}Xe, $t_{1/2}$ = 5.24 days; ^{135}Xe, $t_{1/2}$ = 9 hours) in surrounding soil gases would confirm ongoing fission in the buried waste—and (under optimal conditions) could be used to set limits on leakage rates from the buried waste containers, as well as transport and residence times in the soil gas environment.

ACCOMPLISHMENTS

Initial measurements of soil gases collected near disposal facilities at the U.S. Department of Energy's Hanford site clearly show both stable and radio-xenon isotopic signatures indicative of transuranic waste. The isotopic composition of the stable fission-xenon isotopes closely matches that calculated for production from Hanford's unenriched and enriched Zr-clad fuel (Figure 1A). Radio-xenon isotopes were also detected, and their abundances have been used in a multiphase vadose zone transport model that indicates transport from the waste source is at a sufficient rate to be detected up to 10's of meters away. Additional data will be needed to constrain leakage rates from the waste container.

SIGNIFICANCE OF FINDINGS

Remediation of buried transuranic and other waste is one of the most difficult and costly environmental issues at U.S. Department of Energy sites. This project addresses the DOE need to characterize and assess the location and mobility of wastes in the subsurface. We have demonstrated that xenon isotopes released to the vadose zone from transuranic wastes provide unique tracers for source identification and the study of vadose zone transport processes, as well as having potential for constraining leakage rates from buried containers.

RELATED PUBLICATIONS

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ACKNOWLEDGMENTS

Work on this project at Berkeley Lab was supported by the Director, Office of Science, Office of Basic Energy Sciences, Division of Chemical Sciences, Geosciences, and Biosciences, of the U.S. Department of Energy under Contract No. DE-AC03-76SF00098.

Regional Trends in Helium Isotopes: Evidence for Deep Permeability in the Basin and Range

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RESEARCH OBJECTIVES

The Basin and Range Province of western North America is characterized by an anomalous geothermal gradient that has created a vast region of exceptional potential for geothermal energy development. However, first-order exploration techniques are difficult to apply: by the time deep fluids emerge at the surface, they have re-equilibrated at lower temperatures, overprinting chemical and isotopic compositions that might otherwise provide evidence for deeper high-temperature reservoirs. In essence, the geothermal systems are "hidden." This project maps regional trends in helium isotopic compositions that may detect local zones of deep permeability where surface waters, penetrating deep in the crust, can be heated to form potential geothermal systems.

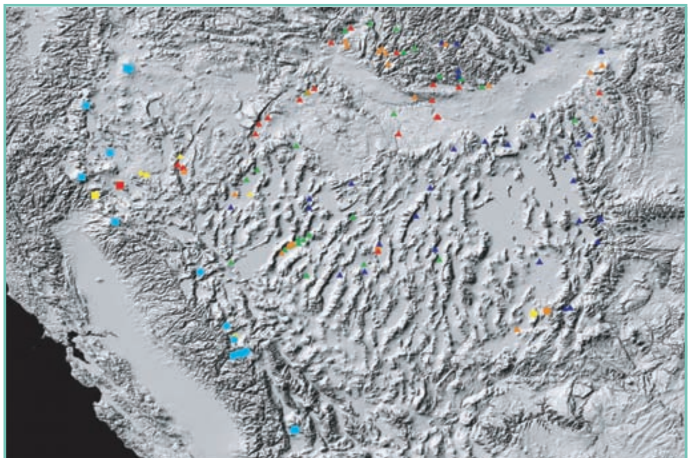

Figure 1. Shaded relief map of the Basin and Range (BR) and nearby surrounding areas. Locations are shown for hot spring and hot well samples for the BR, the Snake River Plain (SRP), the Idaho Batholith (IBL), and for some of the Cascade volcanoes (CV). Some geographical locations are identified. Data from this study, Welhan et al. 1988, and Jenkins, unpublished data (used with permission).

Symbols are shape and color coded to indicate magnitude of $^3He/^4He$ ratio and heat source:
1. Filled circles: BR magmatic heat source or possible BR magmatic heat source.
2. Filled triangles: BR extensional heat source. The samples from the SRP and IBL are included in this catagory until a better assessment of their heat source can be made.
3. Filled squares: CV magmatic heat source.
4. Filled diamonds: BR/CV transitional - unclear heat source: a geothermal well and two springs near Canby, CA.

Color coding is as follows:
Blue ≤ 0.3 Ra; 0.3 > Green ≤ 0.6 Ra; 0.6 > Orange ≤ 1.0 Ra; 1.0 > Red ≤ 2.0 Ra; 2.0 > Yellow ≤ 3.0 Ra; Cyan > 3.0 Ra.

APPROACH

The focus of the project is the relationship between known Basin and Range geothermal resources and the presence of fault-hosted, deep, permeable fluid-flow pathways, as identified by anomalous helium isotopic compositions in surface fluids. The anomalies are defined as high helium-isotopic ratios relative to a regional trend. Helium isotopes are of particular interest because they provide unequivocal evidence for the presence in crustal fluids of mantle-derived volatiles that can only be acquired by deep fluid circulation.

ACCOMPLISHMENTS

We have found that exceptionally high helium-isotopic compositions (~3-6 Ra—Ra is the ratio in air) are confined to the western margin of the Basin and Range (Figure 1) coinciding with a zone of active volcanism, extending along the eastern Sierra into the Cascade volcanic complex of northern California and Oregon. Moving east, there is a general decline to values as low as ~0.1 Ra. Superimposed on this trend are localized zones of high helium-isotopic compositions (e.g., DV, DIV, BRD). A detailed study of one of these "He-spikes" (DV, Dixie Valley) found that high ratios were restricted to fluids emerging directly from an active high-angle normal fault that hosts one of the most successful geothermal fields in Nevada. The high ratios require deep permeability consistent with the presence of high-temperature exploitable fluids rising through the fault. The other "He-spikes" occurring throughout the Basin and Range may also indicate deep permeability and high potential for geothermal development.

SIGNIFICANCE OF FINDINGS

Deep permeable pathways are a necessity in the development of viable nonvolcanic geothermal resources in the Basin and Range. The deep pathways provide access to high temperature and can host fluid convection cells. Helium isotopes may provide the best and perhaps only tool for detecting faults with deep and high-enough permeability to develop economic geothermal systems.

RELATED PUBLICATIONS

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Kennedy, B.M. and M.C. van Soest, Regional and local trends in helium isotopes, Basin and Range Province, Western North America: Evidence for deep permeable pathways. Geothermal Resources Council, Trans (submitted), 2005.

ACKNOWLEDGMENTS

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

Studies of the Formation, Structure, and Reactivity of Nanoparticulate Goethite

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RESEARCH OBJECTIVES

Goethite is a ubiquitous mineral in soils and sediments, and recent work (Van Der Zee et al., 2003) suggests that on the nanoscale it is also the dominant Fe oxyhydroxide in lacustrine and marine sediments. Goethite nanoparticles may have markedly different properties than their larger analogs, including sorption capabilities, surface charges, aggregation, and redox capability (Waychunas et al., 2005). In analogy to our work with nanosize sphalerite (Gilbert et al., 2004), there may also be important phase transformations in both molecular and magnetic structure as a function of size. We thus wish to prepare monodispersed nanogoethite from a few nanometers to 100 nm in diameter, and determine the changes in structure and chemical reactivity over this range.

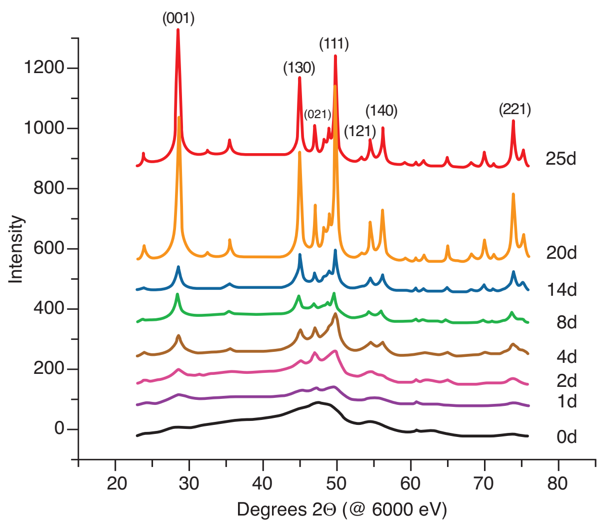

Figure 1. Synchrotron x-ray diffraction patterns of nanogoethite grown for varying periods at 90° C obtained on ALS beamline 7.3.3. Goethite Bragg peaks are labeled with Miller indices. Particle size ranges from 4 nm (0 days) to ~100 nm (25 days).

APPROACH

Nanogoethites were prepared by rapid microwave heating of a ferric nitrate solution, followed by rapid cooling. The resultant solution was aged for up to 33 days at 90°C, with aliquots taken during this period having progressively larger crystallites. Size distributions were obtained via dynamic light scattering (DLS), small angle x-ray scattering (SAXS), and via transmission electron microscopy (TEM) measurements. The crystallization process was also studied in real time by SAXS studies at the Advanced Photon Source (APS). Crystallites were monodispersed and from 4 to 120 nm in diameter, with shape variations during growth. The smallest crystallites were equiaxial, but assembled into rodlike forms in the 30 nm size range. Wide-angle x-ray scattering patterns were obtained for all goethites, including a series over the full coarsening period (Figure 1), and a more detailed analysis of the smallest crystallites at the APS. Sorption of a series of metals (Hg, Zn, As [as arsenate], and Cu) was done over the whole size range, and the samples studied via extended x-ray absorption fine structure (EXAFS) analysis at SSRL.

ACCOMPLISHMENTS

All the sorption studies indicated a change in the character of the metal sorption complexes in the smallest nanogoethites, suggesting differences in the nature of the surface attachment sites. X-ray scattering studies were also consistent, with the smallest crystallites deviating in structure from bulk goethite. Ongoing work involves examining how the nanogoethites change with aging at low temperatures, and the precise nature of aggregation. TEM analysis suggests oriented aggregation processes occur at the smaller size regimes (4–10 nm), leading to nonclassical growth, while larger (30+ nm) nanogoethite grows by classical monomer addition.

SIGNIFICANCE OF FINDINGS

The results verify that nanogoethite reacts differently from larger sized crystallites and has different molecular surface structure. This suggests that studies done with coarser samples may overlook processes that would occur in sediments where goethite is forming. There also may be changes in sorbed species as nanogoethite ages, particularly when oriented aggregation occurs.

RELATED PUBLICATIONS

Gilbert, B., H. Zhang, F. Huang, J. Banfield, Y. Ren, D. Haskel, J. Lang, G. Srajer, A. Jurgensen, and G. Waychunas, Analysis and simulation of the structure of nanoparticles that undergo a surface-driven structural transformation. J Chem Phys, 120, 11785–11795, 2004.

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ACKNOWLEDGMENTS

TEM work was done at the National Center for Electron Microscopy (NCEM) at LBNL. This project was supported by the Director, Office of Science, Office of Basic Energy Sciences, Division of Chemical Sciences, Geosciences, and Biosciences, of the U.S. Department of Energy under Contract No. DE-AC03-76SF00098.

Tube-Wave Effects in Crosswell Seismic Data

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RESEARCH OBJECTIVES

The main goal of this project is to develop a new technology that will improve the quality and resolution of seismic monitoring in natural underground reservoirs. The main innovative part of this technology is the use of tube waves as primary signal-carriers, which will provide a relatively inexpensive seismic monitoring method for use during management of real-time fluid production.

APPROACH

A tube wave is an interface wave for a cylindrical boundary between two media, typically borehole fluid and surrounding elastic rock. These waves have large amplitudes and can propagate long distances without substantial decay. They are traditionally regarded as a source of high-amplitude noise in borehole seismic data, and consequently much effort goes into their suppression and elimination from seismic recordings.

Recently, analysis of crosswell seismic data from a gas reservoir in Texas revealed two previously undetected seismic wave effects, recorded 2,000 ft above the reservoir. The first effect is that the dominant late phases on the recordings are tube waves, generated in the source well and converted into laterally propagating waves through gas/water saturated layers that then convert back to tube waves in the receiver well. This tube-wave train correlated with a multilayered reservoir zone structure, suggesting that the recorded wave field strongly depended on reservoir parameters. The second effect is that the recorded field is composed of multiple low-velocity tube waves. Modeling results suggest that imperfect cementation is the likely cause of this phenomenon.

ACCOMPLISHMENTS

How to interpret the strong late phases arriving in the 0.8–2.0-second interval during the crosshole seismic experiments is the key issue for this project. The relatively small travel time (0.2 seconds) for the direct P-wave arrivals suggests that the late phases belong to waves with long propagation paths and/or rather small velocities. This energy propagated in a different mode from the direct P-waves. Apparent velocities of the strongest phases around the 1-second arrival time were estimated to be in the 1,300–1,500 m/s range, which corresponds to propagating tube waves. High (90–100–200–220 Hz) and low (30–40–80–90 Hz) bandpass-filtered data indicate virtually the same results, which suggests negligibly low dispersion in the frequency band under consideration. The traces were cross–correlated with the first-arriving wave-train interval, which enabled measurement of the main peak travel times to better than 0.01-second accuracy. Measured travel times represent upward propagating waves of varying velocities. The almost perfect lateral homogeneity of the formation suggests that the wave propagation of late arrivals follows a three-legged path: The wave propagates downward as a regular tube wave, then converts into a horizontally propagating wave along some seismically conductive layer. After reaching the receiver well, the wave propagates upwards, splitting into a set of at least six waves of different velocities.

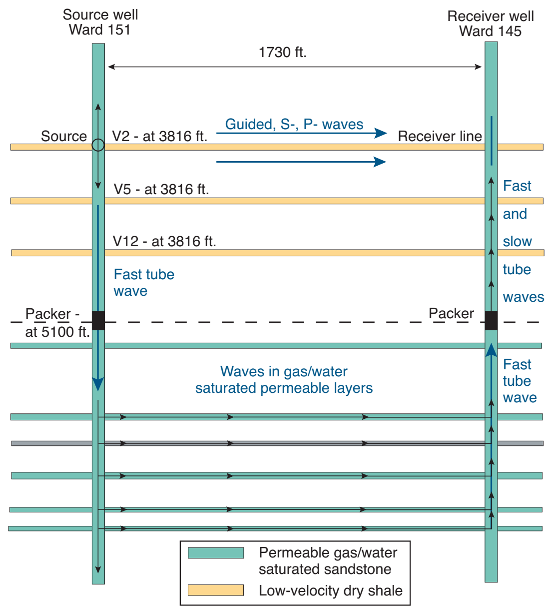

Figure 1. Crosswell experiment scheme and wave paths of the late arrivals

SIGNIFICANCE OF FINDINGS

Because reservoir waves should be affected by reservoir properties (i.e., porosity, permeability, fracture density, and orientation), monitoring based on use of these waves should allow the detection and interpretation of reservoir property changes near production boreholes. These effects can be used to develop a new and promising technology for the imaging and monitoring of underground gas, oil, and water reservoirs.

RELATED PUBLICATION

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ACKNOWLEDGMENTS

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

Lattice-Boltzmann Simulation of Isotopic Kinetics in Crystal Growth

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RESEARCH OBJECTIVES

Isotope information in waters, sediments, and dust samples can be used to identify their sources. The relevant identification techniques utilize the isotope-ratio variations resulting from fractionation effects caused by the mass difference among the isotopes, with diffusion and reaction among the fundamental processes involved. It is especially important to know isotope behavior associated with these processes, because this determines isotope ratios and the degree of fractionation. This study is aimed at evaluating how fractionations affect the isotopic ratios in phase transformations such as evaporation, condensation, and crystal growth.

APPROACH

We used the Lattice-Boltzmann (LB) method to account for fluid flow, diffusion, and reaction in phase transformations. Isotopic kinetics were investigated by considering both diffusion and reaction rates. The effects of reaction relative to that of diffusion were described with a Damkohler number (Da).

ACCOMPLISHMENTS

LB simulations provide new insights into the behavior of isotopes when evaporation, condensation, or crystal growth occur. Results (Figure 1) show the fractionation effects for a crystal growth under different diffusion-reaction conditions. Kinetic considerations also include degree of oversaturation and the original quantity of mass to be deposited. The isotopic distributions are found to be significantly affected by the diffusive strength of the lighter and heavier isotopes in comparison with the reaction rate.

SIGNIFICANCE OF FINDINGS

LB simulation connects the crystal growth processes and isotopic kinetic effects. The simulation results explain the isotopic variation in evaporation/condensation, snow and ice formation, and crystal growth. Judging from this work, LB simulation shows potential as a method by which to evaluate the fractionation of isotopes in natural systems, extending the present simulation capability to investigate the physics bridging molecular dynamics and the conventional continuum domain.

RELATED PUBLICATIONS

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Lu, G., D.J. DePaolo, Q. Kang, and D. Zhang. Lattice Boltzmann simulation of isotopic kinetics in phase growths, J. Geophys. Res. Let. (submitted), 2005.

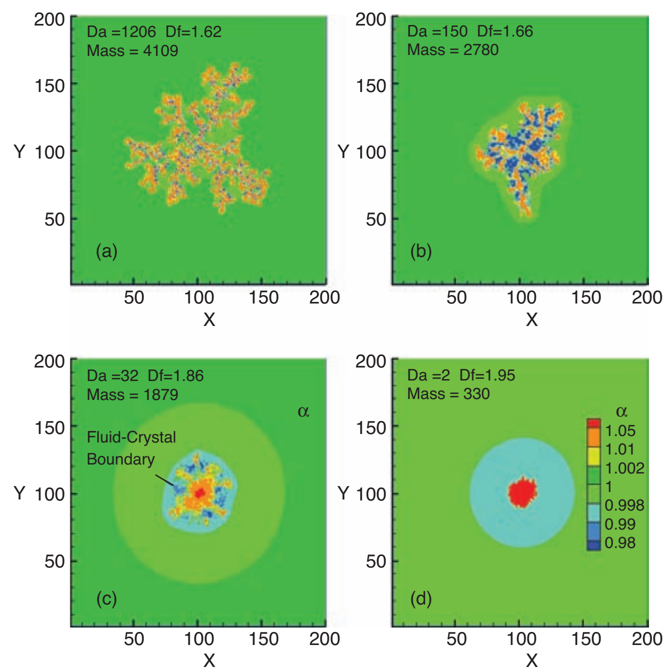

Figure 1. Calculated ^{2}H(D)/H isotopic fractionation effects in phase growth. Supersaturated concentration is set at 1.2, with identical reaction rate and a ^{2}H/H diffusion ratio of 0.972.

ACKNOWLEDGMENTS

This work was supported by Laboratory Directed Research and Development (LDRD) funding from Berkeley Lab, provided by the Director, Office of Science, of the U.S. Department of Energy under Contract No. DE-AC03-76SF0098.

The Mineral Dissolution Rate Conundrum

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RESEARCH OBJECTIVES

The objective of this research is to determine whether mechanistic reactive transport modeling of uranium (U) isotopic profiles and major element chemistry (especially alkalinity and calcium) in marine sediments from the North Atlantic Ocean can be used to determine the origin of the apparent discrepancy between laboratory and field mineral dissolution rates.

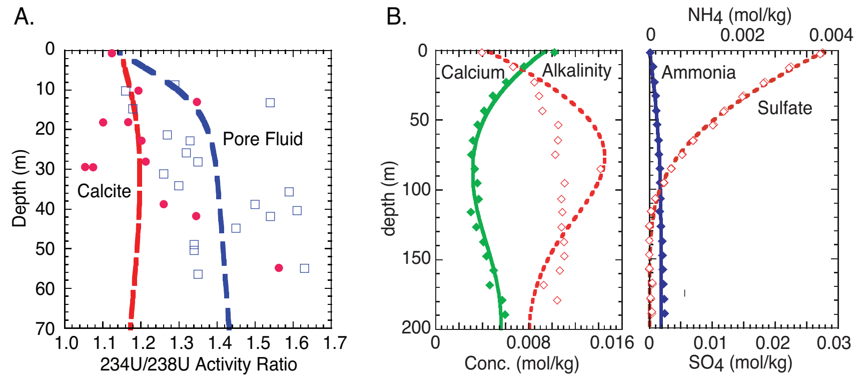

Figure 1A. Uranium isotope activity ratios for calcite (red) and pore fluid (blue). Symbols represent measured values, lines are model results.
Figure 1B. Measured (symbols) and modeled (lines) concentration profiles at Site 984.

APPROACH

Pore-water chemistry and $^{234}U/^{238}U$ activity ratios from fine-grained sediment cored by the Ocean Drilling Project (ODP) at Site 984 in the North Atlantic were used as constraints in modeling *in situ* rates of plagioclase dissolution with the multi-component reactive transport code Crunch. The reactive transport model includes a solid-solution formulation to enable the use of the $^{234}U/^{238}U$ activity ratios in the solid and fluid as a tracer of mineral dissolution.

A suite of reactions, including sulfate reduction and methane production, anaerobic methane oxidation, $CaCO_3$ precipitation, dissolution of plagioclase, and precipitation of secondary clay minerals, along with diffusive transport and fluid and solid burial, control the pore fluid chemistry in Site 984 sediments. The surface area of plagioclase in intimate contact with the pore fluid is estimated to be 3.2 m^2/g, based on both grain geometry and on the depletion of $^{234}U/^{238}U$ in the sediment via α-recoil loss. Various rate laws for plagioclase dissolution are considered in the modeling, including those based on (1) a linear transition state theory (TST) model, (2) a nonlinear dependence on the undersaturation of the pore water with respect to plagioclase, and (3) the effect of Al-inhibition.

RESULTS

The surface area of plagioclase in intimate contact with the pore fluid is estimated to be 3.2 m^2/g, based on both grain geometry and on the depletion of $^{234}U/^{238}U$ in the sediment via α-recoil loss. In the case of the linear TST model, the calculated dissolution rate for plagioclase corresponds to a rate constant that is about 104 to 105 times smaller than the laboratory-measured value. The major element and isotopic methods predict similar dissolution rate constants, if additional lowering of the pore water $^{234}U/^{238}U$ activity ratio is attributed to isotopic exchange via recrystallization of marine calcite, which makes up about 10–20% of the Site 984 sediment. Rate laws based on a nonlinear dependence of the dissolution rate on the solution saturation state, or on inhibition of dissolution by dissolved aluminum, can only account for about one order of magnitude of the apparent discrepancy between laboratory and field rates.

The reactive transport simulations demonstrate that plagioclase dissolution rates depend strongly on the rate of authigenic clay precipitation, since clay precipitation controls both the saturation state of the fluid with respect to plagioclase and dissolved aluminum concentrations. Matching the range of aluminum pore-water concentrations found in deep marine sediments, it appears that slow clay precipitation and/or more soluble clay phases result in close-to-equilibrium conditions with respect to plagioclase, thus effectively removing two to three orders of magnitude from the overall mismatch between laboratory and field rate constants. The remaining two to three orders of magnitude must be attributed to the gradual loss of reactive sites on silicate surfaces with time, which is expected to be more pronounced under close to equilibrium conditions.

SIGNIFICANCE OF FINDINGS

The study indicates that the discrepancy between laboratory and field mineral dissolution rates is real in the case of plagioclase, and that this discrepancy can be attributed to the combination of a control on the saturation state of the plagioclase, exerted by clay precipitation, and the gradual loss of reactivity of the plagioclase surface itself over geologic time.

RELATED PUBLICATIONS

Maher, K., C.I. Steefel, and D. DePaolo, The mineral dissolution rate conundrum: Insights from reactive transport modeling of U isotopes and pore fluid chemistry in marine sediments. Geochimica et Cosmochimica Acta (in press), 2005.

ACKNOWLEDGMENTS

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

Split Hopkinson Resonant Bar Experiment for Fracture Poroelasticity

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RESEARCH OBJECTIVES

The objective of this research is to examine the dynamic poroelastic behavior of single fractures and faults in rock for a range of hydraulic properties. To this day, laboratory experiments on the dynamic properties of single fractures have been conducted nearly exclusively using ultrasonic waves. When extrapolating the laboratory-measured properties to the field, however, large differences in the seismic wave frequencies used in the laboratory (~1 MHz) and the field (~100 Hz–10 kHz) may result, causing significant discrepancies. To overcome this difficulty, we developed an acoustic resonant bar apparatus that can measure the complex elastic moduli of rocks containing fractures in the sonic range (~1 kHz).

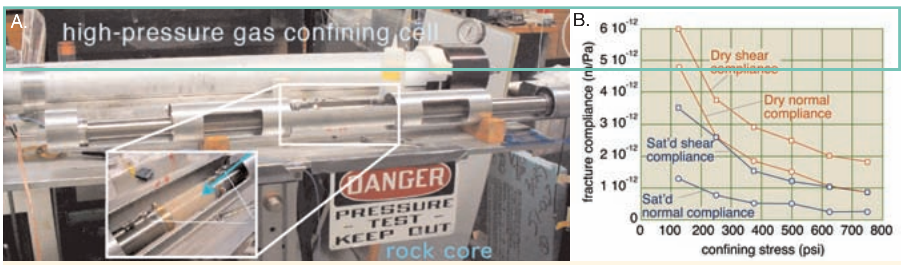

Figure 1. Fracture compliance measurement via split Hopkinson resonant bar tests. A sample assembly containing a short rock core suspended within a metal cage is acoustically resonated within a confining cell (A). Using this setup, normal (compressional) and shear compliances of fractures under dry and water-saturated conditions are measured as a function of applied normal stress (B).

APPROACH

Conventional resonant bar tests have been used since the beginning of laboratory acoustic testing of materials. Typically, a resonant bar test measures a resonance frequency and damping (attenuation) of vibrations in a long, bar-shaped sample and relates them to the complex elastic moduli of the material. Since the frequency, or rather, wavelength, of the resonance is determined by the dimension of the sample, we require a longer sample for measuring the moduli at low frequencies. For testing rocks, this can be a problem, since rock cores longer than several inches (corresponding to frequencies of tens to hundreds of kilohertz) are difficult to obtain.

We have adopted an experimental setup from an acoustic test called the split Hopkinson bar test, which employs a short core or disk-shaped rock sample sandwiched between two long slender metal bars (see Figure 1). While a conventional split Hopkinson bar test measures reflected and transmitted waves across the sample, our setup measures the resonance of the whole system, which allows us to determine the material properties more accurately. Because of the extra length and mass added by the attached metal bars, measured resonance frequencies are reduced, which allows us to measure low-frequency properties of the rock sample. The complex elastic moduli of the rock sample are determined via nonlinear numerical inversion, using a one-dimensional wave propagation model, from measured resonance frequencies and attenuation (measured from the width of the resonance peak). For determining the dynamic properties of a fracture, we conduct two sets of measurements, before and after the fracture is introduced in a rock core. The difference in the apparent elastic moduli of the rock core provides the properties of the fracture.

ACCOMPLISHMENTS

We developed an experimental apparatus for measuring acoustic resonance of short core samples (one to four inches in length) under hydrostatic pressure from high-pressure gas. Concurrently, we developed a complex-elastic moduli inversion technique that allows us to extract the moduli of a sample from measured apparent elastic moduli. An important recent improvement was the consideration of the end-effect, which resulted in an apparent increase in the Young's modulus of a short core sample for materials with a high-Poisson's ratio. A series of experiments was conducted on both synthetic materials with known material properties, and natural geomaterials—including unconsolidated sand, well-consolidated sandstone and carbonates (limestone and chalk), and rock cores containing fractures.

SIGNIFICANCE OF FINDINGS

Experiments for a fractured sandstone core demonstrated that the split Hopkinson resonant bar test is very sensitive to the changes in fracture properties: changes in fracture compliance that result in less than 0.1% of wave transmission coefficient across a fracture can be resolved. This allows us to use the current experimental setup for studying the dynamic poroelasticity of a fracture, with good resolution.

RELATED PUBLICATION

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ACKNOWLEDGMENTS

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Unprecedented Quartz/Water Interface Structure Determined by Phase-Sensitive Sum Frequency Vibrational Spectroscopy

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RESEARCH OBJECTIVES

Natural chemical processes are initiated at interfaces between aqueous solutions and mineral surfaces. Over the past few years, large advances have been made in the elucidation of mineral surface structure in contact with water (e.g., Eng et al., 2000), and metal sorption topologies (Brown and Sturchio, 2002), but much less is understood about the organization of water on surfaces. Water acts to stabilize particular surface molecular geometries, solvate near-surface ions, and promote chemical reactions via proton and electron transfer—but details of these operations are poorly known on a molecular level. Our work seeks to determine water structure on a range of mineral surfaces as a function of pH, ionic strength, and complexation density (Ostroverkhov et al., 2004). We then intend to use this information to bootstrap molecular-dynamics (MD) simulations of interface phenomena, ultimately allowing modeling of interface reactions.

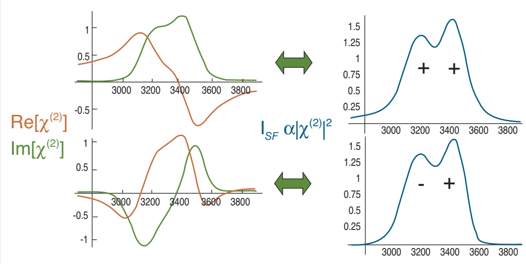

Figure 1. Right: simulated magnitude spectra of interface water having different dipole orientations for the low-frequency (“ice-like”) contribution. The spectra appear identical. Left: Decomposition into real and imaginary parts. The dipole orientation effects are clearly visible.

APPROACH

One of the most powerful tools for investigating interface water structure is sum frequency vibrational spectroscopy (SFVS). SFVS is a two-photon process in which tunable infrared (IR) light is mixed with green light at a mineral surface under solution. As a result of the broken symmetry at the interface, there is a small probability that light at the sum frequency of the two light beams will be generated. Studying this signal allows measurement of the vibrational spectrum only of interface species. SFVS has been used for studying air/liquid, solid/liquid, and other types of interfaces, but as usually employed, the method only detects the spectral amplitude. However, we have developed a method for obtaining SFVS spectra containing both amplitude and phase contributions. This is done by using a reference signal of known phase and allowing it to interfere with the SFVS signal from the interface. By doing this for two different phase reference signals, we can deduce the magnitude and both the real and imaginary parts of the SFVS spectrum. Because the imaginary part yields direct information on the orientation of water dipoles, we can obtain more information on interface water than ever previously measured (Figure 1).

ACCOMPLISHMENTS

By using the Phase-Sensitive (PS)-SFVS technique on quartz (0001) surfaces, we found: (1) that the lower-frequency IR band usually attributed to “ice-like” tetrahedrally bonded water is actually composed of two contributions, and (2) that the “ice-like” water molecules orient themselves quite differentially from interface “liquid water” in response to pH changes (Ostroverkhow et al., 2005). In particular, the “ice-like” water protons resist reorienting as pH is changed until a relatively large surface charge is produced, whereas the “water-like” protons shift positions readily at slight pH changes above the point of zero charge.

SIGNIFICANCE OF FINDINGS

Our results yield new information that can be precisely compared to MD simulations of interface water, and we have already obtained good agreement using MD performed with the Center of Advanced Materials for Purification of Water with Systems, a National Science Foundation Science and Technology Center. This work should lead to a new level in molecular modeling of interface reactions.

RELATED PUBLICATIONS

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ACKNOWLEDGMENTS

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

Infiltration Flux Distributions in Unsaturated Rocks

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RESEARCH OBJECTIVES

The hydrology of unsaturated fractured rocks has received considerable attention over the past two decades. Another category of unsaturated rocks includes talus deposits in mountainous terrain and mine waste rock piles; their hydrology has received little attention. As water percolates through unsaturated rocks, do seepage paths remain uniformly distributed, converge in a manner analogous to river networks, or obey some other principle? This study was aimed at (1) determining whether well-constrained unsaturated flow distributions exist in unconsolidated rock, (2) developing a model consistent with experiments, and (3) identifying similarities between unsaturated flow in unconsolidated rock and in fractured rock.

APPROACHES

Infiltration experiments have been conducted on three different rock types (diabase, sandstone, serpentinite), with rock sizes ranging from 30 mm to 200 mm, and system scales ranging from 1 to 30 rock layers. Water was uniformly applied over the upper surface of the rock packs at various flow rates (all less than 10^{-5} that of the scale-predicted saturated hydraulic conductivity), and spatial distributions of steady state outflow were recorded in arrays of graduated cylinders placed under the lowermost rock layer (Figure 1c). Various flow-path models were developed during the course of this study, allowing individual flow-path trajectories to randomly move downward through successive underlying nearest-neighbor cells.

ACCOMPLISHMENTS

Although individual experiments yielded different spatial distributions of fluxes, we found that probability distributions of fluxes were remarkably similar. Fluxes stabilize into a geometric (exponential) distribution that keeps about half of the system depleted of flow, retains a small fraction of high flow regions, and has a scale equal to the characteristic rock size (Figure 1d). The depth-evolution of the measured flux probability distribution was predicted by modifying a statistical mechanical model, showing that the most probable (maximum entropy) macroscopic distribution of flow paths is equivalent to the Boltzmann distribution.

SIGNIFICANCE OF FINDINGS

These results are important because they have predictive value with respect to probability distributions of fluxes. The geometric distribution of fluxes is expected to be directly applicable to fluxes within talus and waste-rock deposits. Key similarities between infiltration in rock deposits and fractured rock include effectively random downward trajectories (constrained by rock geometry and gravity), balancing of flowpath merging and splitting, and flow occurring at rates many orders of magnitude lower than saturated hydraulic conductivities. These similarities indicate that our results could apply to percolation in fractured rock formations. A better understanding of infiltration path distributions will improve our ability to predict the natural biogeochemical reactive transport rates in unsaturated rocks, as well as help constrain predictions of contaminant migration to underlying groundwaters.

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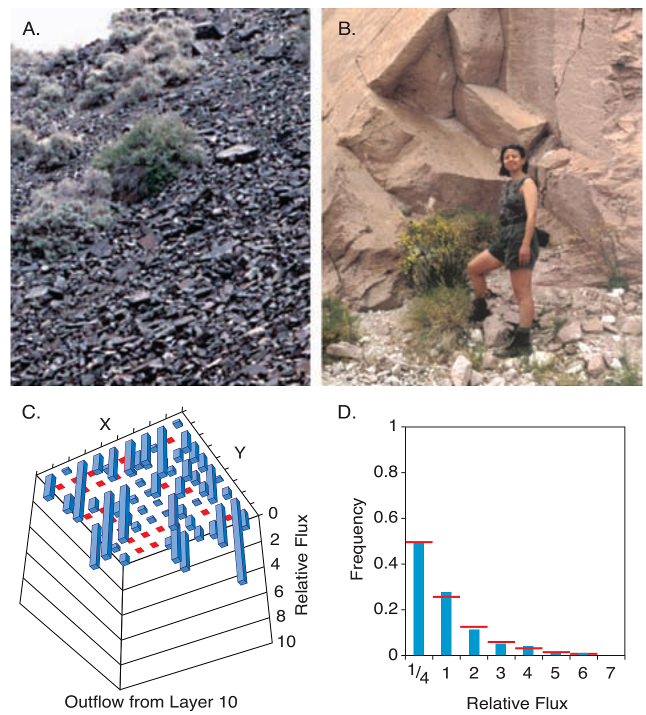

Figure 1A. Talus rock deposit (White Mountains, California); B. Fractured rock (Owens River Gorge, California); C. Spatial distribution of outflow from a rock pack experiment (10 layers); D. Probability distribution of outflow fluxes from a 10-layer rock pack, compared with a geometric distribution model (horizontal red lines).

RELATED PUBLICATION

Tokunaga, T.K., K.R. Olson, and J. Wan, Infiltration flux distributions in unsaturated rock deposits and their potential implications for fractured rock formations. Geophys. Res. Lett. 32, L05404, doi:10.1029/2004GL022203, 2005. Berkeley Lab Report LBNL-57399.

ACKNOWLEDGMENTS

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

Intragranular Diffusion of Uranium in Sands

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RESEARCH OBJECTIVES

Transport of solutes, including contaminants, in soil and groundwater systems can be complex because of the very wide range of time scales associated with basic processes. Although this complexity can be overlooked in volume-averaged measurements of sufficient size (Figure 1a), more mechanistic understanding of reactive transport requires several progressively finer levels of resolution. One such basic scale in porous media is defined by sizes of individual grains. Intragranular diffusion is often invoked to explain slow mass transfer and reaction rates. Our study uses synchrotron x-ray fluorescence microtomography to directly measure intragranular uranium(VI) diffusion in sediments from Oak Ridge National Laboratory, a DOE facility where uranium (U) contamination has occurred.

APPROACH

Experiments involved exposing 50 to 100 μm sand grains from an uncontaminated area of Oak Ridge to U(VI) solutions, and then obtaining fluorescence microtomographs of intragranular U distributions at different times. The sand grains and U(VI) solutions were contained in sealed micropipette tips and scanned at GSECARS beamline 13ID-C, Advanced Photon Source. In addition to fluorescence microtomography, we applied micro-x-ray absorption near-edge structure (μ-XANES) spectroscopy to determine the oxidation state of U within grains.

ACCOMPLISHMENTS

Fluorescence microtomography maps of U were obtained in real time, over two days of intragranular diffusion. Two-dimensional maps within sands (5 μm resolution) revealed very heterogeneous migration of U into individual grains (Figure 1b). Rates of U uptake inferred from the fluorescence maps of grains are consistent with time scales observed in bulk sorption experiments, indicating that intragranular diffusion is in fact the rate-limiting step. Micro-XANES spectra confirmed that U remained as U(VI) during intragranular sorption. Some spatial correlation between U and Fe was also indicated, as expected from the high sorption affinity of U(VI) to Fe(III)-oxide surfaces.

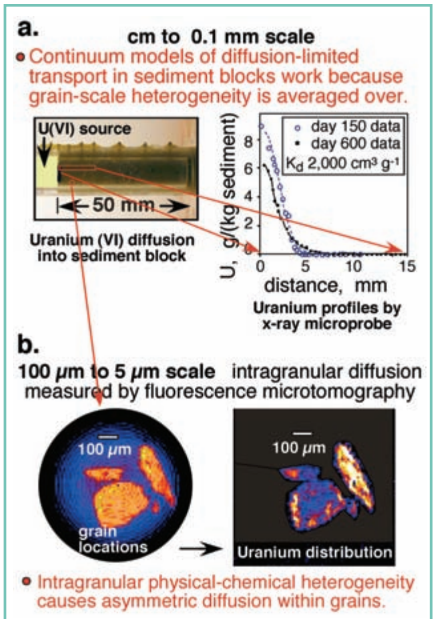

Figure 1. Uranium(VI) diffusion measured at two different scales: (a) at the sediment column scale, diffusion averages over many grains and pores, such that continuum descriptions are directly applicable; (b) at the grain scale, differences associated with mineralogy, secondary coatings, and intragranular properties result in highly heterogeneous U diffusion patterns and control rates for achieving local equilibrium.

SIGNIFICANCE OF FINDINGS

These results provide proof that intragranular diffusion exerts a major influence on time scales needed for sorption equilibrium of U(VI) in sediments. The fact that most of the sorbed U(VI) in Oak Ridge sediments occurs in intragranular regions has important implications on its reactivity. If most of the U(VI) diffuses into intragranular regions, it does so through typically less than 100 nm pores that would exclude bacteria. Therefore, intragranular redox transformations of U could not occur via direct contact with bacteria, but instead through other redox active solids and solutes, including electron shuttles.

RELATED PUBLICATION

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ACKNOWLEDGMENTS

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

Natural Abundance and Mobile Fractions of Nanoparticles in Soils

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RESEARCH OBJECTIVES

The current growing interest in nanomaterials and nanotechnology has stimulated the geoscience community to evaluate the roles of nanoparticle phenomena in many of the earth's natural processes. There is currently little quantitative information available on the abundance and mobility of nanoparticles in the subsurface. The importance of natural nanoparticles in facilitating chemical transport can only be evaluated based on knowledge of their inventories and mobility. The objective of this research is to address these two most basic questions: how abundant and how mobile are nanoparticles in the subsurface?

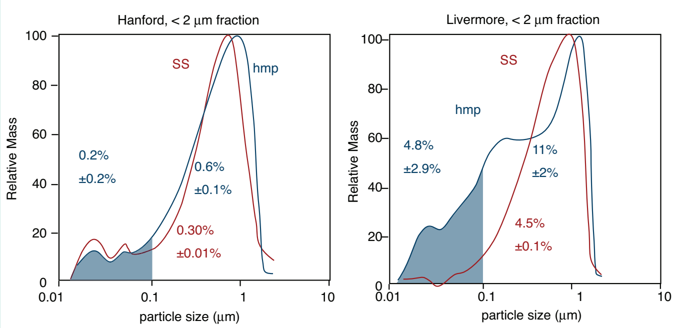

Figure 1. Examples of measured potentially mobile mass (red and ≤ 0.1 μm) vs. mass of total colloid (including nanoparticle) inventory (blue shaded area). For the Hanford soil (pH 8.0), all the dispersible nanoparticle mass is potentially mobile. For the Livermore soil (pH 6.7), only a small fraction of the total dispersible nanoparticle inventory is potentially mobile.

APPROACH

To quantify the influences of soil properties on nanoparticle abundance and mobility, we collected representative types of soils from DOE facilities, including the Oak Ridge, Hanford, Livermore, and Savannah River Sites, all having different mineralogy, soil texture, and pH. Batch equilibrium and column-leaching experiments were conducted using two different kinds of solutions. One was Na-hexametaphosphate, a strong dispersing agent, used to obtain maximum particle releases, thereby defining the total inventories of nanoparticles. The other was a diluted soil pore solution, used to determine potentially mobile fractions of nanoparticles. In these tests, nanoparticles were defined by an upper effective diameter of 100 nm.

ACCOMPLISHMENTS

We found that: (1) nanoparticles are ubiquitous in soils, and the inventories are proportional to their clay and organic matter fractions; (2) natural nanoparticles in soils consist primarily of common clay minerals and organic matter; and (3) the mobility of nanoparticles is highly pH dependent. No mobile fractions were detected in acidic soils, even when their total nanoparticle inventories were large.

SIGNIFICANCE OF FINDINGS

This research has provided the first survey of mobile nanoparticle inventories of sediments from a variety of subsurface environments. The finding that mobile nanoparticle fractions in natural acidic soils are practically undetectable is an important new insight for the environmental nanogeosciences. These studies will help constrain calculations of subsurface transport associated with nanoparticles.

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ACKNOWLEDGMENTS

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

As(V) Sorption on Hematite: Complexation Geometry Obtained from Combined Surface X-Ray Diffraction and Grazing-Incidence X-Ray Absorption Spectroscopy

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[1]University of Alaska, Fairbanks, [2]University of Chicago
[3]U.S. Geological Survey, Menlo Park , [4]Stanford Synchrotron Radiation Laboratory
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RESEARCH OBJECTIVES

The objectives of this work were to combine surface x-ray diffraction results of wet hematite surfaces, with arsenate complexation structure derived from surface extended x-ray absorption fine structure (EXAFS) measurements. Using these two techniques together, it is now possible to describe the geometry of sorbed metal complexes with unrivaled detail. This enables testing of both structural and thermodynamic models for sorption and surface complexation, and direct comparisons with molecular-dynamics (MD) simulations of surface reactions.

APPROACH

Surface diffraction of the wet hematite (0001) and (1–102) surfaces can be done using crystal truncation rod (CTR) measurements to obtain the reconstructed or relaxed configuration of surface ions. This has been done (Trainor et al., 2005) and shows that the wet hematite surface is highly defective, with iron atoms missing from the double layers that characterize the bulk structure. The missing atoms are those that would ordinarily share FeO_6 polyhedral faces with one another. We then obtained polarized EXAFS structure functions for arsenate sorbed on the wet (0001) and (1-102) hematite surfaces at SSRL beamline 11-2, and used the hematite surface structure to interpret the results.

ACCOMPLISHMENTS

The results show details of surface complexation that could not have been recovered without these methods (Figure 1). In particular, there is an abundance of "edge-sharing" arsenate-FeO_6 units on the surface, which results from the high proportion of available edge-sharing sites, but relative scarcity of adjacent FeO_6 units allowing "corner-sharing" arsenate attachment. The measurements also demonstrated self-consistency of the hematite surface structure model, and thus helped to verify the CTR diffraction work. We also determined that the method could be applied to complexation coverages as low as about 5% of one monolayer.

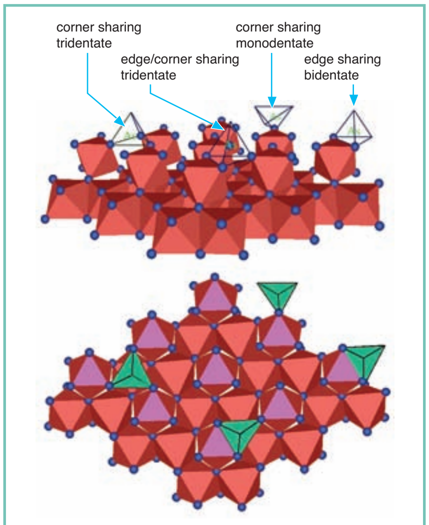

Figure 1. Cartoon showing two views of arsenate complexes (green tetrahedral) as they could sorb on a wet hematite (0001) surface. Of these types, only the edge-sharing bidentate complex is actually observed. Note that the hematite surface is only partially populated by FeO_6 unit (red octahedral) as indicated by CTR work.

SIGNIFICANCE OF FINDINGS

The results indicate the powerful nature of such combined surface probes of interfacial reactions. Prior to this type of study, the surface structure information would not have been accurate enough to derive a proper model of the complexation. We can now proceed to develop MD simulations of surface reactions with a detailed knowledge of the expected complexation geometries. This work is continuing with other surface sorbants, including silicate, phosphate, and selenate, and the CTR work is being extended to include refinements with sorbates present on the scattering surfaces.

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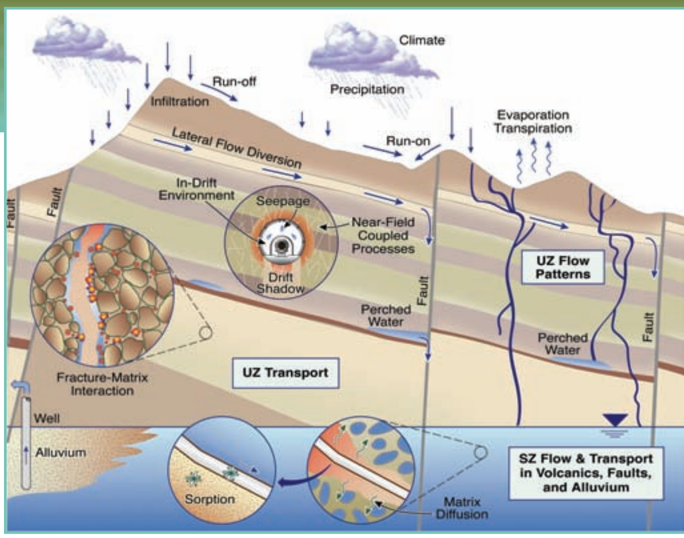
ACKNOWLEDGMENTS

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

Research Program

Nuclear Waste



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Geological isolation of spent nuclear fuels and high-level radioactive waste is currently the preferred means of disposal for many countries worldwide. The role of ESD's Nuclear Waste Program (NWP) is to assist the U.S. Department of Energy, the United States, and other countries in achieving the safe disposal of high-level radioactive waste—by means of high-quality scientific analyses that encompass modeling, laboratory and field experiments, and technology development. The majority of research within NWP relates to Yucca Mountain, the proposed site for the permanent storage of high-level nuclear waste in the USA; although NWP has also collaborated on nuclear-waste disposal issues with countries such as Japan, Finland, Switzerland, Spain, Sweden, and China.

The geologic repository program in the United States is at a point where the Department of Energy (DOE) is close to completing the license application for repository construction at Yucca Mountain to the Nuclear Regulatory Commission. If the license application process proceeds as planned by DOE, the Yucca Mountain repository is scheduled to start accepting waste in 2010. The safe performance of a high-level nuclear waste repository hinges on the multiple-barrier concept—namely, that the natural system and the engineered system would each contribute significantly to prevent radionuclides from leaving the repository and entering the biosphere. The proposed repository at Yucca Mountain, consisting primarily of fractured volcanic tuffs that vary in degree of welding, will be located about 350 m below ground surface within a thick unsaturated zone (UZ) above the water table. Over the last decade, NWP's work at Yucca Mountain consists of site characterization studies aimed at understanding the barrier function of the UZ, through field testing in an underground facility, an 8 km long underground tunnel known as the Exploratory Studies Facility (ESF). Complex numerical models have also been developed to simulate and understand the relevant processes related to multiphase, nonisothermal flow and transport through the UZ. Some of the key questions addressed by NWP scientists include:

- How much water percolates through the UZ to the repository at Yucca Mountain?
- What fraction of the water flows in fractures and what fraction flows through the rock matrix blocks?
- How much of this water will seep into the emplacement drifts (tunnels)?
- How will the radionuclide migration from the repository to the water table be retarded?
- How will coupled TH (thermal-hydrological), THC (thermal-hydrological-chemical), and THM (thermal-hydrological-mechanical) processes affect flow and transport?

Apart from the above studies that pertain to the barrier function of the UZ and its contribution to the safety case of the license application, NWP scientists have also conducted research under a new Office of Science and Technology International Program (OST&I) within the DOE Office of Civilian Radioactive Waste Management (OCRWM). Distinct from, but in parallel to, the licensing effort at the Yucca Mountain, the role of OST&I is to advance technologies not previously considered, to identify new or substantially revised scientific methods or tools that would provide a better understanding of the repository environment. The OST&I program is a well-integrated, focused research and technology program that aims to reduce cost, reduce uncertainty, enhance performance, develop new technologies, and overall greatly enhance the repository system, its performance, and its defensibility during and beyond the license application defense. The OST&I program funds proposals from national laboratories and universities and is currently organized into four Targeted Thrust areas: (1) Source Term, (2) Material Performance, (3) Radionuclide Getters, and (4) Natural Barriers.

Berkeley Lab's Earth Sciences Division is the Lead for the Natural Barriers Thrust. The goal for the Natural Barriers Thrust is to focus on research that would provide the essential scientific basis and demonstration of large contributions to repository performance by the unsaturated and saturated volcanic rocks at Yucca Mountain. The enhanced understanding of the different processes in the natural system would lead to reduction of uncertainty and obviate the need for overconservatism. NWP scientists are conducting studies pertaining to:

- In-drift processes, integrating thermal-hydrologic-chemical-transport (THCM) models that simultaneously consider source term, corrosion, and the hydrological-chemical environment around waste package processes and conditions—and synthesize these complex processes into transparent, realistic, and defensible process models
- Near-drift processes, such as found in laboratory, field, and analogue studies to confirm the drift shadow concept, and the fact that it will lead to a large delay and sorption of radionuclides in the near-drift region
- Processes and conditions that will retard or mitigate flow and transport through the unsaturated and saturated volcanic rocks

FUNDING

Funding for research in the Nuclear Waste Program comes primarily from the Department of Energy, through the Director, the Office of Civilian Radioactive Waste Management.

Evaluating Near-Field TH Processes at Yucca Mountain: The Impact of Natural Convection

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RESEARCH OBJECTIVES

The heat output of the waste to be emplaced at Yucca Mountain will strongly affect the thermal-hydrological (TH) conditions in and near the geologic repository. Recent analysis of gas flows within emplacement drifts has demonstrated that the open tunnels will act as important conduits for natural convection processes. As a result, water will evaporate from the drift walls in elevated-temperature sections of the drifts, migrate along the drifts, and condense in cooler sections (i.e., the end sections with no emplaced waste). Thus, evaporation driven by natural convection has great potential for reducing the moisture content in the near-drift fractured rock, which in turn would reduce the potential for formation of pore water drops at the drift wall (and subsequent dripping into the opening). However, up to now, natural convection processes have been neglected in predictions of future TH behavior in the fractured porous rock at Yucca Mountain. We have developed a new simulation method that couples existing tools for simulating TH conditions in the fractured formation (Birkholzer et al., 2004) with modules that approximate natural convection and evaporation conditions in heated emplacement drifts.

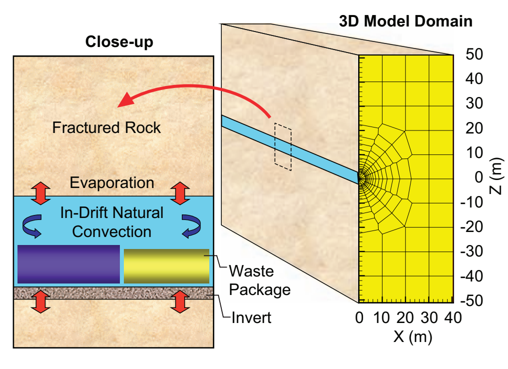

Figure 1. Schematic showing 3-D model domain with emplacement drift and fractured rock

APPROACH

The new simulation method simultaneously handles (1) the flow and energy transport processes in the fractured rock; (2) the flow and energy transport processes in the open drifts; and (3) the heat and mass exchanges at the interface between the rock formation and the cavity. This integrated modeling approach ensures consistency between the thermal-hydrological conditions in the fractured rock and those in the open drift. In-drift convection and turbulent mixing is approximated with a lumped-parameter approach, following a procedure developed by scientists at Sandia National Laboratories for estimating condensation processes in waste emplacement drifts (BSC, 2004). A lumped-parameter approximation means that the turbulent mixing is not solved in detail, but approximated as a binary diffusion process, with effective diffusion coefficients estimated from supporting computational-fluid-dynamics analyses. The lumped-parameter simulations are conducted with a newly developed version of the multiphase, multicomponent simulator TOUGH2, which includes a new module for in-drift convection.

ACCOMPLISHMENTS

We have successfully applied the new modeling methodology to study future TH conditions in a three-dimensional model domain comprising a representative emplacement drift and the surrounding fractured rock (Figure 1). Sensitivity studies were conducted simulating different degrees of convective mixing within the open tunnels. Our results have shown that natural convection can indeed remove significant amounts of vapor from the heated fractured rock. For cases with relatively strong convective mixing, evaporative conditions will prevail over long stretches of emplacement drifts for several thousand years after emplacement. At early times, vapor is driven from the formation into the drifts by both convective flow (from pressure buildup caused by boiling) and diffusive flow (resulting from vapor concentration gradients). At later times, diffusive flow dominates.

SIGNIFICANCE OF FINDINGS

Compared to previous models that neglect in-drift convection, this new modeling approach predicts TH conditions that are much less favorable for seepage of formation water into emplacement drifts. Application of this method to drift seepage prediction models would significantly reduce the expected seepage rates at Yucca Mountain and thereby improve the predicted performance of the repository. The new model could also be used to assess innovative emplacement designs that deliberately utilize natural convection processes, to generate an in-drift environment beneficial to the performance of natural and engineered barriers (less seepage, less humidity).

RELATED PUBLICATIONS

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ACKNOWLEDGMENTS

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

A Temperature-Profile Method for Estimating Flow Processes in Geologic Heat Pipes

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RESEARCH OBJECTIVES

Above-boiling temperature conditions, as encountered, for example, in geothermal reservoirs and in geologic repositories for the storage of heat-producing nuclear wastes, may give rise to strongly altered liquid and gas flow processes. Evaluating the magnitude of such flux alterations is a challenging task, because the direct *in situ* measurement of such quantities is virtually impossible. Thermally induced fluxes can be particularly strong in geologic heat pipes, where vaporization and subsequent condensation of pore water creates a continuous recirculation at significant rates. The energy transported with these fluxes generates characteristic features in temperature profiles. We have developed a temperature-gradient method that uses these characteristic features to derive the flux perturbation occurring in geologic heat pipes. Since field measurements of temperature are relatively simple and accurate in subsurface systems, our method can offer fast and reliable first-order estimates of heat pipe fluxes.

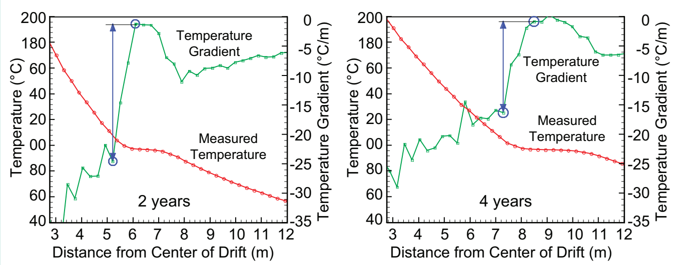

Figure 1. Temperature profiles measured in Borehole 137 of the Drift Scale Test at Yucca Mountain, at 2 years and 4 years of heating. Plot shows measured temperature at sensor location and average gradient between adjacent sensors. The blue arrow depicts the gradient difference at the boiling end of the heat pipe. The estimated liquid fluxes are 470 mm/yr at 2 years and 340 mm/yr at 4 years.

APPROACH

The detailed theoretical framework for the temperature-gradient method is presented in Birkholzer (2005a,b). In essence, differences between the temperature gradients measured at both sides of the boiling end of a heat pipe are used to estimate the amount of energy available to vaporize water (Figure 1). For stationary heat pipes, the estimated energy is directly proportional to the liquid reflux in the heat pipe. For transient heat pipes, some fraction of the supplied energy is used to change the temperature and to boil the resident pore water of downstream regions encountered when the heat pipe moves out from the heat source. Application of the method requires temperature profile data with sufficient resolution in time and space, knowledge of thermal properties, and a general idea of the geometry of heat transfer conditions. The starting point of each application is a thorough analysis of the measured temperature profiles. A valuable practice for identifying heat pipes and determining gradient differences is to calculate the gradients between two adjacent sensors and to plot these together with the temperature profile (Figure 1).

ACCOMPLISHMENTS

The proposed method was tested in comparison with various one-dimensional and two-dimensional example cases in porous and fractured media, for which model simulations were conducted to provide simulated temperature and flux results. The temperature results were fed as "measured data" input to the temperature-gradient method. It turned out that the fluxes estimated from applying the temperature-gradient method to these "measured data" were in excellent agreement with the simulated fluxes, demonstrating that the temperature-gradient method works in principle. In a second step, a temperature-profile analysis was performed with measured data from a large-scale *in situ* heater test at Yucca Mountain, demonstrating the general feasibility of the method in field situations. Fluxes were estimated for selected boreholes drilled from the heated tunnel in a vertical direction into the surrounding rock. All boreholes showed clearly detectable heat-pipe signatures, as evident from strong temperature-gradient changes and extended constant-temperature plateaus. The maximum fluxes estimated from the temperature-gradient method were as high as 470 mm/yr—much larger than site ambient percolation.

SIGNIFICANCE OF FINDINGS

The proposed temperature-gradient method offers a promising approach for quantifying liquid and gas flow processes in complex thermal-hydrological settings. The flux estimates obtained for the large-scale heater test at Yucca Mountain provide an additional piece of evidence for calibrating and validating numerical simulation models for predicting future thermal-hydrological conditions at Yucca Mountain.

RELATED PUBLICATIONS

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ACKNOWLEDGMENTS

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

Analyzing Drift Seepage at Yucca Mountain in a Performance-Assessment Framework

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RESEARCH OBJECTIVES

In relation to the proposed geologic repository for high-level radioactive wastes at Yucca Mountain, seepage is defined as the amount of water that drips into the waste emplacement tunnels (drifts), potentially contacting waste packages and dissolving the waste form. Predicting the amount of seepage into drifts is thus essential in assessing the long-term performance of the proposed repository. The Total System Performance Assessment Model (TSPA Model) for Yucca Mountain therefore evaluates the amount and spatial distribution of drift seepage. In support of TSPA, we have developed an integrated probabilistic–deterministic seepage module for the TSPA Model, a module that accounts for the spatial and temporal variability and inherent uncertainty of all seepage-relevant properties and processes. This module calculates the seepage rate (amount of seepage per time) and the seepage fraction (the fraction of waste packages affected by seepage) as a function of time and location in the repository.

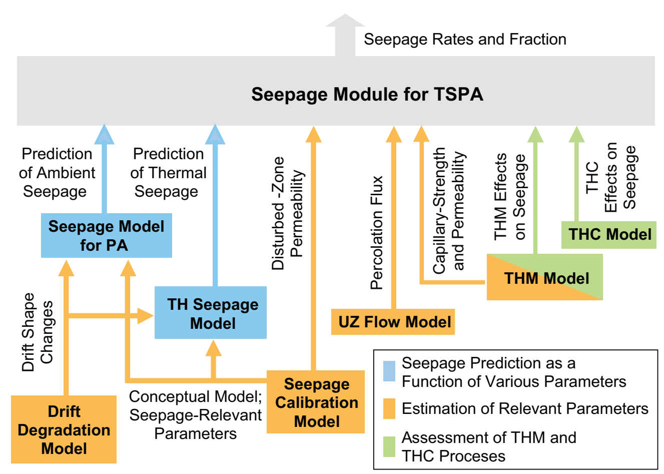

Figure 1. Schematic showing information flow between various predictive process models and the seepage module for TSPA

APPROACH

The basic processes involved in seepage phenomena in unsaturated fractured tuff have been presented elsewhere (e.g., BSC, 2004). In short, experimental and modeling studies have demonstrated that seepage at ambient, idealized conditions can be described as a function of a few key hydrological properties. Using various data sources from site characterization, *in situ* testing, and predictive modeling, we developed appropriate spatial variability and uncertainty distributions for these key properties. Additional factors important for seepage are, for example, flux perturbations as a result of increased temperatures near heat-producing waste packages, changes in hydrological properties caused by mechanical and chemical effects, changes in the drift shape caused by drift degradation, and the presence of rock bolts used for ground support (see Figure 1). Information on these factors was available from various experimental and modeling studies, but not enough to allow for a probabilistic treatment. Our seepage module therefore involves two steps: First, ambient seepage at idealized conditions is calculated based on a probabilistic approach that accounts for the variability and uncertainty of seepage-relevant properties at ambient conditions. Second, the impact of additional factors affecting seepage is evaluated by adjusting the probabilistic seepage rates in a simplified, deterministic manner, based on input provided from various experimental and modeling studies (e.g., studies evaluating geomechanical and geochemical processes at Yucca Mountain). To incorporate uncertainty, the simplifications made in this second step realistically bound the expected seepage behavior.

ACCOMPLISHMENTS

A seepage module was developed that incorporates processes and properties relevant for seepage estimation, yet is sufficiently simple, efficient, and transparent such that it can be incorporated into the overall performance assessment of the proposed geological repository at Yucca Mountain. The new seepage module is a key element of the TSPA Model supporting the license application of the proposed Yucca Mountain repository.

SIGNIFICANCE OF FINDINGS

Results from the integrated probabilistic–deterministic seepage model show that the fraction of waste canisters affected by seepage will be rather small over the lifespan of the repository. The seepage rates are usually much smaller than the local percolation fluxes arriving at drift sections. These findings illustrate the importance of the natural barrier formed by the unsaturated rock at and above the repository horizon.

RELATED PUBLICATION

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ACKNOWLEDGMENTS

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

Nopal I Uranium Deposit as an Analogue for Radionuclide Transport

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RESEARCH OBJECTIVES

The primary objective of this collaborative analogue study is to develop conceptual and numerical models for radionuclide transport at the Nopal I uranium (U) mine in the Peña Blanca district, Chihuahua, Mexico. These models can be used to evaluate the Yucca Mountain Total System Performance Assessment (TSPA) model. The models will be constrained through field and laboratory studies of the geology, geochemistry, and hydrology of the Nopal I system.

APPROACH

The Nopal I deposit has a number of characteristics that are similar to those of the planned high-level waste repository at Yucca Mountain, characteristics that make it a good analogue for evaluating the long-term transport of radionuclides. Both areas have thick (>200 m) unsaturated zones, are located in Basin and Range horst structures comprised of Tertiary rhyolitic ash-flow tuffs overlying limestones, and have semi-arid to arid climates. In addition, the secondary uranium mineral assembly at Nopal I is similar to the fuel rod alteration assemblage predicted to develop within a geologic repository.

This study consists of eight different subprojects that are being conducted jointly by researchers at Berkeley Lab, Los Alamos National Laboratory, University of Tennessee-Knoxville, University of Texas-El Paso, the University of Southern California, the Instituto de Ecología, and the Autonomous University of Chihuahua. Berkeley Lab is a primary participant in four of these research areas: (1) characterization of rock and hydrologic properties; (2) adit seepage studies; (3) characterization of the role of colloids in radionuclide transport; and (4) development of numerical flow and transport models.

Figure 1. Photomosaic of back (ceiling) of +00 adit of Nopal I mine. Seepage occurs preferentially along the iron stained fracture within the left frame. Metal frame (12′ by 5′) is part of a seepage collection system.

ACCOMPLISHMENTS

Work completed thus far includes the characterization of the stratigraphy for the Nopal I area, collection of representative samples of each unit from the PB-1 core for rock-property measurements, and installation of a seepage collection system and characterization of fractures within the +00 adit (Figure 1). To develop a hydrologic flow model for the region, we have also collected water samples from wells, springs, and the adit, reviewed regional hydrologic data, and conducted water table measurements in wells in the Nopal I area. Future work includes refining the hydrologic model, completing rock-property analyses, conducting seepage studies within the adit, and developing conceptual and numerical models for fluid flow, colloids, and radionuclide transport.

SIGNIFICANCE OF FINDINGS

Initial results from the hydrologic study indicate that the primary subsurface flow direction is towards the Laguna El Cuervo basin to the east. Seepage within the adit appears to be focused along specific faults and fractures, suggesting that flow through the welded ash-flow tuffs is dominated by fracture flow. The concentrations of U in water collected from wells immediately adjacent to the deposit are significantly higher than those recorded in regional water wells (< 10 ppb), but these concentrations have steadily declined with time, suggesting that the initial elevated values (up to >10 ppm) were caused by contamination resulting from drilling.

RELATED PUBLICATIONS

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ACKNOWLEDGMENTS

This work was supported by the Director, Office of Civilian Radioactive Waste Management, Office of Science and Technology and International, of the U.S. Department of Energy under Contract No. DE-AC03-76SF00098.

Calibration of a Large-Scale Groundwater Flow Model Using Transient Pressure Data

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RESEARCH OBJECTIVES

It is quite challenging to build a reliable model for simulating groundwater flow in a large body of rock mass, particularly when the rock is fractured. Large-scale groundwater flow models are typically calibrated to the steady-state pressure head data. However, because steady-state head data are largely controlled by the boundary conditions and less sensitive to the permeability structure, they alone are not sufficient for building a reliable predictive model. Large-scale, active stressing of the system can help greatly increase the reliability of the model. The overall objective of this project is to develop a methodology for reducing the uncertainty and increasing the reliability of such a model.

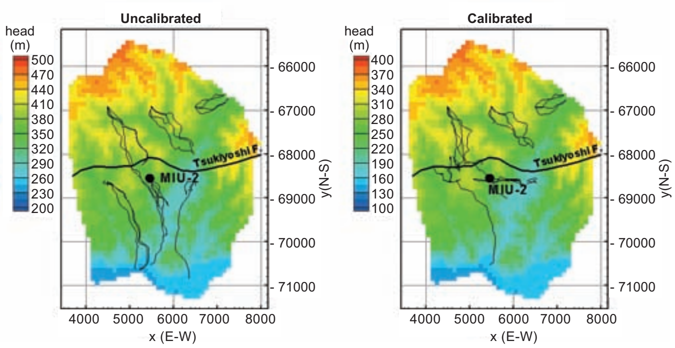

Figure 1. Particle trajectories before and after calibration. Travel times increase by a factor of 100 primarily due to decreases in permeability and increases in porosity. Well MIU-2 and the surface trace of the Tsukiyoshi fault are also shown. Well MIU-2 intersects the fault at a depth of approximately 1,000 m.

APPROACH

Starting with regional geographic, geologic, surface and subsurface hydrologic, and geophysical data for the Tono area in Gifu, Japan, we developed an effective continuum model to simulate subsurface flow and transport in a 4 km × 6 km by 3 km thick fractured granite rock mass overlain by sedimentary layers. Continuum permeability and porosity distributions are assigned stochastically, based on well-test data and fracture density measurements. Lithologic layering and one major fault—the subvertical, E-W striking, Tsukiyoshi Fault—are assigned deterministically. Well MIU-2 penetrates through the Tsukiyoshi fault, and when a packer system was removed prior to long-term pump tests, the open wellbore provided a high-permeability pathway for flow from the high-head foot wall, to the lower-head hanging wall. The pressure in the foot wall declined, and the pressure in the hanging wall increased in response. Thus, the removal of the packer effectively created two simultaneous well tests. We use this transient pressure response to the packer removal in Well MIU-2, in addition to the steady-state hydraulic head profiles of several wells in the MIU area, to calibrate the model. The calibrated model is then used to predict travel times from specified monitoring points to the model boundaries.

ACCOMPLISHMENTS

We successfully constrained a groundwater flow model by using transient pressure data. The disturbance caused by the removal of a packer string in effect served as an inadvertent large-scale well test. We concluded that the effective porosity of granite may be one to two orders of magnitude larger than that previously predicted. The calibration process serves to lengthen the travel times through the model by a factor of about 100.

SIGNIFICANCE OF FINDINGS

Large-scale pressure tests may be an effective tool for estimating the large-scale porosity of a large body of granite.

RELATED PUBLICATION

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ACKNOWLEDGMENTS

This work was supported by Taisei Corporation of Japan, through the U.S. Department of Energy Contract No. DE-AC03-76SF00098.

Estimating Large-Scale Permeability by Using Independent Lines of Evidence

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RESEARCH OBJECTIVES

In hydrogeological characterization of sedimentary rocks, the hydraulic properties of faults and caprock structure play a key role in determining the flow and transport through the formation. Although the reliability of a hydrogeological model usually increases with the amount of geologic and hydrogeologic data obtained (mainly from boreholes), it is nonetheless important to construct a model using limited available data at an early stage of the field investigation, and continue to refine the model as more data become available. The objective of this study is to develop an effective methodology for refining and improving a model incorporating both hydrologic and nonhydrologic data.

APPROACH

The numerical inversion code iTOUGH2 was applied to a 40 km × 40 km × 5 km area of the Horonobe Underground Research Laboratory (URL) site in Hokkaido, Japan. The basic hydrogeological model was constructed using existing geological survey data, assuming a low-permeability caprock. The top boundary was set as the fixed head boundary at the ground surface, and the bottom and lateral boundaries were closed. Using the steady-state hydraulic head distribution from some ten boreholes as the observation data, the permeability of the caprock was calculated using numerical inversion.

The steady-state hydraulic head distribution was well reproduced by the model. However, the recharge estimate from river flow data indicates that the average permeability of the hydrogeologic model should be approximately 20 times larger than the original estimate based on borehole tests. In addition to hydraulic head data, groundwater temperature data at the nearby hot spring and the salt concentration data at two boreholes were available. Using all these data, we carried out heat flow and saltwater washout simulation with TOUGH2-EWASG, varying the permeability values. The initial salt concentration was set as that of seawater throughout the model, and the top boundary was set as that of a constant freshwater boundary.

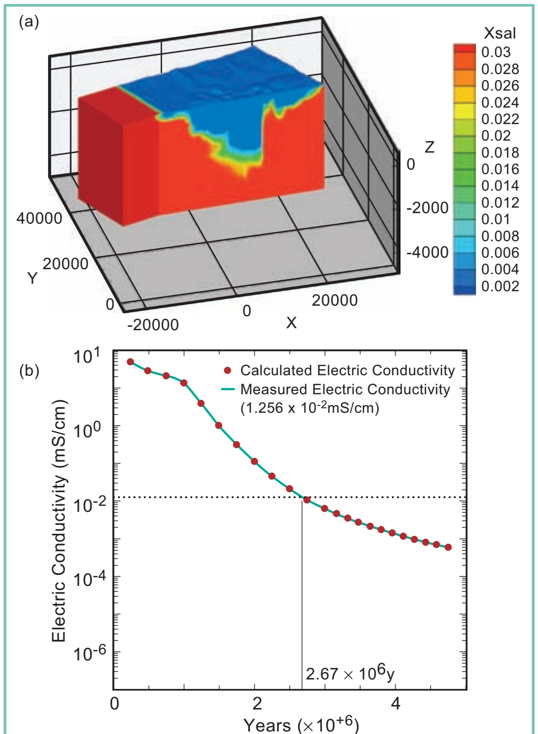

Figure 1. Result of saltwater washout simulation: (a) salt concentration distribution after 2 million years; (b) time-dependent change of electric conductivity at a monitoring borehole

ACCOMPLISHMENTS

Results from the hydrothermal simulations indicate that the permeability should be increased by ~20–50 times to match the temperature data observed in the borehole at the nearby hot spring area. This result is consistent with the permeability estimation based on the recharge rate.

Saltwater washout simulation with the increased permeability also corroborates the 20-fold increase. Figure 1 shows the salt concentration distribution after 2 million years and the electric conductivity distribution along a monitoring borehole. After 2.7 million years, the salt concentration matches with the observed electrical conductivity data. The geological survey indicated that the age of the sedimentary rocks in this area is no more than several million years.

SIGNIFICANCE OF FINDINGS

This work is an example of how independent lines of evidence can be used to enhance confidence in a hydrologic model. Hydrothermal and salinity simulations both corroborated a substantial increase in the average permeability, based on the river flow data. These results show that the use of nonhydraulic data for the calibration of a hydrological model can reduce uncertainties in the large-scale model, enabling a more realistic model to be constructed.

RELATED PUBLICATIONS

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ACKNOWLEDGMENTS

This work has been supported by Japan Nuclear Cycle Development Institute (JNC) under U.S. Department of Energy Contract No. DE-AC03-76SF00098.

Finding the Drift Shadow in Nature

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RESEARCH OBJECTIVES

The drift shadow is a region (within the unsaturated zone) of limited water flow and chemical transport beneath an underground opening, such as a cave or mined tunnel. This region is partially sheltered from downward-percolating water by the existence of the opening and preserved because capillarity is not strong enough to immediately draw the water laterally back under the opening (see Figure 1). Because the drift shadow is sheltered, there is less water there, and the water present moves slower than in other regions; thus, transport rates there are reduced. The drift shadow has not been observed in nature, but its existence has been predicted by analytical and numerical models of flow and transport through unsaturated media. Our research objective is to demonstrate the presence of the drift shadow in nature.

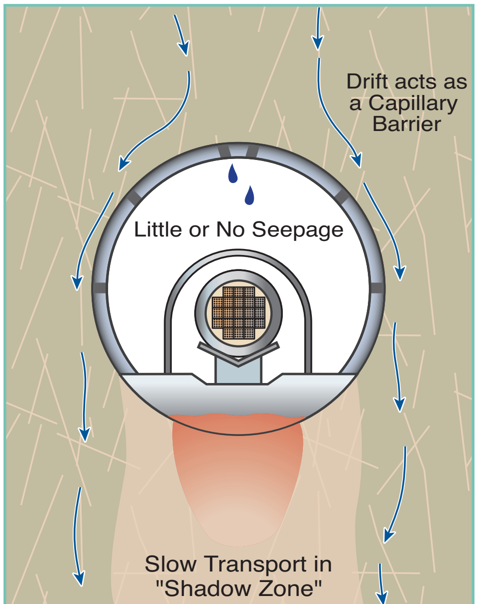

Figure 1. Conceptual model of flow around a drift showing the capillary barrier at the drift crown, and the drift shadow below the drift.

APPROACH

We will use passive and active tests at a field site to demonstrate the drift shadow presence. Passive tests will include making measurements of water potential in the rock surrounding a drift, analyzing geochemical signals caused by the drift shadow, and using ground-penetrating radar and neutron logging to measure the water content of rock surrounding the drift. Active tests could include introducing water with or without tracers above an existing drift, and looking for the presence and concentration of the tracer at locations around the drift. The field measurements will be compared with a detailed site-specific model, to build confidence in the ability to model unsaturated flow.

ACCOMPLISHMENTS

Extensive modeling of the drift shadow has been performed to understand the theoretical definition and drift shadow extent for various sets of conditions. The results of this modeling effort have led to refined site-selection criteria. Many potential analogue sites, including caves, mines, and concrete pads, have been investigated and evaluated, and we have tentatively selected the Hazel-Atlas sand mine in Antioch, California, a mine that has been closed since the 1940s. Preliminary cores have been obtained and analyzed for moisture. Chemical and mineralogical analyses and measurements to obtain hydrological parameters are in progress.

SIGNIFICANCE OF FINDINGS

Demonstration of the presence of a predicted drift shadow will provide another line of evidence to build confidence in the theory of flow and transport in unsaturated media and its numerical extension. In addition, it will allow the consideration of significantly reduced rates of transport from waste emplacement drifts at the proposed high-level nuclear waste repository at Yucca Mountain, Nevada, where waste canisters are expected to be placed in near-horizontal drifts in the unsaturated zone.

RELATED PUBLICATION

Houseworth, J.E., S.A. Finsterle, and G.S. Bodvarsson, Flow and transport in the drift shadow in a dual-continuum model. Journal of Contaminant Hydrology, 62–63, 133–156, 2003. Berkeley Lab Report LBNL-49868.

ACKNOWLEDGMENTS

This work was supported by the Director, Office of Civilian Radioactive Waste Management, Office of Science and Technology and International, of the U.S. Department of Energy under Contract No. DE-AC03-76SF00098.

Confirmation of the Scale Dependence of the Effective Matrix Diffusion Coefficient

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RESEARCH OBJECTIVES

Matrix diffusion in fractured rock refers to the exchange (through molecular diffusion) of solute mass between fractures and surrounding rock matrix. Owing to the much slower water velocity in the rock matrix compared to fractures, matrix diffusion can significantly retard contaminant transport and increase the spreading of a contaminant plume. The effective matrix diffusion coefficient is an important parameter controlling this process. Matrix-diffusion-coefficient values measured from small-scale rock samples in the laboratory have often been used for modeling large-scale contaminant transport processes at many different sites, including the proposed Yucca Mountain nuclear waste repository site. In a recent study, Liu et al. (2003) indicated that the effective matrix diffusion coefficient may be scale dependent and generally increases with test scale. The major objective of this work is to confirm this scale-dependent behavior, based on a data set from a comprehensive literature survey.

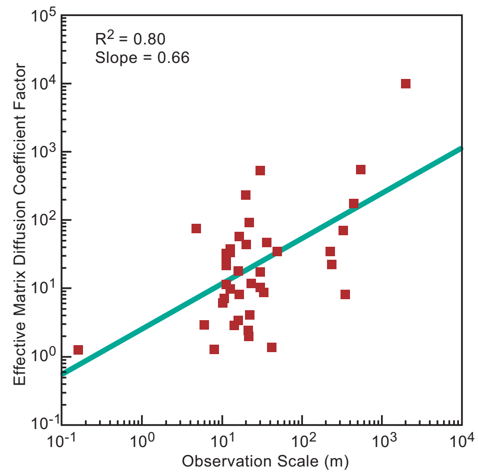

Figure 1. Effective matrix diffusion coefficient factor as a function of test scale

APPROACH

We conducted a comprehensive literature survey of field tracer tests, with scales ranging from 5 to 2,000 m and corresponding effective diffusion coefficient values (Zhou et al., 2005). Forty field tracer tests at 15 fractured geologic sites were selected for this study, based on data availability and quality. For the field tracer tests without reported matrix-diffusion-coefficient values, reanalysis of the tracer breakthrough curves was performed to calibrate transport parameters that included the effective matrix diffusion coefficient. This reanalysis was conducted using an analytic solution for linear flow and a semi-analytic solution for radial flow. To compare data from tests associated with different tracers, we compiled the ratio of an estimated effective matrix diffusion coefficient to its local value (corresponding to a small core sample), called the "effective matrix-diffusion-coefficient factor," as a function of test scale (Figure 1).

ACCOMPLISHMENTS

Based on results from the comprehensive literature survey (Figure 1), our work confirms that the effective matrix diffusion coefficient is scale dependent and generally increases with test scale. In addition, the surveyed data indicate that field-scale longitudinal dispersivity also increases with observation scale, which is consistent with previous studies. A preliminary explanation for the scale dependence of the effective matrix diffusion coefficient was reported in Liu et al. (2003), based on the argument that solute travel paths in a fracture network are fractal, and therefore the fractal-matrix interface area (contributing to the effective matrix diffusion coefficient) is scale dependent. Further investigation into the scale-dependence mechanisms is ongoing.

SIGNIFICANCE OF FINDINGS

While the scale dependence of permeability and dispersivity has been an active research topic for many years, this study confirms that the effective matrix diffusion coefficient, an important parameter controlling matrix diffusion processes, is also scale dependent. This finding has many important implications for problems involving matrix diffusion. For example, the performance of the Yucca Mountain site may be significantly underestimated when this scale dependence is not considered. This is because a large degree of matrix diffusion significantly retards radionuclide transport and decreases the concentration of (by increasing the spreading of) the radionuclide plume.

RELATED PUBLICATIONS

Liu, H.H., G. Zhang, and G.S. Bodvarsson, The active fracture model: Its relation to fractal flow behavior and a further evaluation using field observations. Vadose Zone Journal, 2, 259–269, 2003. Berkeley Lab Report LBNL-52824.

Zhou, Q., H.H. Liu, F.J. Molz, Y. Zhang, and G.S. Bodvarsson, Field-scale effective matrix diffusion coefficient for fractured rock: Results from literature survey. Water Resour. Res. (in review), 2005. Berkeley Lab Report LBNL-57368.

ACKNOWLEDGMENTS

This work was supported by the Director, Office of Civilian Radioactive Waste Management, Office of Science and Technology and International, of the U.S. Department of Energy under Contract No. DE-AC03-76SF00098.

Neptunium Solubility Effect in the Unsaturated Zone at Yucca Mountain

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RESEARCH OBJECTIVES

The mobility of radionuclides (such as neptunium) in natural waters is affected by various factors—acidity, oxidation and reduction (redox) states, temperature, and aqueous composition. At Yucca Mountain, where high-level nuclear waste is to be stored in an underground geological repository, it is especially important to know the solubility of radionuclide minerals, because their solubility determines whether they will precipitate at this site. This study is aimed at evaluating the use of solubility models, in conjunction with aqueous chemical data, to quantify the mobility of radionuclides in the Yucca Mountain unsaturated zone.

APPROACH

The solubility of neptunium (Np) minerals was investigated using two representative controlling solids, the moderately soluble $Np_2O_{5(s)}$ and the highly insoluble $NpO_{2(c)}$ among a total of nine known Np minerals. Aqueous speciation is calculated in terms of each of the controlling solids, assuming equilibrium and employing the thermodynamic databases generated from the Yucca Mountain Project and the pertinent literature. A fixed concentration of total carbonate was used for speciation calculations.

ACCOMPLISHMENTS

Solubility calculations provide new insights into the behavior of Np nuclides in the unsaturated zone at Yucca Mountain. Results (Figure 1) emphasize the effects of pH and the redox potential, Eh. The effect of temperature was also investigated, and the solubilities of all the Np minerals were compared. Np solubility drops about 1 to 2.5 orders of magnitude in response to the pH conditions in the flow paths, which are slightly acidic in waters contacting waste package surfaces, and slightly alkaline in pore water within the tuffs of the Topopah Spring (TSw) and Calico Hills (CHn) units. The solubility of Np decreases with rising temperature. When the temperature rises from 25°C to 100°C, the solubility drops about 1 to 1.5 orders of magnitude.

SIGNIFICANCE OF FINDINGS

Solubility data provide chemical evidence of radionuclide precipitation as a likely mechanism for naturally enhanced radionuclide retardation in the Yucca Mountain unsaturated zone. The trends for Np_2O_5 solubility also hold for the highly insoluble NpO_2, and the solubility of the latter is in a comparable order of magnitude to that of the former at higher redox conditions. The results indicate that solubility investigations could provide a method by which to evaluate the mobility of radionuclides in natural systems.

RELATED PUBLICATION

Lu, G., Impact of neptunium solubility on radionuclide retardation in the unsaturated zone at Yucca Mountain. Applied Geochemistry (submitted), 2005.

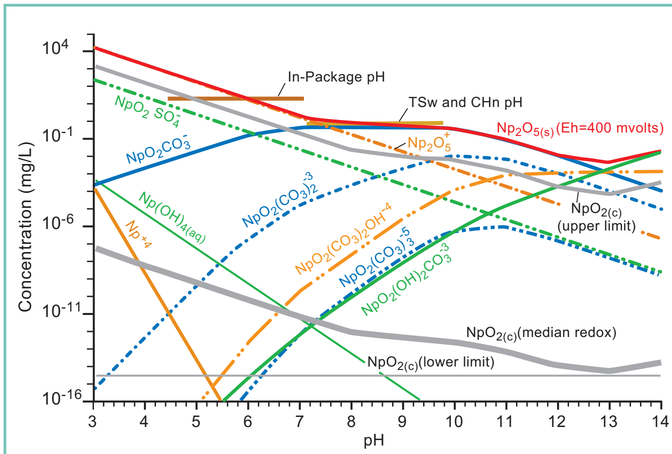

Figure 1. Calculated $Np_2O_{5(s)}$ solubility of neptunium (total aqueous carbonate = 115 mg/L, $[SO_4^-]$ = 60 mg/L, temperature at 25°C, and Eh at 400 mV for $Np_2O_{5(s)}$), contributing species are in color. In the background are total solubility curves (in solid gray) for $NpO_{2(c)}$, with Eh covering the water redox stability field ranges.

ACKNOWLEDGMENTS

This work was supported by the Director, Office of Civilian Radioactive Waste Management, U.S. Department of Energy, through Memorandum Purchase Order EA9013MC5X between Bechtel SAIC Company, LLC, and the Ernest Orlando Lawrence Berkeley National Laboratory (Berkeley Lab). The support is provided to Berkeley Lab through the U.S. Department of Energy Contract No. DE-AC03-76SF0098.

Impact of Coupled Thermal-Hydrological-Chemical Processes on Seepage Into Emplacement Drifts at Yucca Mountain

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RESEARCH OBJECTIVES

Seepage refers to flow of liquid water into the emplacement drifts (tunnels) at the proposed repository site of Yucca Mountain. Seepage may enhance corrosion of waste packages, resulting in release of radioactive materials from the drifts into the surrounding rock. Understanding seepage is therefore critical for reliable prediction of repository performance. Substantial experimental and modeling studies have been undertaken to investigate seepage under ambient conditions. These studies have concluded that seepage (or its absence) is controlled by the fracture permeability heterogeneity and fracture capillary strength parameters of the repository host rock. Additionally, models have been developed to analyze the impact of coupled thermal-hydrological (TH) processes on seepage. These TH models have predicted that seepage at Yucca Mountain could occur only under considerably elevated infiltration fluxes. In this study, it is demonstrated that other factors may also influence seepage, particularly the coupled thermal-hydrological-chemical (THC) changes in the host rock.

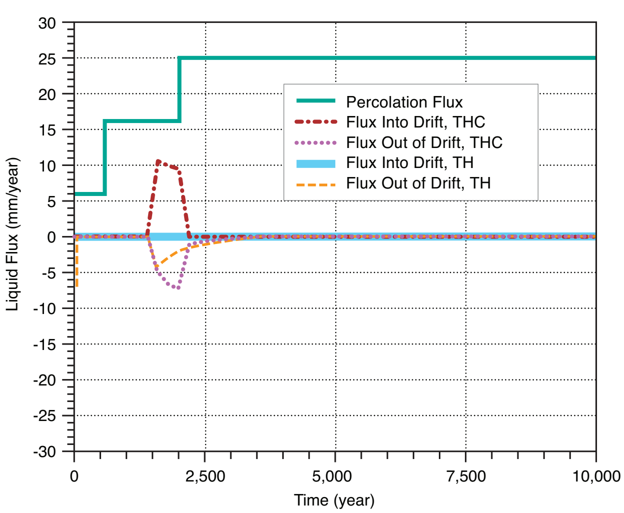

Figure 1. Seepage prediction for TH and THC simulations

APPROACH

Heat emanating from the waste keeps rock temperatures near the emplacement drifts above boiling for a considerable period of time. Boiling of water generates vapor that migrates away from the drifts, then condenses in cooler regions and drains through the fracture network, resulting in redistribution of moisture. The elevated temperature and moisture redistribution also cause changes in pore-water and gas compositions, as well as mineral dissolution and precipitation. Mineral dissolution and precipitation can result in porosity and permeability changes in the rock, which lead to altered flow paths and flow focusing. In this study, these THC processes are simulated with the TOUGHREACT reactive transport software. TH and THC simulations are performed in a two-dimensional vertical model domain extending from the ground surface to the water table. Heterogeneous fracture-permeability distributions are generated using measured air-permeability data from the host rock. The fracture capillary strength parameter of the host rock is obtained by calibrating data from ambient liquid-release tests at Yucca Mountain. Fractured rock is modeled as two separate but interacting continua, one for the rock matrix and the other for the fractures.

ACCOMPLISHMENTS

The impact of THC processes on seepage can be seen in Figure 1, which shows the amount of water entering and exiting the emplacement tunnel for one realization of the heterogeneous permeability field. Infiltration fluxes are shown with the solid green lines. The model predicts a finite amount of seepage between 1,400 and 2,000 years with the THC simulations. However, when only TH processes are simulated, no seepage is observed. (This can be attributed to the THC Processes of mineral precipitation and dissolution altering the porosities and permeabilities of the rock. They also introduce dynamic heterogeneities in the capillary characteristics. Such changes in hydrologiic properties causes focusing of flow into zones of higher permeability, leading to seepage even under circumstances not predicted by ambient or TH-only simulation.)

SIGNIFICANCE OF FINDINGS

Alternations in hydrological properties, arising from coupled THC processes, may lead to local flow focusing and seepage even under nonelevated infiltration fluxes. Further experimental and modeling studies are therefore needed to study hydrological property changes caused by THC processes.

RELATED PUBLICATION

Mukhopadhyay, S., E.L. Sonnenthal, and N. Spycher, Impact of coupled thermal-hydrological-chemical processes on seepage into emplacement tunnels in unsaturated fractured rock. Journal of Hydrology (in preparation), 2005.

ACKNOWLEDGMENTS

This work was supported by the Director, Office of Civilian Radioactive Waste Management, U.S. Department of Energy, through Memorandum Purchase Order QA-B004220RB3X between Bechtel SAIC Company, LLC and the Ernest Orlando Lawrence Berkeley National Laboratory (Berkeley Lab). The support is provided to Berkeley Lab through the U.S. Department of Energy Contract No. DE-AC03-76SF00098.

Infiltration-Seepage Responses: Effects of Capillary Barriers on Flow Partitions

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RESEARCH OBJECTIVES

Possible water seepage into waste emplacement tunnels (drifts) in response to infiltration at the land surface is a major concern for performance evaluation of the proposed nuclear waste repository at Yucca Mountain, Nevada. To address this issue, investigators have recently conducted an infiltration seepage experiment at the site. However, data collected from this experiment showed complicated infiltration-seepage responses that were difficult to interpret, even with a sophisticated multiple-continuum numerical model. The objectives of this work are (1) to study the coupled effects of different processes on infiltration-seepage responses, and (2) to develop a more realistic 3-D numerical model that could quantitatively interpret the measured seepage into the alcove, as well as analyze the conditions under which seepage into drifts could occur.

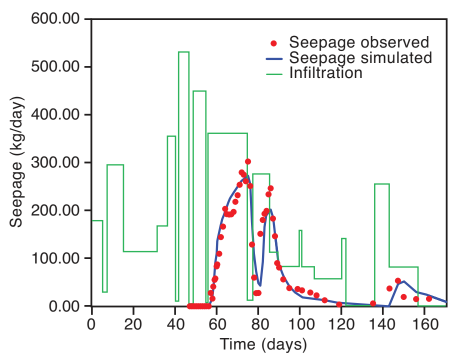

Figure 1. Comparison between the simulated (blue line) and the observed (red dots) seepage responses under given infiltration (light green line).

APPROACH

In the infiltration-seepage experiment, infiltration water was applied to the land surface through a drip irrigation system. The resulting seepage was collected and measured in an alcove 32 m below, sealed by a bulkhead (door). The basic approach for this study was to (1) incorporate site information about the flow system, and realistic experimental conditions into the previous model; (2) refine conceptual framework for the 3-D numerical model; (3) match model predictions to the observed seepage data, and to identify underlying key processes and mechanisms.

Specifically, the following new features were incorporated in the developed model:

- A sloping (about 40%) land surface with a soil cover of 30 cm is included in the numerical model. The soil layer is represented as a single continuum porous medium.
- A unique third L-continuum is introduced into the model to represent the portion of the fractured tuff that is not included in either F-continuum (the fast flow path) or M-continuum (the extremely slow flow path).
- The general flow simulator TOUGH2 was modified to accommodate the above features.

ACCOMPLISHMENTS

A 3-D, triple-continuum numerical model was developed to successfully simulate water percolation through fractured porous media. The simulated seepage compared well with the measured data. Furthermore, it was observed that seepage, in responding to the infiltration pulse, is highly nonlinear (Figure 1). When the internal saturation was low, even high infiltration pulses could be entirely damped, and no seepage occurs. After an adequate saturation condition was established, the peak seepage responses to the infiltration pulses could be very quick (e.g., <1 day). However, the slower responses in the tailing part, as a result of contributions from the L- and M-continua, were still visible. When the infiltration rate was reduced to a certain level, almost no seepage was observed. A likely explanation for the above phenomena is that, on the way from the land surface to the alcove, several "lateral" flow paths "compete" for the water from seepage. These paths are (1) the downslope flow in the soil layer, (2) imbibition to the L- and M-continuum, and (3) flow into the fracture network outside of the collection area. The capillary barriers at the soil/tuff interface and the alcove ceiling act as two "lower dams" that regulate the flow partitions between the competing flow paths, working with the suction forces in the unsaturated media.

SIGNIFICANCE OF FINDINGS

Our new approach shows significant improvement over previous methods in capturing the observed infiltration-seepage responses and the percolation processes behind them. The results also show that seepage into an emplacement drift (which would be located deeper than the test alcove) would not likely occur under the current local (i.e., desert) climate and geological conditions at Yucca Mountain. However, special attention should be paid to the strongly broken zones (i.e., the zones along the deep faults) where natural capillary barriers may be weak.

RELATED PUBLICATION

Pan, L., K. Zhang, Y.S. Wu, and G.S. Bodvarsson, Percolation through heterogeneous fractured porous media under transient infiltration: Reconciling measured and predicted seepage into a mined opening. The 68th Annual Meeting for Soil Science Society of America, Seattle, Washington. Agronomy Abstracts. American Society of Agronomy, Madison, Wisconsin, Oct. 31–Nov. 4, 2004.

ACKNOWLEDGMENTS

This work was supported by the Director, Office of Civilian Radioactive Waste Management, U.S. Department of Energy, through Memorandum Purchase Order QA-B004220RB3X between Bechtel SAIC Company, LLC and the Ernest Orlando Lawrence Berkeley National Laboratory (Berkeley Lab). The support is provided to Berkeley Lab through the U.S. Department of Energy Contract No. DE-AC03 -76SF00098.

Coupled Thermal-Hydrological-Mechanical Modeling of an *In Situ* Experiment in Fractured Rock

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RESEARCH OBJECTIVES

The objective of this work is to increase our understanding of coupled thermal-hydrological-mechanical (THM) processes in unsaturated welded tuff, and to test a numerical simulator used for analysis of coupled THM effects at a proposed future geological nuclear waste repository at Yucca Mountain.

APPROACH

A numerical simulation of coupled multiphase fluid flow, heat transfer, and mechanical deformation was carried out to study the coupled THM processes involved in the Yucca Mountain Drift Scale Test (DST). Coupled THM processes, and the capability of the numerical simulator, TOUGH-FLAC, to model relevant coupled THM processes at the DST, were studied by comparison of numerical results to *in situ* measurements of temperature, water saturation, displacement, and fracture permeability. Of particular relevance in this study are thermally induced rock-mass stress and deformations, with associated changes in fracture aperture and fractured rock permeability.

ACCOMPLISHMENTS

Through the numerical analysis and by comparison to measured THM responses at the DST, an increased understanding of coupled THM processes in unsaturated fractured welded tuff was achieved. The generally good agreement between simulated and measured temperature, displacement, and changes in air permeability (Figure 1) indicated that the numerical model and underlying conceptual model were appropriate for simulating relevant coupled THM processes at the DST. Specifically, thermally induced rock-mass deformation and accompanying changes in fracture permeability were reasonably well predicted using a continuum elastic model, although some individual measurements of displacement and permeability indicated inelastic mechanical responses. It is concluded that fracture closure/opening caused by a change in thermally induced normal stress across fractures is an important mechanism for changes in intrinsic fracture permeability at the DST, whereas fracture shear dilation appears to be less significant. Observed and simulated maximum permeability changes at the DST are within one order of magnitude.

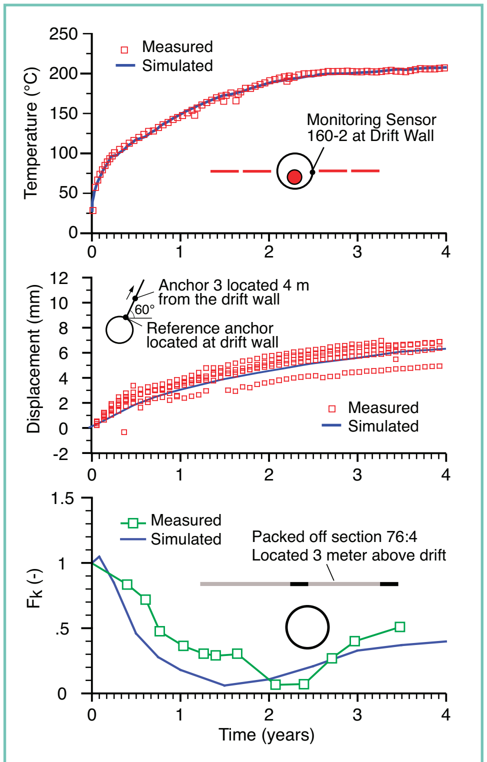

Figure 1. Comparison of simulated and measured temperature, displacement, and permeability change factors (Rutqvist et al., 2005b)

SIGNIFICANCE OF FINDINGS

A solid understanding of the underlying mechanisms for observed THM responses at the DST, including THM-induced changes in permeability, is essential for analysis of THM effects at a future repository at Yucca Mountain. Moreover, the observed and simulated maximum permeability changes at the DST are important information for bounding model predictions of potential changes in rock-mass permeability at a future repository.

RELATED PUBLICATIONS

Rutqvist, J., D. Barr, R. Datta, A. Gens, M. Millard, S. Olivella, C.-F. Tsang, and Y. Tsang, Coupled thermal-hydrological-mechanical analysis of the Yucca Mountain Drift Scale Test—Comparison of field results to predictions of four different models. Int. J. Rock Mech. & Min. Sci (in press), 2005a. Berkeley Lab Report LBNL-56267.

Rutqvist, J., Tsang, C.-F., and Y. Tsang, Analysis of coupled multiphase fluid flow, heat transfer, and mechanical deformation at the Yucca Mountain Drift Scale Test. Proceedings of the 40th U.S. Rock Mechanics Symposium, Anchorage, Alaska, USA, June 25–29, 2005: American Rock Mechanics Association ARMA, Paper No. 893, 2005b. Berkeley Lab Report LBNL-57323.

ACKNOWLEDGMENTS

This work was supported by the Director, Office of Civilian Radioactive Waste Management, U.S. Department of Energy, through Memorandum Purchase Order EA9013MC5X between Bechtel SAIC Company, LLC, and the Ernest Orlando Lawrence Berkeley National Laboratory (Berkeley Lab). The support is provided to Berkeley Lab through the U.S. Department of Energy Contract No. DE-AC03-76F00098.

Investigations of Flow in Fractured Welded Tuffs

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RESEARCH OBJECTIVES

Preferential flow in fractured rock suggests channeling of flow through a subsection of the possible flow field. In recent years, investigations evaluating sites for geological disposal of high-level nuclear waste have been particularly focused on preferential flow, because of the potential for rapid movement of water to waste containers, and the subsequent migration of radionuclides that could escape from these containers.

The broad objective of this research effort was to study flow in fractured welded tuff. Specifically, the goal was to identify and characterize flow paths that developed as water was released under ponded conditions along a 12 m^2 infiltration plot. Of particular interest were features of flow paths such as flow velocities, size, spatial distribution, and temporal dynamics.

APPROACH

This experiment involved the release of ~22 m^3 of ponded water (at a pressure head of ~0.04 m) over a period of 7 months, directly onto a 12 m^2 infiltration plot located on a fractured welded tuff surface. As water was released, changes in moisture content were monitored along an array of horizontal boreholes located in the formation ~19–22 m below, with specially designed sensors to detect the arrival and persistence of flow through fractured rock.

ACCOMPLISHMENTS

This investigation has provided insights into specific features of flow zones that developed from the ponded release of water into fractured rock. To our knowledge, such specific flow zone features in unsaturated fractured rock have not been observed in previous studies at this spatial (i.e., >20 m vertical flow) and temporal scale (i.e., months).

SIGNIFICANCE OF FINDINGS

Observations from this investigation suggest that existing conceptual models could be improved in their representation of some fundamental aspects of water movement through unsaturated fractured rock. Specifically:

- Flow encompasses numerous fractures of various sizes to form flow conduits. Therefore, rather than individual fractures, the geometry of the fracture network forming these flow conduits is likely the dominant mechanism controlling flow through fractured tuffs.
- The inclusion of numerous fractures in individual flow conduits suggests that the area across which fracture-matrix interactions occur is significantly greater than would be expected from a model of focused flow along a fracture.
- Gravity-driven flow can have a significant lateral component likely dictated by the geometry of fracture networks.
- Flow conduits do not necessarily interact.
- Capillary barriers may increase the area through which flow seeps into an excavated cavity, by diverting water from the ceiling to sidewalls.
- The range in velocities for the leading edge of flow paths suggests a vertical spread, rather than a uniform edge, to the wetting front.

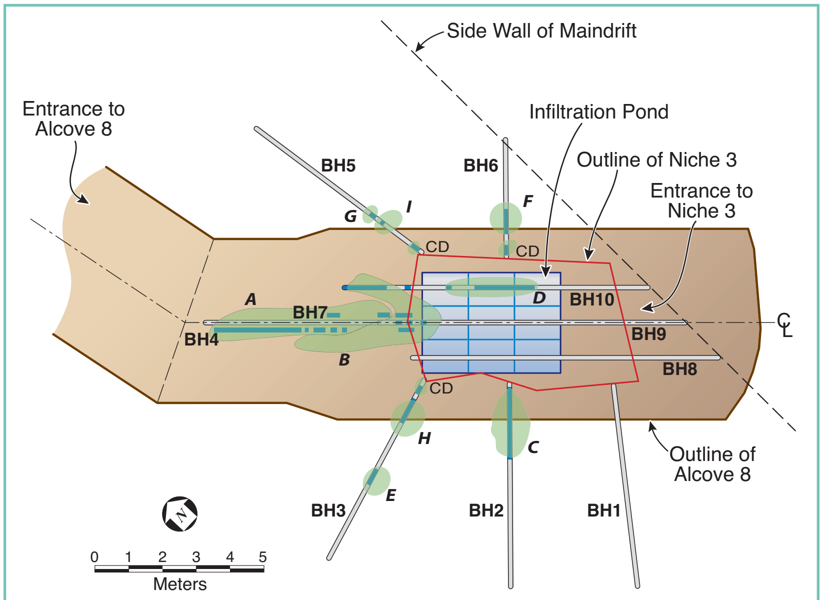

Figure 1. Plan view of the test bed showing the location of the infiltration plot (upper boundary) relative to monitoring boreholes surrounding Niche 3 (lower boundary). The letters A–H indicate the location of flow zones defined by wetting-front velocity and location.

RELATED PUBLICATION

Salve, R., Observations of preferential flow during a liquid-release experiment in fractured welded tuffs. Water Resour. Res. (in press), 2005. Berkeley Lab Report LBNL-56265.

ACKNOWLEDGMENTS

This work was supported by the Director, Office of Civilian Radioactive Waste Management, U.S. Department of Energy, through Memorandum Purchase Order QA-B004220RB3X between Bechtel SAIC Company, LLC, and the Ernest Orlando Lawrence Berkeley National Laboratory (Berkeley Lab). The support is provided to Berkeley Lab through the U.S. Department of Energy Contract No. DE-AC03-76SF00098.

Water Vapor Transport in an Underground Mined Opening

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RESEARCH OBJECTIVES

During periods of suppressed ventilation, liquid water was observed as droplets on nonporous surfaces (such as metal surfaces and cables) and small pools of water (<1 liter) on impermeable surfaces in one of two large tunnels (i.e., the Cross Drift) at Yucca Mountain (Figure 1). Rust on steel surfaces and dense mold populations on some nonmetallic nonporous surfaces also suggest the presence of water. However, despite the presence of liquid water, there has been no evidence to suggest that this water is from seepage through localized flow paths. We hypothesize that the observed water entered the nonventilated drift through natural fractures as water vapor, and then condensed along sections of the drift.

The goal of this research effort is to develop an understanding of water vapor dynamics in the near-drift environment at Yucca Mountain, specifically to:

- Identify conditions resulting in the transformation between liquid- and vapor-phase moisture (evaporation and condensation processes) in the near-drift environment.
- Evaluate microclimates created by the configuration of drifts.
- Quantify the potential movement of water vapor through ventilated and nonventilated drifts.
- Quantify rates at which surrounding rock will yield water vapor during continuous ventilation of drifts.
- Develop numerical models for vapor-phase movement of water in the near-drift environment.

APPROACH

Over the last four years, we have monitored temperature and relative humidity to understand the microclimate in the terminal section of the Cross Drift. We have compared these observations to results from analytical and numerical models, to investigate processes associated with the movement of water vapor between the tunnel bore and the surrounding fractured rock formation.

Future work will include the creation of thermal gradients in nonventilated sections of the drift, to study the development of microclimates as well as the processes of condensation and evaporation. Gas tracer tests will be performed to evaluate internal drift flow, drift-scale air dynamics, and interaction with the mountain air flow.

ACCOMPLISHMENTS

We have analyzed observations of moisture and temperature dynamics made along the terminal ~1.2 km of the Cross Drift, using three numerical models. These models included the advection of air through the mountain (a mixed tank model), molecular diffusion into the drift from a 100% relative humidity (RH) boundary at the drift wall, and diffusion of water vapor from a 100% RH boundary within the rock through the fracture network (with fluid flow assumed to be inactive) into the drift. Our analyses suggest that fractures can be primary paths for vapor flow driven by a potential gradient within the unsaturated zone in the immediate vicinity of emplacement drifts.

SIGNIFICANCE OF FINDINGS

A model that incorporates fracture-dominated vapor-flow conditions would be a strong departure from existing conceptual models, which postulate the overwhelming importance of liquid traveling through fractures as the primary water-transport mechanism. However, such a model is required to explain recent observations and may be required to predict moisture dynamics under conditions encountered in an operating repository.

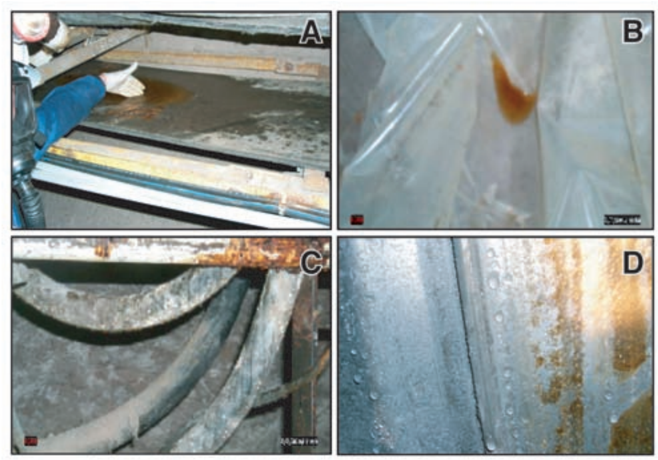

Figure 1. Observations of moisture in nonventilated sections of the Cross Drift: (A) pool of water on lower conveyor belt; (B) pool of water on plastic sheet; (C) mold on electrical cables and rust on metal surfaces; and (D) droplets on ventilation tube.

RELATED PUBLICATION

Salve, R., and T. Kneafsey, Vapor-phase transport in the near-drift environment at Yucca Mountain. Water Resour. Res., 41, doi:10.1029/2004WR003373, 2005. Berkeley Lab Report LBNL-55212.

ACKNOWLEDGMENTS

This work was supported by the Director, Office of Civilian Radioactive Waste Management, U.S. Department of Energy, through Memorandum Purchase Order QA-B004220RB3X between Bechtel SAIC Company, LLC, and the Ernest Orlando Lawrence Berkeley National Laboratory (Berkeley Lab). The support is provided to Berkeley Lab through the U.S. Department of Energy Contract No. DE-AC03-76SF00098.

A Model for Calcite Precipitation in an Elevated Geothermal Gradient at Yucca Mountain over 10 Million Years

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RESEARCH OBJECTIVES

In an earlier study, Xu et al. (2003) simulated the precipitation of calcite in the unsaturated zone (UZ) of Yucca Mountain over a ten million year (Ma) period and compared the results to data collected by the U.S. Geological Survey. The objective of this study was to evaluate the relationship between infiltration rate and calcite abundance; therefore, simulations were performed using the present-day geothermal gradient and a range of infiltration rates. Abundant evidence indicated that the majority of the calcite in the UZ precipitated from downward flowing water of meteoric origin. Recent fluid-inclusion data (from University of Nevada, Las Vegas) showed that calcite precipitated under elevated temperatures for several Ma. Temperatures in the Topopah Spring Tuff at the level of the Exploratory Studies Facility (ESF) prior to approximately 6 Ma may have been around 45–60°C, with a maximum value of 83°C. The latter findings have been used as evidence by some that hydrothermal circulation of upwelling fluids was responsible for the calcite. This new study evaluates the effect of an elevated geothermal gradient on calcite precipitation in the Yucca Mountain UZ.

APPROACH

Based on the temperature history inferred from fluid inclusions, a variable temperature lower boundary at the water table was developed to approximate the inferred paleotemperatures in the Topopah Spring Tuff. The temperature was set initially at 95°C at the base of the 1-D model at 10 Ma and allowed to decrease through conductive and advective cooling into the overlying rock and with the atmosphere. The infiltration rate was set to 5.92 mm/yr with a simplified geochemical system composed of primarily calcite and silica polymorphs as well as several aqueous and gaseous species. The simulation was carried out using the nonisothermal reactive geochemical transport code TOUGHREACT developed at Berkeley Lab.

ACCOMPLISHMENTS

Simulated calcite abundances under elevated temperatures, compared to those for the ambient geothermal gradient and the measured values, are shown in Figure 1. Somewhat greater abundances result from higher temperatures, yet the overall pattern and magnitude is similar to that for the steady-state ambient temperature distribution. Higher temperatures result in lower calcite solubility and somewhat higher calcite abundances, yet the abundances are dominated by the Ca flux into the unsaturated zone. The variable temperature simulation equally captures the U.S. Geological Survey measured data for the TCw, TSw, and CHn hydrostatigraphic units, and equally overestimates abundances in the PTn. Such deviations in the PTn may result from processes not treated in the simulations, such as reactions with feldspars and glass, and cation exchange with zeolites.

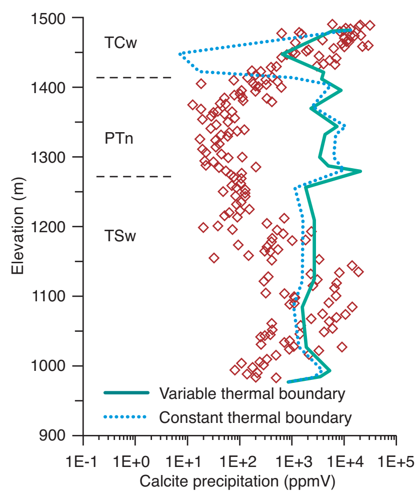

Figure 1. Total (fracture plus matrix) calcite abundances (volume fraction) obtained with two types of thermal conditions applied at the bottom boundary (WT-24 column, after 10 million years). Diamonds represent bulk rock calcite abundances measured by the U.S. Geological Survey.

SIGNIFICANCE OF FINDINGS

Even with a temperature of 95°C at the base of the UZ, the system remains unsaturated and gravity-driven flow is dominant, as opposed to hydrothermal circulation in saturated systems driven by differences in fluid density. The elevated temperatures showed somewhat greater abundances of calcite in most units compared to those at ambient temperature, yet the trends with depth are similar and did not change the overall relationship between calcite abundance and infiltration rate (as documented in the first study). Thus, the current study provides support for the widely held view that calcite precipitation was the result of downward infiltrating meteoric water at long-term average rates on the order of 10 mm/yr.

RELATED PUBLICATIONS

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ACKNOWLEDGMENTS

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

A Particle-Tracking Approach to Modeling Transport in a Complex Fracture

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RESEARCH OBJECTIVES

Nearly all of the studies of flow and transport in fractured rocks assume that a fracture can be modeled as an open space between two rock surfaces with constant or variable separation. Field observations of rock fractures have shown that a fracture in the field can in fact be much more complex. Recent studies indicate that a complex fracture can be characterized as a thin fracture zone having several interconnected subfractures (Figure 1), which can contain mechanically dislodged and chemically altered materials with enhanced porosity. Our objective is to develop a model for flow and transport through a fracture that incorporates these complexities.

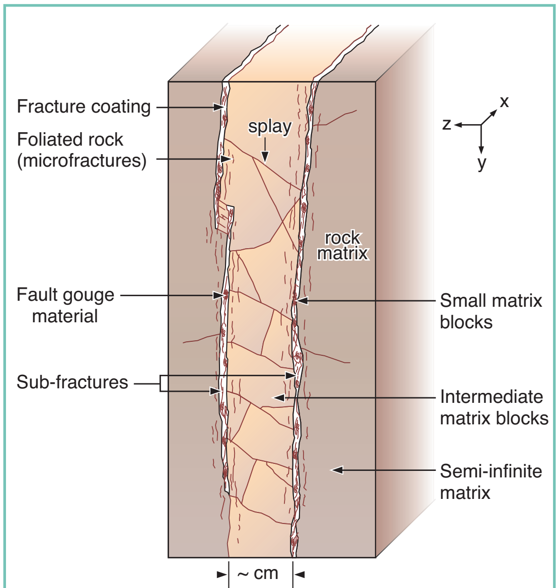

Figure 1. Structure of a complex fracture or master fault

APPROACH

We use a particle-tracking approach to calculate solute transport in a complex fracture, accounting for transmissivity variability over the fracture plane, and incorporating structures in the fracture thickness normal to the fracture plane. These structures include subfractures, dead-end pores, gouge materials, small blocks of altered rock, and the adjacent "semi-infinite" rock matrix. The subfractures provide alternative flow paths for advection, whereas the remaining features all provide material in which solute diffusion and sorption can occur (Figure 1). Flow through the fracture plane is calculated numerically using a finite-difference method, and advective transport is modeled with particle tracking. For each particle, flow is distributed among the subfractures; then, for each gridblock, a time delay is added to the advective residence time to account for diffusion and sorption into adjacent lower-permeability materials. The time delay for each particle is obtained stochastically, by inverting an analytical solution for diffusion and sorption into finite-sized matrix blocks.

ACCOMPLISHMENTS

The above approach has been applied to a field study of a single complex fracture on the 15 m scale. Fracture mapping and pump-test results were used to characterize the transmissivity distribution within the fracture plane. Tracer tests using sorbing and nonsorbing tracers were analyzed to infer the near-fracture parameters of the complex fracture model, including distribution of flow between subfractures as well as diffusion and sorption into gouge and intermediate matrix blocks. Short-term tracer tests are less sensitive to properties of the semi-infinite rock matrix, so laboratory analyses of unaltered rock samples should be used to obtain those properties. When considering time scales of thousands of years, as needed for nuclear waste storage performance assessment, properties of the semi-infinite matrix have a much more significant role. Results show that the proposed method is feasible, efficient, and can match field tracer-test data. Additionally, the parameter dependence and sensitivity are reasonable for both short-term (site characterization) and long-term (performance assessment) studies.

SIGNIFICANCE OF FINDINGS

If a simple fracture model, based on the conventional advective-dispersive equation, is used to match the tracer breakthrough curves obtained from a complex fracture, serious problems arise. In the simple fracture model, multiple flow paths within the fracture and diffusion and sorption into gouge materials and intermediate blocks are ignored, and thus their effects have to be represented by the property values of the semi-infinite rock matrix. This leads to calibrated values significantly larger than laboratory measurements of the rock matrix samples, which in turn leads to significant errors in long-term (performance assessment) models. This may be one significant source of the so-called scaling effect.

RELATED PUBLICATIONS

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ACKNOWLEDGMENTS

Work is supported by the Japan Nuclear Cycle Development Institute (JNC) through a bi-national JNC/DOE Agreement between JNC and the U.S. Department of Energy (DOE), under the overview of DOE's Office of Environmental Management, Office of Science and Technology, and conducted at the Ernest Orlando Lawrence Berkeley National Laboratory, under the auspices of DOE Contract No. DE-AC03-76SF00098.

A Mountain-Scale Thermal-Hydrological Model for Evaluating Repository Thermal Effects on Multiphase Flow in the Yucca Mountain Unsaturated Zone

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RESEARCH OBJECTIVES

The primary objective of this study is to develop a multidimensional, mountain-scale, thermal-hydrological (TH) numerical model for investigating the impact of decay heat from radioactive waste on unsaturated flow behavior at the proposed repository in Yucca Mountain, Nevada. This mountain-scale TH model includes heat-driven processes occurring both near and far away from the emplacement drifts. The model simulations predict thermally perturbed liquid saturation, gas- and liquid-phase fluxes, and water and rock temperature elevations, as well as the changes in water flux driven by evaporation/condensation processes and drainage between drifts—to assess the repository performance under thermal loading and future climates.

APPROACH

The mountain-scale TH model, which consists of both two-dimensional (2-D) and three-dimensional (3-D) representations of the UZ repository system, is based on the current repository design, drift layout, geometry, thermal loading scenarios, and estimated current and projected future climate conditions. Specifically, the TH model implements the current hydrogeological conceptual model and incorporates the current, best-estimated input parameters into modeling studies of two-phase flow and heat transfer using the TOUGH2 code. Fracture-matrix interaction is conceptualized by a rigorous dual-permeability modeling approach. The 3-D representation explicitly includes every waste emplacement drift of the repository, as designed. Current and future climatic conditions are represented using a time-dependent net infiltration map with a three-step increase, in which the present-day climate lasts up to 600 years, the monsoon climate then covers the period from 600–2,000 years, and the glacial transition climate follows thereafter. The model simulations predict the TH evolution of the UZ system under repository thermal load and provide insight into moisture conditions and percolation fluxes in the UZ.

ACCOMPLISHMENTS

The multidimensional, mountain-scale, thermal-hydrologic (TH) numerical model for the repository at Yucca Mountain has been recently calibrated against borehole temperature data at ambient geothermal conditions. The TH processes represented in the model have also been verified against field test data on a drift scale. This mountain-scale TH model has been used to simulate the repository response of two-phase flow and heat transfer under two thermal loading scenarios, with or without ventilation operations, within the first 50 years after waste emplacement. In particular, the TH model has been used to provide predictions of repository heating effects on far-field UZ flow and TH conditions for hundreds and thousands of years after waste emplacement,

SIGNIFICANCE OF FINDINGS

Since laboratory studies and field heater experiments, however necessary, cannot adequately recreate or represent the space and time scales relevant for a geological repository, numerical modeling plays a crucial role in providing an understanding of nuclear-waste-repository performance. The mountain-scale TH model has provided large-scale quantitative predictions and scientific understanding of TH processes in the UZ of Yucca Mountain under the designed schedule of repository thermal load and ventilation operations. In particular, model simulations have shown the ability to predict thermally perturbed liquid saturation, gas- and liquid-phase fluxes, and water and rock temperature elevations, as well as changes in water flux driven by evaporation/condensation processes and drainage between drifts. In this way, the developed model is crucial for assessing repository performance under thermal loading and future climate conditions.

RELATED PUBLICATION

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ACKNOWLEDGMENTS

This work was supported by the Director, Office of Civilian Radioactive Waste Management, U.S. Department of Energy, through Memorandum Purchase Order QA-B004220RB3X between Bechtel SAIC Company, LLC, and the Ernest Orlando Lawrence Berkeley National Laboratory (Berkeley Lab). The support is provided to Berkeley Lab through the U.S. Department of Energy Contract No. DE-AC03 -76SF00098.

A Triple-Continuum Model for Flow and Transport Processes in Fractured Rock

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RESEARCH OBJECTIVES

The objectives of this study are (1) to explore a triple-continuum concept for studying the effect of small-scale fractures on flow and transport processes in fractured rock, (2) to develop a methodology for determining the model input parameters of the proposed model, and (3) to show how the proposed model can apply to site characterization of the Yucca Mountain unsaturated zone (UZ). In particular, we investigate the triple-continuum behavior of flow and transport processes in the fractured Yucca Mountain UZ, using both numerical and analytical solutions.

APPROACH

As conceptualized, the triple-continuum media consist (as the name implies) of three continua: a single porous-medium rock matrix and two types of fractures: (1) "large" fractures globally connected and (2) "small" fractures locally connected to the "large" fractures and the rock matrix. This concept is a natural extension of the dual-permeability or double-porosity models, in that it treats small-scale fractures as an additional connection between large fractures and the matrix. With this triple-continuum approach, flow and transport processes in fractured rocks are described using a triplet of governing equations for the two fracture and matrix continua. This conceptualization results in a set of partial differential equations for flow and transport in each continuum, which are in the same form as that for a single porous medium.

We have developed both analytical and numerical approaches to the triple-continuum model. Analytical solutions are obtained under single-phase flow and simple flow-geometry conditions only, while numerical implementation of such a triple-continuum model is based on the TOUGH2 framework, i.e., the mass- and energy-conservation equations are discretized in space using an integral finite-difference method, and the resulting discrete nonlinear equations are solved using a Newton iteration scheme.

ACCOMPLISHMENTS

Our new triple-continuum conceptual model, developed for modeling flow and transport through heterogeneous fractured rock, has been implemented into both analytical and numerical approaches. The model has been used for performing theoretical studies characterizing transient flow behavior in a triple-continuum formation. In field applications, the triple-continuum model has been employed in a sensitivity study of flow and transport in the Yucca Mountain UZ. This new conceptual model was first used to estimate model-related fracture-matrix parameters from field observation data using an inverse-modeling approach. Then, the estimated parameters were incorporated into the triple-continuum model for 3-D site-scale flow and transport simulations. The triple-continuum modeling results have indicated that small fractures may have a significant impact on radionuclide transport in the Yucca Mountain UZ system, as shown in Figure 1.

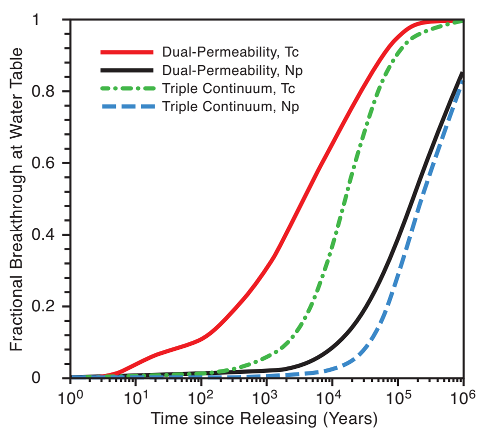

Figure 1. Comparison between cumulative breakthrough curves at the water table, simulated for conservative (Tc) and reactive (Np) tracer transport from the repository with dual-permeability and triple-continuum 3-D models, respectively

SIGNIFICANCE OF FINDINGS

This study shows that small fractures may have an important effect on radionuclide transport within Yucca Mountain, and provides a new capability in modeling flow and transport through heterogeneous fractured rock. As an extension of the dual-continuum concept, the triple-continuum model, with its analytical solution and numerical approach, will find further applications in the analysis of flow and transport through multifractured reservoirs, which typically contain a large number of small fractures, cavities, and different-scale heterogeneities. In general, such fractured reservoirs cannot be described using conventional dual-continuum models. In addition, the methodology developed in this study for determining model properties with the triple-continuum model, using observed data, will prove to be useful for parameter estimation in application.

RELATED PUBLICATION

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ACKNOWLEDGMENTS

This work was supported by the Director, Office of Civilian Radioactive Waste Management, U.S. Department of Energy, through Memorandum Purchase Order QA-B004220RB3X between Bechtel SAIC Company, LLC, and the Ernest Orlando Lawrence Berkeley National Laboratory (Berkeley Lab). The support is provided to Berkeley Lab through the U.S. Department of Energy Contract No. DE-AC03 -76SF00098.

A Physically Based Approach for Modeling Multiphase Fracture-Matrix Interaction in Fractured Porous Media

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RESEARCH OBJECTIVES

The objective of this study is to develop a physically based upstream weighting scheme. Such a scheme would be used for determining relative permeability functions or mobility terms that could be generally applicable to calculating multiphase flow between fractures and the rock matrix, using a dual-continuum concept. The physically based numerical approach overcomes the limitation of most numerical models for dealing with fracture-matrix interaction in selecting correct relative permeability values. Most such models use a single-point upstream weighting scheme by which to estimate flow mobility for fracture-matrix flow terms. However, such a scheme is prone to selecting incorrect mobilities for calculating fracture-matrix flow, which may lead to unphysical solutions or significant numerical errors.

APPROACH

Our modified upstream weighting scheme by which to select the appropriate mobility for fracture-matrix interaction is based on (1) the principle that the capillary pressure is continuous at the fracture-matrix interface and (2) the assumption that there is an instantaneous local pressure equilibrium for each phase on the matrix surface between fracture and matrix systems. These conditions should be reasonable for most fractured reservoirs, because fracture aperture is normally small, and dynamic changes in fractures, such as capillary pressures, could be instantaneously equilibrated locally at contacted matrix surfaces. Therefore, the new scheme, when the upstream direction for fracture-matrix flow is at fractures, uses a matrix relative permeability function as a function of fracture capillarity to calculate the mobility. Physically, this approach is equivalent to evaluating flow through the fracture-matrix interface into the matrix with the effective matrix permeability at that interface, which is still an upstream weighting scheme.

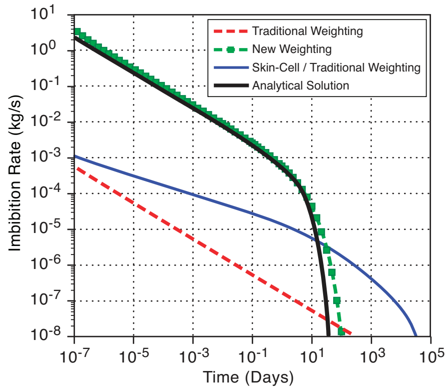

Figure 1. Comparison of calculated water imbibing rates from analytical and numerical solutions into a cubic matrix block

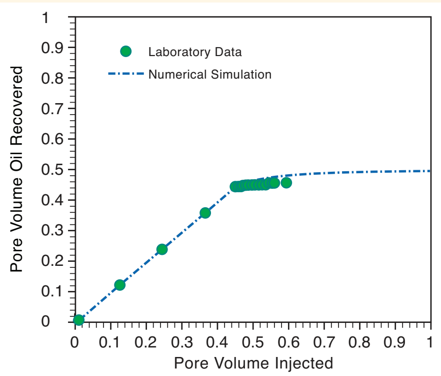

Figure 2. Comparison of simulation results with experimental data (Kazemi, 1979)

ACCOMPLISHMENTS

This physically based modeling approach for estimating physically correct relative permeability, in calculating multiphase flow between fractures and the matrix, has been implemented into two multiphase reservoir simulators. It has also been verified using both analytical solutions and laboratory experimental data (see Figure 1 for comparison of the proposed model results with laboratory tests involving a water-oil displacement experiment using fractured cores). The new method is demonstrated to be accurate, numerically efficient, and easy to implement in dual- or multiple-continuum models.

SIGNIFICANCE OF FINDINGS

The physically based upstream weighting scheme overcomes a serious flaw that exists in most current, conventional simulation practice when estimating flow mobility for fracture-matrix flow terms. Numerically, the new scheme uses exactly the same dual-continuum grids as the traditional dual-continuum approaches. Without requiring an additional computational burden or using refined grids, we achieve not only accurate but also physically correct results for fracture-matrix interaction.

RELATED PUBLICATION

Wu, Y. S., L. Pan, and K. Pruess, A physically based approach for modeling multiphase fracture-matrix interaction in fractured porous media. Advances in Water Resources, 27, 875–887, 2004. Berkeley Lab Report LBNL-54749.

ACKNOWLEDGMENTS

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

Numerical Investigation of the Temporal Damping Effect in the Unsaturated Fractured Rock of Yucca Mountain

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RESEARCH OBJECTIVES

Performance assessment of the Yucca Mountain unsaturated zone (UZ) as an underground repository of radioactive waste is based on a key assumption that physical processes in the unsaturated zone can be approximated as a steady-state condition. Justification of such an assumption relies mainly on the temporal damping effects of certain geological units within the unsaturated formations—in particular, the nonwelded tuff of the Paintbrush Group (PTn unit), above the repository horizon at Yucca Mountain. The main objective of this study is to investigate the damping function of the PTn unit via a three-dimensional (3-D) mountain-scale model and one-dimensional (1-D) column flow and transport models.

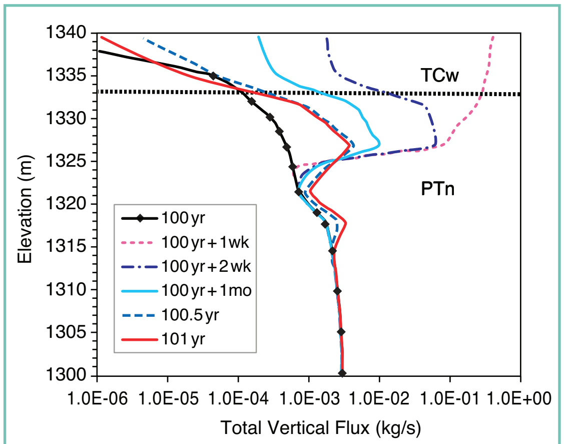

Figure 1. Flux distribution along column f96 at different times: right before an applied infiltration pulse (100 years), and right after an applied infiltration pulse (100 years+1 week), and afterwards

APPROACH

The 3-D mountain-scale model incorporates a wide variety of updated field data for the highly heterogeneous formation at Yucca Mountain. The model is first run to steady state and calibrated using field-measured data under present-day mean infiltration. Then, pulse infiltrations are applied to the model top boundary. The episodic infiltration boundary condition is implemented by concentration of the present-day mean infiltration of 50 years into one week as infiltration pulses. Flux changes at the bottom of the PTn unit and inside the unsaturated layers are examined under episodic infiltration boundary conditions. The 1-D column model consists of a single vertical column extracting directly from the 3-D mountain-scale model. The 1-D model is used to examine the long-term response of the flow system to higher infiltration pulses. The damping effect is also investigated through examining tracer transport in the UZ under episodic infiltration conditions.

ACCOMPLISHMENTS

This study provides insights into unsaturated zone flow behavior under episodic infiltration conditions and the role of the PTn unit in damping of pulse percolation. The large-scale transient 3-D flow model and 1-D models have been run to investigate vertical flux inside and at the bottom of PTn. Damping mechanisms have been analyzed by looking into the flux allocation inside the UZ vertical columns. Flux can be imbibed into dryer rock matrix, diverted to faults or other flow paths, detained along fractures, or continue percolating downward. Figure 1 shows vertical fluxes within a typical column at the repository area at different times.

SIGNIFICANCE OF FINDINGS

Model results show that the total fluxes at the PTn bottom gradually approach the average mean-infiltration-rate value for the entire period, with the probability that the system would eventually reach a dynamic equilibrium condition under the uniform pulses of infiltration. Episodic infiltration, once crossing the PTn, can be approximated as steady state. Results from the 1-D model with higher infiltration scenarios confirm that higher infiltration pulses will not weaken the damping effect. The transport model results further reveal that the damping effect exists specifically in the PTn unit. Flux allocation analyses suggest that the damping effect at nonfault columns is mainly caused by matrix rock water storage, absorbing and releasing water at different periods. Along fault columns, both lateral flow and rock water storage play an important role, with the importance of these two damping components being location-dependent.

RELATED PUBLICATION

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ACKNOWLEDGMENTS

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

Reactive Transport Modeling of Acid Gas Generation and Condensation

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RESEARCH OBJECTIVES

Yucca Mountain, Nevada, is a proposed site for geologic storage of high-level nuclear waste. The safety case for the proposed repository greatly depends on the integrity of the engineered barrier system, especially where waste packages would be located. Of concern is the possible presence of corrosive brines or acid gases via evaporation of pore water on top of hot waste packages after seepage into waste emplacement tunnels. Pulvirenti et al. (2004) recently conducted a laboratory evaporation/condensation experiment on a synthetic solution of primarily calcium chloride. This solution represents one potential type of evaporated pore water at Yucca Mountain. These authors reported that boiling this solution to near dryness (a concentration factor >20,000 relative to actual pore waters) leads to the generation of acid condensate (pH <1.5), presumably due to volatilization of HCl (and minor HF and/or HNO_3). The objective of this study was to evaluate the experimental results of Pulvirenti et al. (2004), so as to better understand processes leading to acid gas generation and condensation, and their potential implications for Yucca Mountain.

APPROACHES

The experiment of Pulverenti et al. (2004) was simulated with a multicomponent and multiphase reactive transport code (TOUGHREACT, Xu et al, 2004), including boiling, gas transport, and condensation. A Pitzer ion-interaction model was implemented into this simulator to allow calculations at high ionic strength. In addition, the code was modified to take into account vapor-pressure lowering caused by the increased salinity.

ACCOMPLISHMENT

The simulation of the experiment captures the observed increase in boiling temperature (up to 144°C and higher at ~1 bar) resulting from elevated concentrations of dissolved salts (up to 40 m ionic strength). The computed HCl fugacity (up to ~10^{-3} bars) generated by boiling under these conditions is not sufficient to lower the pH of the condensate (cooled to 80 and 25°C) down to observed values, unless the H_2O mass fraction in gas is reduced below ~2%. This is because the condensate becomes progressively diluted by H_2O gas condensation. However, when the system is modeled to remove water vapor, the computed pH of instantaneous condensates decreases to negative values (Figure 1), consistent with the Pulverenti experiment. The results also show that the HCl fugacity increases, and calcite, gypsum, halite, sylvite, and hydrated calcium chloride precipitate sequentially with increasing concentration factors.

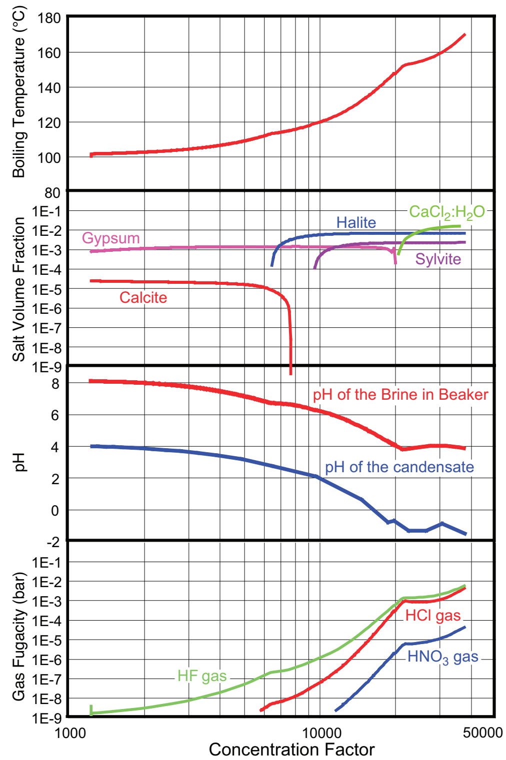

Figure 1. Simulated boiling temperature, salts volume fraction, pH, and fugacity

SIGNIFICANCE OF FINDINGS

The acid gases generated from boiling Yucca Mountain unsaturated zone pore water lead to an acid condensate in the experiment, which was successfully simulated with the addition of a Pitzer ion-interaction model into TOUGHREACT. However, these experimental conditions—corresponding to equipment of ~15 m^3 of seepage water, and highly localized condensation within a closed system—are not anticipated in the drift environment at Yucca Mountain. Hence these extreme pH observations are irrelevant to the Yucca Mountain.

RELATED PUBLICATIONS

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Xu, T., E. Sonnenthal, N. Spycher and K Pruess, TOUGHREACT User's Guide: A simulation program for nonisothermal multiphase reactive geochemical transport in variably saturated geologic media. MOL.20050125.0172, 2004. Berkeley Lab Report LBNL-55460.

ACKNOWLEDGMENTS

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A Sensitivity Study on the Impact of Fracture-Matrix Heat Transfer in Hot Fractured Rock

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RESEARCH OBJECTIVES

The objective of this research is to improve our understanding of thermal seepage (seepage of water into drifts at above-boiling average temperatures in the near-drift fractured rock) by evaluating the applicability and impact of fracture and matrix (F-M) interface reductions in heat-transfer problems. Our goals are to (1) demonstrate that our predictive thermal-hydrological (TH) model used for Yucca Mountain can explain the seepage observations from a laboratory heater experiment conducted at the Center for Nuclear Waste Regulatory Analyses (CNWRA experiment), (2) to identify the F-M area formulation best suited for this purpose, and (3) to evaluate whether the test conditions and observations of the CNWRA experiment are representative of the TH conditions expected at Yucca Mountain.

APPROACH

We first developed a conceptual framework for dual-continuum modeling of TH processes that can handle flow channeling in fractures and the related interface reduction in F-M heat transfer. Then, in a sensitivity analysis, we varied the degree of F-M interaction by applying different interface reduction formulations known from ambient flow and solute transport studies. The sensitivity study was performed using the CNWRA experiment (Figure 1) as a simulation example. Both experimental conditions and simulation results are compared with what is expected at Yucca Mountain.

ACCOMPLISHMENTS

Our simulation results stress the importance of understanding and adequately simulating the degree of heat transfer between the matrix and flowing water in fractures: Simulation cases featuring interface reduction for heat transfer exhibit early and consistent arrival of water at the drift crown, even though the matrix temperatures remain above boiling. Thermal seepage is possible under these conditions, which is consistent with the findings from the CNWRA experiment. In contrast, if interface reduction is not considered at all or is only applied to liquid-exchange processes, water is prevented from arriving at the drift crown by a fully efficient vaporization barrier. We conclude that the sensitivity cases featuring interface reduction for F-M heat transfer are generally better suited to represent the CNWRA test results than those assuming that heat is conducted over the full geometric area.

SIGNIFICANCE OF FINDINGS

That the thermal seepage observations in the CNWRA experiment could be reproduced with models that account for reduction of heat transfer between fractures and matrix provides confidence in the predictive TH models for Yucca Mountain, which utilize similar conceptual approaches for F-M interface reduction. Our simulation analysis furthermore indicates that the CNWRA experiment was operated at conditions extremely favorable for thermal seepage, in particular (1) the rather small boiling region near the drift, and (2) the strong gravity-driven downward flow in response to forced water release from the top. These conditions are not representative of those expected at Yucca Mountain, where the boiling region is much larger and the downward flow characteristics are much different in magnitude and temporal evolution.

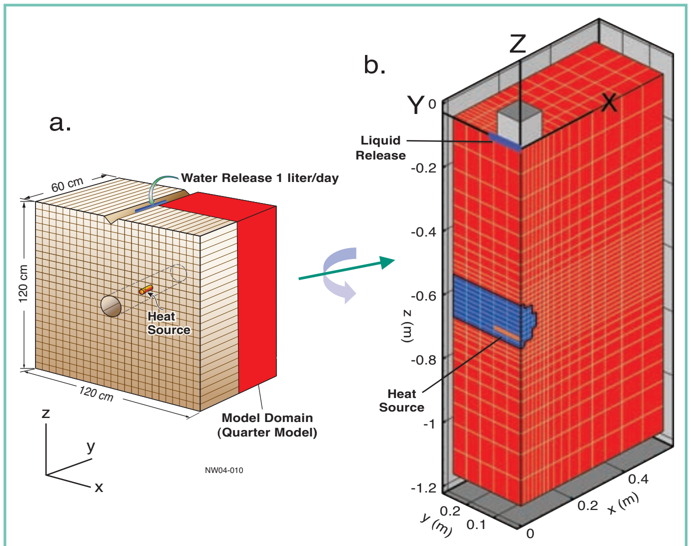

Figure 1. Schematic of (a) CNWRA heater experiment and (b) simulation domain

RELATED PUBLICATIONS

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Birkholzer, J.T., and Y. Zhang, On water flow in hot fractured rock—A sensitivity study on the impact of fracture-matrix heat transfer. Vadose Zone Journal (submitted), 2005. Berkeley Lab Report LBNL-57667.

ACKNOWLEDGMENTS

This work was supported by the Director, Office of Civilian Radioactive Waste Management, U.S. Department of Energy, through Memorandum Purchase Order QA-B004220RB3X between Bechtel SAIC Company, LLC, and the Ernest Orlando Lawrence Berkeley National Laboratory (Berkeley Lab). The support is provided to Berkeley Lab through the U.S. Department of Energy Contract No. DE-AC03-76SF00098.

Research Program

Energy Resources

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

OIL AND GAS EXPLORATION AND DEVELOPMENT

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

International and national concern about the variable climatic effects of greenhouse gases produced by burning of fossil fuels is increasing, while it is also recognized that these fuels will remain a significant energy source well into the 21st century. In response to these concerns, ER has initiated research focused on development of technologies that will minimize the impact of fossil-fuel usage on the environment. Methane hydrates constitute a tremendous potential fuel source with lower carbon emissions than coal or oil. ER researchers are developing and evaluating possible methods for producing gas from such deposits. Geophysical data acquisition and inversion methods developed in the ER program are also being applied in a new project on geologic sequestration of CO_2 carried out in the Climate Change and Carbon Management Program within the Earth Sciences Division.

Principal research activities include:

- Development of microwell seismic technology, including instrumentation, acquisition, and processing
- Applications of seismic methods for characterization of fractured reservoirs
- Laboratory measurement of the seismic properties of poorly consolidated sands
- Evaluation of seismic stimulation methods and their application to different classes of oil reservoirs
- Improved inversion methods for reservoir characterization, with a focus on combining production and geophysical data
- Application of x-ray computed tomography and nuclear magnetic resonance 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 increasing drilling efficiency
- Development of new methods to mitigate environmental effects of petroleum refining and use
- Enhancement of refining processes using biological technologies
- Numerical simulation of subsurface methane hydrate systems

Since 1994, the major part of the Oil and Gas Exploration and Development program has been funded through the

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

Partnership technology areas are:

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

GEOTHERMAL ENERGY DEVELOPMENT

There are two main objectives of ER's geothermal energy development program: (1) to reduce uncertainties associated with finding, characterizing, and evaluating geothermal resources, and (2) to develop and understand the enhancement of current geothermal systems to significantly increase production. The ultimate purpose is to lower the cost of geothermal energy for electrical generation or direct uses (e.g., agricultural and industrial applications, aquaculture, balneology). The program encompasses theoretical, laboratory, and field studies, with an emphasis on a multidisciplinary approach to solving the problems at hand. Existing tools and methodologies are upgraded, and new techniques and instrumentation are developed for use in the areas of geology, geophysics, geochemistry, and reservoir engineering. Cooperative work with industry, universities, and government agencies draws from Berkeley Lab's 25 years of experience in the area of geothermal research and development.

In recent years, DOE's geothermal program has become more industry-driven, and the Berkeley Lab effort has been directed toward technology transfer and furthering our understanding of the nature and dynamics of geothermal resources under production.

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

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

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

FUNDING

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

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

A Stochastic Model for Base-Of-Salt Mapping Using Gravity Data

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RESEARCH OBJECTIVES

Mapping base-of–salt using gravity and gravity gradient data is subject to a large degree of uncertainty, because of measurement errors and ambiguity in those data. Deterministic methods are limited for characterizing this uncertainty, since the optimal estimates of base-of-salt rely on starting models, and sensitivity-analysis methods often underestimate the actual uncertainty in the estimation. Our goal in this study is to develop a stochastic model for mapping base-of-salt using gravity and gravity-gradient data. The model should provide not only the estimates of base-of-salt at each location, but also uncertainty information at the location, such as mean, variance, ranges, and possible multiple modes.

APPROACH

In this study, we assume that the seafloor and top-of-salt of a continuous salt body are known through seismic surveys. We consider the thickness of the salt body at each location in the area as a random variable and strive to estimate the probability distribution function (instead of a single value) of the thickness, using gravity and gravity-gradient data. First, we define a joint posterior probability distribution function for all the unknown thicknesses, using a Bayesian framework. Second, we develop a Markov chain Monte Carlo (MCMC) method to obtain many samples of each unknown variable. Finally, we estimate the mean, variance, density function, and predictive intervals of each unknown variable. We also compare the results obtained using stochastic models with those obtained using deterministic methods.

ACCOMPLISHMENTS

We tested our stochastic model using a simple synthetic data set, based on a seismic model of a Gulf of Mexico site (Gemini) with one salt body, and a field data set collected from a North Sea site. We also explored the efficiencies of a variety of sampling methods, which included methods using gradient information, methods updating by columns, and methods updating by blocks. An image based on the Gemini data set is shown in Figure 1. Salt thickness uncertainty information at four locations is shown in Figure 2, where locations were chosen at which the estimated thickness of salt is distributed bi-modally, with intermediate thickness less likely, given the measured gravity and gravity gradient data.

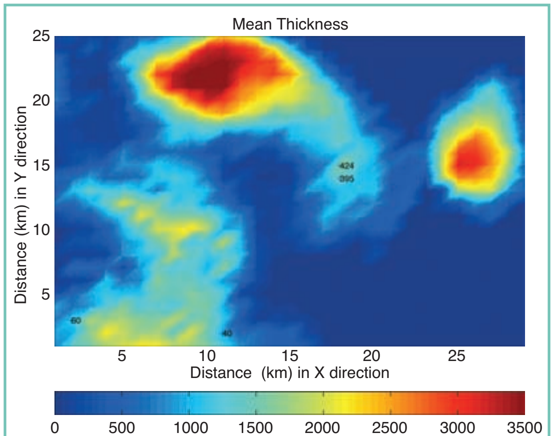

Figure 1. The estimated thickness of the salt body based on data collected from the Gemini data set. The numbers in the image show several locations where the thickness may have bi-modes.

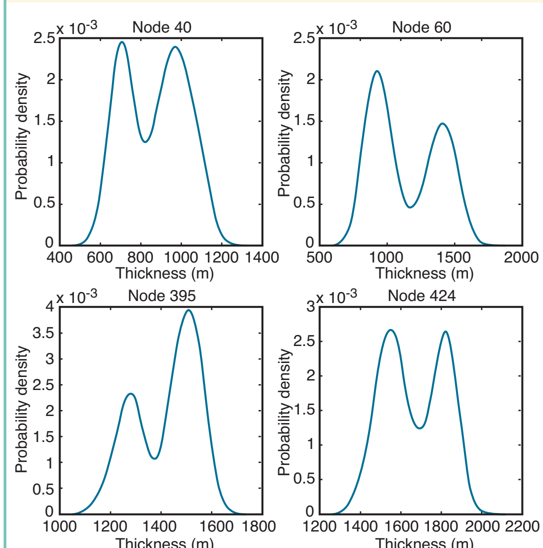

Figure 2. Probability densities for the salt-body thicknesses at the four locations, where the thickness may have bi-modes

SIGNIFICANCE OF FINDINGS

Our stochastic model for mapping base-of-salt provides an effective approach for characterizing uncertainty in the estimation of base-of-salt, since it gives us not only the estimates of base-of-salt but also the possible modes, ranges, and distributions at the location. The stochastic model, if used together with a deterministic model, can significantly reduce the number of forward calculations needed for the MCMC sampling method. For example, we can start from the optimal solutions obtained from deterministic models and draw many samples from the initial values.

RELATED PUBLICATION

Chen, J., M. Hoversten, and T. Smith, Stochastic inversion of gravity data for mapping the base-of-salt. Geophysics (in preparation), 2005.

ACKNOWLEDGMENTS

This study was supported primarily by the Anadarko Company and the U.S. DOE Assistant Secretary for Energy Research, Office of Biological and Environmental Research, under Contract No. DE-AC03-765SF00098.

Simulation of Reservoir Rock Formation: Sedimentation, Compaction, and Diagenesis

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RESEARCH OBJECTIVES

The microstructure of sedimentary rock determines its transport, electric, and mechanical properties. An efficient rock modeling procedure would enable characterization of the pore space geometry and compute the desired macroscopic properties of the rock. The objective of this project is to develop methods for modeling the formation of sedimentary rocks suitable for prediction of rock-transport properties directly from analysis of microscopic pore-space geometry.

APPROACH

The dynamic geologic processes of grain sedimentation and compaction are simulated by solving a dimensionless form of Newton's equations of motion for an ensemble of grains. The Lattice-Boltzmann method is used to simulate viscous fluid flow in the pore space of natural and computer-generated rock samples.

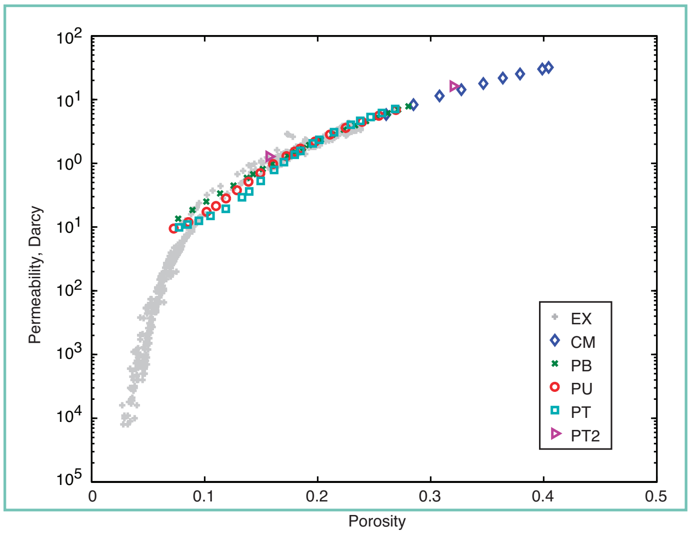

Figure 1. The evolution of absolute permeability of the modeled unconsolidated Fontainebleau sandstone with progressive compaction (CM), various modes of cementation (PB, PU, and PT), and different diagenetic history (PT and PT2), and the measurements on the real Fontainebleau sandstones

ACCOMPLISHMENTS

An integrated approach for estimating the absolute permeability of unconsolidated and consolidated reservoir rock has been developed. This procedure consists of two major steps: (1) obtaining an image from a computed tomography (CT) scanner or simulation of sedimentary rock formation; and (2) simulating viscous fluid flow in the pore space of a tomographic or computer-generated rock image. The results are confirmed by the quantitative comparison of computed permeability with experimental data. The computations-based porosity-permeability relationship of the modeled Fontainebleau sandstone is in good agreement with the laboratory measurements in real rocks (Figure 1).

SIGNIFICANCE OF FINDINGS

Our approach can be used to study the evolution of sedimentary rock porosity, permeability, and strength during arbitrary rock deformations and fracturing. The obtained knowledge can be used to predict rock properties from the grain size distribution and diagenetic history. The crucial factors controlling rock properties can be identified by running various “what-if” simulations. Our model is particularly suitable for analysis of unconsolidated sands whose cores or microtomographic images cannot be obtained.

RELATED PUBLICATIONS

Jin, G., T. Patzek, and D. Silin, Dynamic reconstruction of sedimentary rock using the distinct element method. SPE Journal (submitted), 2004. Berkeley Lab Report LBNL-55038.

Jin, G., T. Patzek, and D. Silin, Direct prediction of the absolute permeability of unconsolidated and consolidated reservoir rock. SPE Paper 90084, Presented at SPE Annual Technical Conference and Exhibition, Houston, Texas, 2004. Berkeley Lab Report LBNL-55339.

ACKNOWLEDGMENTS

This research was supported by the Assistant Secretary for Fossil Energy, Office of Natural Gas and Petroleum Technology, through the National Petroleum Technology Office, Natural Gas and Oil Technology Partnership, under U.S. Department of Energy Contract No. DE-AC03-76SF00098. Partial support was also provided by gifts from ChevronTexaco, Phillips Petroleum, and Statoil to UC Oil, Berkeley. Synchrotron CT images of Fontainebleau sandstone were provided by

Measuring and Observing Methane Hydrate Behavior Under Natural Conditions

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RESEARCH OBJECTIVES

Naturally available gas hydrates present in suboceanic and permafrost environments are thought to contain a vast amount of natural gas, amounts that could eventually be exploited as an energy source. Efficiently tapping this incompletely comprehended energy source will require strong modeling capabilities and significant laboratory and field efforts to determine modeling parameters and constitutive models. Natural samples are difficult to obtain for testing purposes because the hydrates are unstable at atmospheric pressure and typically dissociate upon recovery.

Our research objective is to provide model parameters and constitutive models for the Berkeley Lab simulator TOUGH-Fx/HYDRATE. To do this, we make laboratory measurements under realistic conditions on samples of hydrate in porous media, which we synthesize to model natural samples. Monitoring pressure and temperature, we use x-ray computed tomography (CT) to make detailed observations of density changes during tests.

APPROACH

We synthesize large methane hydrate samples in partially water-saturated sand samples in an x-ray-transparent pressure vessel contained within a temperature-controlled heat exchanger. Temperature is monitored at multiple locations, pressure is monitored during hydrate synthesis and dissociation tests, and we use CT to monitor density changes that occur in response to changes in temperature and pressure.

ACCOMPLISHMENTS

We have synthesized methane hydrate in the pore space between mineral grains, with our samples being the largest laboratory samples in the world. We have dissociated the hydrate by both thermal stimulation and depressurization, and have used our measurements to determine the thermal conductivity of the hydrate-bearing medium, and to estimate the parameters of dissociation kinetics. From this work, we have learned that the presence of hydrate in the pore space alters the capillary pressure-saturation curve affecting water movement, and that formation and dissociation of hydrate in partially saturated sand may induce mechanical changes that cause the sample size to change (Figure 1).

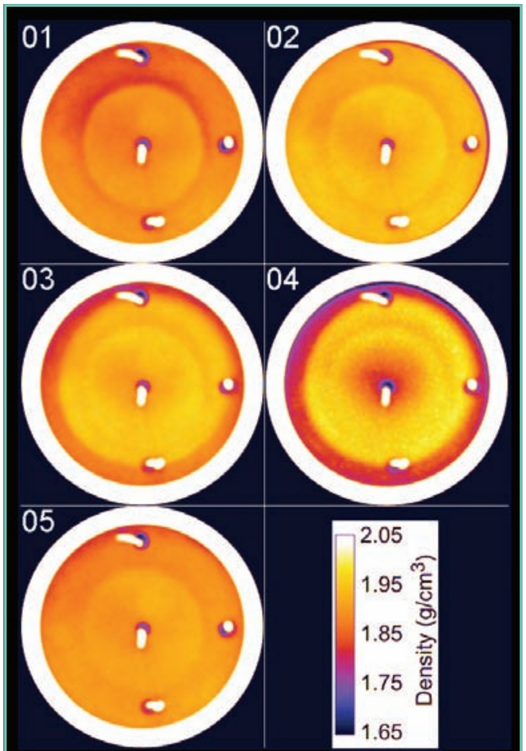

Figure 1. CT scans showing the average density in the 7.6 cm diameter x 26 cm cylindrical sample: (1) initial condition, (2) after hydrate formation, (3) after thermal stimulation from the outside, (4) after secondary hydrate formation, and (5) after complete dissociation. Note the dark rind at the upper right contact between the vessel (white circle) and the sample inside, indicating sample shrinkage on hydrate formation in (2) and (4). The short white lines within the white circle are thermocouples.

SIGNIFICANCE OF FINDINGS

We have begun to develop parameters and constitutive models that are useable to model gas production from hydrate accumulations, in addition to observing processes via CT. We are the first to use CT to quantitatively measure changes during hydrate formation and dissociation, leading to improvements in conceptual models.

RELATED PUBLICATIONS

Kneafsey, T.J., L. Tomutsa, G.J. Moridis, Y. Seol, B. Freifeld, C.E. Taylor, and A. Gupta, Methane hydrate formation and dissociation in a partially saturated core-scale sand sample. Journal of Petroleum Science and Engineering (submitted), April 2005. Berkeley Lab Report LBNL-57300.

Moridis, G.J., Y. Seol, and T.J. Kneafsey, Studies of reaction kinetics of methane hydrate dissociation in porous media. In: Fifth International Conference on Gas Hydrates, Trondheim, Norway, 2005. Berkeley Lab Report LBNL 57298.

ACKNOWLEDGMENTS

This work was supported by the Assistant Secretary for Fossil Energy, Office of Natural Gas and Petroleum Technology, through the National Energy Technology Laboratory, under U.S. DOE Contract No. DE-AC03-76SF00098.

Detection of Hidden Geothermal Systems Based on Near-Surface CO_2

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RESEARCH OBJECTIVES

The majority of hydrothermal systems with obvious surface expressions in the U.S. have been explored to determine their development potential. Consequently, discovery of new geothermal systems will require exploration of areas where the resources are hidden. Emissions of moderate-to-low solubility gases may be one of the primary near-surface signals from hidden geothermal systems, and detection of anomalous gas emissions may be a tool by which to discover new resources. Carbon dioxide shows promise because it is the major noncondensible gas present in geothermal systems, has moderate solubility in groundwater, and is measurable by numerous technologies. The objective of this work is to design an integrated measurement, modeling, and analysis strategy to identify geothermal CO_2 in the near-surface environment, with the goal of discovering hidden geothermal systems.

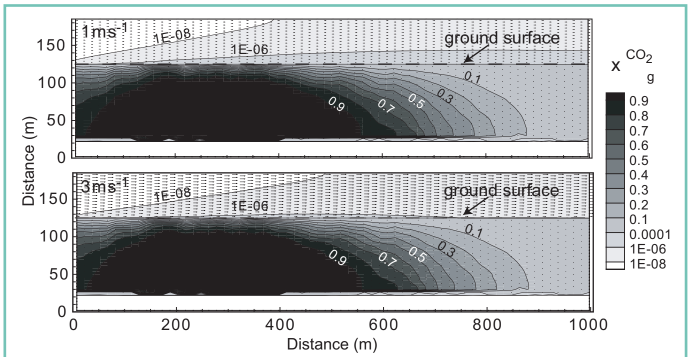

Figure 1. Coupled CO_2 subsurface migration and surface-layer mixing at t = 200 years for one heterogeneous permeability realization, source CO_2 flux = 576 g m^{-2} d^{-1}, and constant wind speeds of 1 m s^{-1} (upper plot) and 3 m s^{-1} (lower plot). CO_2 concentration is in mole fraction.

APPROACH

Simulations were conducted using the numerical code T2CA, a coupled subsurface-atmospheric surface layer flow and transport model, to estimate near-surface CO_2 concentrations and fluxes that might result when CO_2 leaks from a hidden geothermal system at depth. The geologic framework of the modeled hidden geothermal system was based on an arid Basin and Range Province system. Observed sources, as well as the spatial and temporal variability of natural background CO_2 fluxes and concentrations in the near-surface environment, were also evaluated. Methods were designed to detect geothermal CO_2 emissions within the background variability of CO_2, integrating field measurement technologies with statistical analysis and modeling approaches.

ACCOMPLISHMENTS

Near-surface CO_2 fluxes and concentrations were simulated for different geothermal source CO_2 fluxes, homogeneous and heterogeneous permeability structures, and constant wind speeds. Results show that CO_2 concentrations can reach high levels in the shallow subsurface, even for relatively low geothermal source CO_2 fluxes (Figure 1). However, winds are effective at dispersing CO_2 seepage. Technologies to detect CO_2 in the near-surface were evaluated for detection capability and cost. An exploration strategy was proposed involving integrated measurement, modeling, and statistical analysis to characterize the spatial and temporal variability and source of CO_2 in a background system and the area targeted for exploration. Emphasis was placed on using time- and cost-efficient methods to determine whether CO_2 derived from a geothermal source is present, and if so, the spatial extent of the anomaly.

SIGNIFICANCE OF FINDINGS

The proposed near-surface CO_2 monitoring and analysis strategy is designed to search for relatively small geothermal CO_2 signals within the background variability of CO_2, using relatively low-cost and time-efficient methods. Further geophysical measurements, installation of deep wells, and geochemical analyses of deep fluids can be guided by the results of the near-surface CO_2 investigation.

RELATED PUBLICATION

Lewicki, J.L., and C.M. Oldenburg, Near-surface CO_2 monitoring and analysis to detect hidden geothermal systems. Proceedings, 30th Workshop on Geothermal Reservoir Engineering, Stanford University, Stanford, California, 2005. Berkeley Lab Report LBNL-56900.

ACKNOWLEDGMENTS

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

The Application and Use of Microdrilling for Vertical Seismic Profiling and Monitoring Reservoir Performance

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RESEARCH OBJECTIVES

Microhole technology (providing inexpensive access to the subsurface) has the potential to be the most significant technology advance for the energy industry in the last 50 years. It has the potential to be a catalyst for creating a quantum leap in imaging technology, which could lead to a much clearer understanding of subsurface processes. A critical application is the placement of sensors in the subsurface for use with seismic techniques such as vertical seismic profiling (VSP), crosswell, microseismic, and even high-resolution surface seismic to image and monitor previously unknown or unresolved resources. To achieve this goal, we are pursuing an integrated program of testing, evaluation, and development of the technology required to deliver, process, and interpret the data.

APPROACH

The technology exists today to achieve many of these goals. To a large degree, it is a matter of tailoring this technology for the energy industry rather than starting from scratch. The DOE National Energy Technology Laboratory (NETL) oil program has undertaken and sponsored an integrated program of modeling, instrumentation evaluation/testing, and data acquisition and processing. This effort is tightly coupled with the microdrilling program at Los Alamos National Laboratory (LANL), and with field testing at the Rocky Mountain Oil Testing Center (RMOTC) at Teapot Dome in Wyoming (as well as at other sites of opportunity), to test and develop the technology. In the first year, the focus of the effort was modeling, design, and processing of multiple shallow VSP's (500 to 700 ft deep) in microdrilled holes within a well-characterized area. Follow-on tasks extended this work, with continued evaluation of sensors for use in microholes, optimizing the employment of sensors using innovative clamping and deployment mechanisms, partnering with industry for data acquisition and sensor evaluation, and processing/interpreting data derived from field tests.

ACCOMPLISHMENTS

In 2004 and early 2005, Berkeley Lab deployed a 20-level (with 5 m spacing) hydrophone and geophone string in the 750 ft deep microhole that LANL drilled at RMOTC. The purpose was to compare the difference between a fluid coupled sensor and a directly clamped sensor. The overall objective, however, was to determine the image volume and resolution that could be obtained from microholes drilled to depths above a target. For example, most VSP wells are drilled to the target or just above a target. In this case, our target was 1,500 ft (two well depths) below the well. Because of the small size of the microholes, a new type of clamping system had to be developed for the geophones. This "vacuum assisted" clamping mechanism is used to minimize the overall size of the package such that it will fit down the well. Another prime objective was to develop low-cost instrumentation that could be deployed in a low-cost manner (most VSP surveys cost from 50 K to 250 K per well to collect the data). Modeling of the shot-hole locations was performed prior to the field work to estimate shot spacing, total distance for the well, etc. Two complete VSP multi-offset (12 shot locations each) with offset distances from 35 ft to 2,700 ft (every 250 ft) were completed using a 20-level hydrophone string and a 20-level geophone string. In total, 40 levels were recorded for each set of sensors, using 12 different shot locations. A vibroseis was used as a source (Enviroseis from IVI Inc.) to minimize ground disturbance and maximize its high-frequency content (up to 300 Hz). Figure 1 shows one of the VSP results from the survey. As can be seen, the reflections are coming from well below the target depth. This was a relatively near offset, but it does show good reflections.

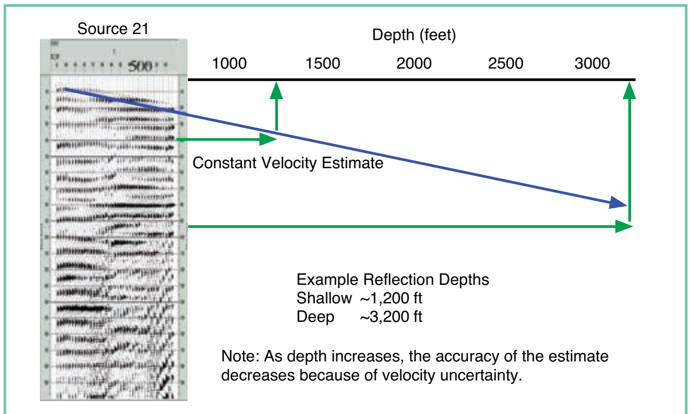

Figure 1. The estimate of the depth of reflections from the VSP in the 650 ft depth well; note the reflections at the 3,000 ft depth.

SIGNIFICANCE OF FINDINGS

All objectives were met in the evaluation of the microhole technology for VSP. In addition, a baseline study was obtained in preparation for future CO_2 injection monitoring. Direct arrivals were observable from source offsets of 2,800 ft, and reflections were observable as deep as 3,000 ft. As more microholes are drilled, additional data can be acquired to expand the image to accommodate larger CO_2 injections.

ACKNOWLEDGMENTS

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

Evaluating and Managing the Impact of Induced Seismicity at the Geysers Geothermal Field

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RESEARCH OBJECTIVES

As the demand for energy increases, it is obvious that geothermal resources must play a growing part in meeting our energy needs. Water injection into geothermal systems, to affect enhanced geothermal systems (EGS), has become an often-required strategy to extend and sustain production of geothermal resources. Critical questions that need to be addressed are how injection will affect seismicity of an area, what does seismicity imply for injection strategy, and how will seismicity and injection together impact the local community, as well as field operations.

The two prime objectives of this project are: (1) to understand the impact of EGS operations on induced seismicity and its environmental impact on the surrounding community, and (2) to use microearthquake monitoring to intelligently manage the effects of fluid injections and stimulations, so as to ensure the optimization of EGS projects.

APPROACH

The Geysers, in Sonoma County, California, is a prime candidate for EGS because of its very high heat content—injection is one of the few economic means by which to mine the heat stored there in the subsurface rock. This site constitutes a unique opportunity for obtaining data before injection and increased production begin. Additional opportunities exist in the Basin and Range to monitor seismicity associated with hydrofracturing and using microearthquake (MEQ) monitoring to track the induced fracturing. In addition to natural fracture systems, hydrofracturing may be a possible means to enhance the fracture area and permeability of geothermal reservoirs. MEQ monitoring is a means to track the hydrofracture and estimate the success of the hydrofracturing operations.

Besides collecting data to address the environmental impact of EGS operations, we are also part of an International Energy Agency implementing agreement to participate in assessing and mitigating the environmental effects of these operations, specifically induced seismicity. The work scope of this international group is "to pursue a collaborative effort to address an issue of significant concern to the acceptance of geothermal energy in general, and EGS in particular. The objective is to investigate these (induced) events to obtain a better understanding of why they occur, so that they can either be avoided or mitigated. Understanding requires considerable effort to assess and generate an appropriate source-parameter model, testing of the model, and then calculating the source parameters in relation to the hydraulic injection history, stress field and the geological background. An interaction between stress modeling, rock mechanics, and source-parameter calculation is essential. Once the mechanism of the events is understood, the injection process, the creation of an engineered [enhanced] geothermal reservoir, or the extraction of heat over a prolonged period may need to be modified to reduce or eliminate the occurrence of large [seismic] events."

ACCOMPLISHMENTS

Data are being routinely gathered and analyzed in real time and sent to the U.S. Geological Survey for archiving. Figure 1, a typical map of a month's seismicity at The Geysers, shows the lack of seismicity in the northwest Geysers (Aidlin area), where injection has not yet started. Results will include a unique data set for a geo-thermal area, a set that will be available to the public and research community. Initial correlation has shown that although the numbers of events are increasing at The Geysers, the overall energy release is level or decreasing (do EGS areas eventually gain stability?). Also, as can be seen from Figure 1, the larger events occur outside of the main clusters (green stars).

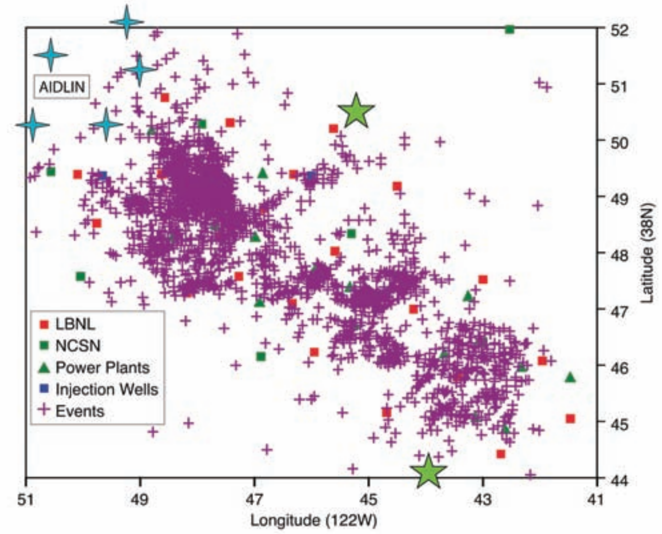

Figure 1. Locations of events in Nov. of 2004, Geysers wide—note the lack of events in the Aidlin area prior to high-rate injection; injection will proceed in the fall/early winter of 2005. The Blue stars are the new Berkeley Lab stations installed in FY 04. Green stars are Magnitude 4 events (February 2004, December 2004).

SIGNIFICANCE OF FINDINGS

Never-before resolution and coverage will allow detailed analysis to correlate and investigate the link of induced seismicity to injection and production at The Geysers. Real-time public display will allow the community to gain confidence and assurance that the operators are acting in a responsible fashion.

ACKNOWLEDGMENTS

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

Application of Seismic Methods for Fracture Characterization

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RESEARCH OBJECTIVES

A five-year (2000–2004), comprehensive, joint industry, university, and national laboratories project was carried out to develop and apply multiscale seismic methods for detecting and quantifying fractures in naturally fractured gas reservoirs.

APPROACH

This project took place within a 20-square-mile area at a producing gas field in the northwest part of the San Juan Basin in New Mexico. Three-dimensional surface seismic, multi-offset 9-C vertical seismic profiling (VSP), 3-C single-well seismic, and well-logging data were complemented by geologic/core studies to model, process, and interpret the data. The overall objective was to determine the seismic methods most useful in mapping productive gas zones.

ACCOMPLISHMENTS

Data from nearby outcrops, cores, and wellbore image logs suggested that natural fractures were probably numerous in the subsurface reservoirs at the site selected, and trend north-northeast/south-southwest despite the apparent dearth of fracturing observed in the wells logged at the site (Newberry and Moore wells). Estimated fracture spacing is on the order of 1–5 m in Mesaverde sandstones, less in Dakota sandstones. Fractures are also more frequent along fault zones, which in nearby areas trend between north-northeast/south-southwest and northeast-southwest—and are probably spaced a mile or two apart. The maximum *in situ* horizontal, compressive stress in the vicinity of the seismic test site trends approximately north-northeast/south-southwest. The data are few, but they are consistent.

The seismic data present a much more complicated picture of the subsurface structure. Faulting inferred from surface seismic had a general trend of SW–NE, but with varying dip, strike, and spacing. Studies of P-wave anisotropy from surface seismic showed some evidence that the data did have indications of anisotropy in time and amplitude. However, compared to the production patterns, there is little correlation with P-wave anisotropy. One conclusion is that the surface seismic reflection data are not detecting the complexity of fracturing controlling the production. Conclusions from the P-wave VSP studies showed a definite 3-D heterogeneity in both P- and S-wave characteristics. The analysis of shear-wave splitting from 3-D VSP data gave insight into the anisotropy structure with depth around the borehole. In the reservoir, the VSP shear-wave splitting data do not provide sufficient constraints against a model of lower symmetry than orthorhombic, so that the existence of more than one fracture set must be considered. It was also demonstrated that vertical transverse isotropy (VTI) and orthorhombic symmetry could be well defined from the field data by analyzing shear-wave splitting patterns. The detection of shear-wave singularities provides clear constraints to distinguish between different symmetry systems. The P-wave VSP common-depth-point (CDP) data showed evidence of fault detection at a smaller scale than the surface seismic showed, and in directions consistent with a complicated stress and fracture pattern. The single-well data indicated zones of anomalous wave amplitude that correlated well with high gas shows. The high amplitude single-well seismic data could not be explained by wellbore artifacts, nor could it be explained by known seismic behavior in fractured zones. Geomechanical and full-wave elastic modeling in 2- and 3-D provided results consistent with a complicated stress distribution induced by the interaction of the known regional stress and faults mapped with seismic methods.

SIGNIFICANCE OF FINDINGS

Sophisticated modeling capability was found to be a critical component in quantifying fractures through seismic data. Combining the results with the historical production data showed that the surface seismic analysis provided a broad picture consistent with production, but not detailed enough to consistently map complex structuring, which would allow accurate well placement. VSP and borehole methods show considerable promise in mapping the scale of fracturing necessary for more successful well placement. Integration of these methods at one field site enables investigators to give specific recommendations for the scale at which each method and fracture complexity would be appropriate.

ACKNOWLEDGMENTS

This work was supported by the Assistant Secretary for Fossil Energy, Office of Oil and Natural Gas, Department of Natural Gas Exploration, Production, and Storage, through the National Energy Technology Laboratory, of the U.S. Department of Energy under Contract No. DE-AC03-76SF00098.

The Reaction Kinetics of Methane Hydrate Dissociation in Porous Media

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RESEARCH OBJECTIVES

The objective of this study is to describe the kinetic dissociation of CH_4-hydrates in porous media, and to determine the corresponding kinetic parameters. Knowledge of the kinetic dissociation behavior of hydrates can play a critical role in evaluating the gas production potential of gas-hydrate accumulations in geologic media.

APPROACH

We analyzed data from a sequence of tests of CH_4-hydrate dissociation by means of thermal stimulation. These tests had been conducted on sand cores partially saturated with water, hydrate, and CH_4 gas, and contained in an x-ray-transparent aluminum pressure vessel. The pressure, volume of released gas, and temperature (at several locations within the cores) were measured. To avoid misinterpreting local changes as global processes, x-ray computed tomography scans provided accurate images of the location and movement of the reaction interface during the course of the experiments. After first determining the thermal properties of the hydrate-bearing medium, we obtained estimates of the kinetic parameters of the hydration reaction in porous media by means of inverse modeling (history matching) of the laboratory data, using the TOUGH-Fx/Hydrate code. Comparison of the results from the hydrate-bearing porous media cores to the known kinetic parameters of dissociation of pure CH_4-hydrate samples provided a measure of how the porous medium affected the kinetic reaction.

ACCOMPLISHMENTS

This is the first-ever determination of the kinetic parameters of hydrate dissociation in porous media. The excellent agreement between observations and numerical predictions validated the kinetic parameters determined through the inversion process, confirmed the hypothesis of their intrinsic character (and, thus, of their invariant values), provided increased confidence in (and further verification of) the numerical model used to describe the hydrate behavior in porous media, and indicated that the thermal conductivity model (developed as part of a related study) was not inconsistent with the overall system behavior.

SIGNIFICANCE OF FINDINGS

Knowledge of the kinetic rate of dissociation for gas hydrates is of critical importance in predicting the rate of gas production from natural hydrate accumulations, because it can provide an estimate of their technical and economic viability as potential energy sources.

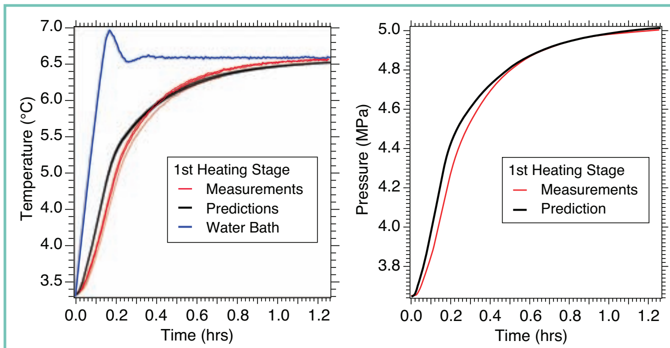

Figure 1. Comparisons between the evolution of the observed and predicted (based on the new estimates of kinetic dissociation) temperature and pressure in the hydrate-bearing core samples

RELATED PUBLICATIONS

Kneafsey, T., L. Tomutsa, G.J. Moridis, Y. Seol, B. Freifeld, C.E. Taylor and A. Gupta, Methane hydrate formation and dissociation in partially saturated sand—Measurements and observations. Proceedings of the 5th International Conference on Gas Hydrates (in press), Trondheim, Norway, June 13–16, 2005. Berkeley Lab Report LBNL-57300.

Moridis, G.J., Y. Seol, and T. Kneafsey, Studies of reaction kinetics of methane hydrate dissociation in porous media. Proceedings of the 5th International Conference on Gas Hydrates (in press), Trondheim, Norway, June 13–16, 2005. Berkeley Lab Report LBNL-57298.

ACKNOWLEDGMENTS

This work was supported by the Assistant Secretary for Fossil Energy, Office of Natural Gas and Petroleum Technology, through the National Energy Technology Laboratory, under U.S. DOE Contract No. DE-AC03-76SF00098.

A Similarity Solution for Gas Production from Dissociating Hydrate Accumulations

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RESEARCH OBJECTIVES

The main objective of this study is to demonstrate that the problem of single-well gas production from dissociating hydrate-bearing geologic systems accepts a similarity solution. Such solutions are invariant when plotted against the similarity variable r^2/t; can form the basis of simplified, yet robust, graphical methods to estimate gas production from natural gas hydrate accumulations; and can serve as a tool to test the validity and accuracy of numerical simulators.

APPROACH

This study was motivated by the realization that there is a direct analogy between the phases of a pure H_2O system and a composite CH_4-H_2O hydrate system. Following the approach used in the development of the H_2O-based systems, we used the Boltzman transformation to reduce the partial differential equations (PDEs) of fluid flow and heat transfer in a hydrate-bearing geologic system, the boundary conditions, and the initial conditions into a set of ordinary differential equations (ODEs) of a form entirely consistent with prior similarity solutions. The transformation was conducted without any thermophysical simplifications or reduction in the strong nonlinearities of the PDEs. To prove the existence of a similarity solution, the ability to transform the original equations into a form known to accept a similarity solution is a necessary and sufficient condition. Thus, it is not necessary to solve the transformed system of equations; rather, it suffices to solve the original (coupled and strongly nonlinear) PDEs, and to demonstrate the invariance of any of the parameters (e.g., pressure, temperature, phase saturations) with respect to the similarity variable $r/t^{1/2}$.

ACCOMPLISHMENTS

Using the TOUGH-Fx/Hydrate numerical simulator of system behavior in hydrate-bearing geologic media, we demonstrated that the problem of gas production from natural hydrate accumulations admits a similarity solution. We established that such similarity solutions apply to all methods of hydrate dissociation (i.e., depressurization, thermal stimulation, and the effect of inhibitors), both individually and in any combination.

SIGNIFICANCE OF FINDINGS

Because the problem admits a similarity solution, the distributions of any of the variables (e.g., pressure, temperature, phase saturation) are invariant when plotted against r^2/t. Therefore, a single set of results is sufficient to describe system behavior and performance at any time.

The similarity solution can provide a simple and robust tool for evaluating the production potential of hydrate deposits. To accomplish this, we can develop simple graphical solutions for very complex problems by obtaining a family of similarity graphs for different conditions, thus avoiding lengthy numerical simulations.

Additionally, because we showed that the hydrate problem has a similarity solution, any numerical solution must be invariant when plotted against r^2/t. This is a robust tool for evaluating the accuracy of any numerical simulator of hydrate behavior. If the simulator is inaccurate, then the solutions at different times will not coincide.

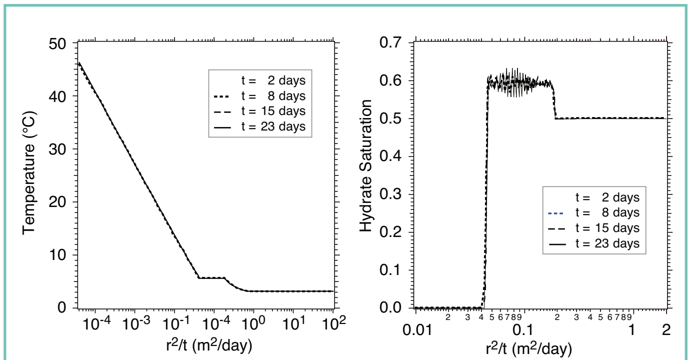

Figure 1. Numerically determined similarity solution of temperature and hydrate saturation vs. r^2/t at different times, for a 1-D radial problem of gas production from hydrate through thermal stimulation

RELATED PUBLICATION

Moridis, G.J., M. Kowalsky, and K. Pruess, TOUGH-Fx/HYDRATE User's Manual: A Code for the Simulation of System Behavior in Hydrate-Bearing Geologic Media. Berkeley Lab Report LBNL/PUB-3185, 2005.

ACKNOWLEDGMENTS

This work was supported by the Assistant Secretary for Fossil Energy, Office of Natural Gas and Petroleum Technology, through the National Energy Technology Laboratory, under U.S. DOE Contract No. DE-AC03-76SF00098.

Slot-Shaped Borehole Breakout within Weakly Cemented Sand under Anisotropic Stresses

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RESEARCH OBJECTIVES

Boreholes drilled within weakly cemented sand can suffer excessive sand production that may hinder, or even stop, production of oil—and ultimately cause collapse. Further, in recent years, there has been increasing evidence of a unique, slot-shaped borehole failure within weak, high-porosity sandstones, which may have a significant impact on the stability and sand production of boreholes.

The primary objectives of this research are: (1) to establish quantitative relationships between grain-scale properties of weakly cemented sand and macroscopic properties such as failure mode and rock strength; (2) to understand the process and mechanism of fracture formation and failure of a borehole in a realistic stress and flow environment; and (3) to develop a predictive capability for borehole stability and sand production, through a series of laboratory experiments.

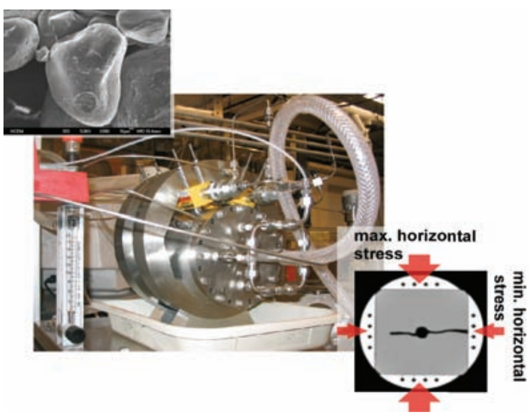

Figure 1. Block samples of weakly cemented sand (upper left, SEM photograph. Sand grain size~150 micrometers), containing a single borehole, are compressed anisotropically within a portable "true-triaxial" cell with fluid circulation through the borehole (middle). A slot-shaped borehole breakout develops in the direction perpendicular to the maximum horizontal stress direction around the borehole (lower right, x-ray CT image). The diameter of the borehole is approximately 1 cm (0.39 inches).

APPROACH

Because field cores of weakly cemented rocks are difficult to recover from oil and gas reservoirs, we developed a new laboratory technique to fabricate weakly cemented synthetic sandstone samples for our experiments. Using synthetic samples also allowed us to conduct parametric studies for a range of controlled sample properties, including the strength of intergranular bonds and porosity. These samples are made of pure quartz sand cemented together by a soda-lime glass micropowder melted under a high temperature. We also developed a "true-triaxial" loading cell (loads can be applied in the three perpendicular directions independently), capable of circulating fluid at a controlled rate through a borehole drilled in a rectangular block-shaped sample (3 inches x 3 inches x 6 inches).

ACCOMPLISHMENTS

Using the synthetic sandstone samples and the "true-triaxial" loading cell, we successfully produced a slot-shaped borehole breakout within the samples under anisotropic stresses and with fluid flow through the borehole (Figure 1). Experiments were conducted for a range of sample strength, borehole fluid flow rate, and stress anisotropy around the borehole axis. After each experiment, the geometry of the resulting breakout was examined via x-ray CT.

The results of the experiment showed that the width of the breakout decreased with increasing intergranular cohesion and strength of the samples, possibly because a larger zone of damage (process zone) formed near the edge of a breakout for weaker samples, which was subsequently washed away by the fluid flow. Further, for stronger samples, the growth of the breakout was rapid and catastrophic, while weaker samples exhibited the slow, stable growth of a breakout.

SIGNIFICANCE OF FINDINGS

Slot-shaped borehole breakout within well-cemented sandstone is commonly believed to form when the rock undergoes local compaction at the leading edge of the breakout, resulting in crushing of sand grains. In contrast, the slot failure within weakly cemented sand involves little grain failure, which indicates that compaction is not necessarily a critical mechanism of the failure. This indicates that the slot-shaped failure can occur at low stresses that do not involve grain crushing. Further, a numerical stress analysis based on a static boundary-element method indicates that, as long as the produced debris can be removed from the edge of the breakout, the growth of the slot-shaped breakout cannot be stopped, since the stress concentrations at the breakout-tip increases monotonically with the breakout length.

RELATED PUBLICATION

Nakagawa, S., and L.R. Myer, Mechanical and acoustic properties of weakly cemented granular rocks. 38th U.S. Rock Mech. Symp., Washington, DC, 3–10, 2001. Berkeley Lab Report LBNL-50814.

ACKNOWLEDGMENTS

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

Characterizing Thermal and Hydrological Properties of Hydrate-Bearing Sediments

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RESEARCH OBJECTIVES

Predicting natural gas recovery from reservoirs containing gas hydrates requires knowledge of both the reservoir properties and the properties and processes of hydrate dissociation. The main objective of this study is to perform laboratory tests to determine the thermal and physical properties of hydrate-bearing porous media, including thermal conductivity, kinetic parameters, and relative permeability.

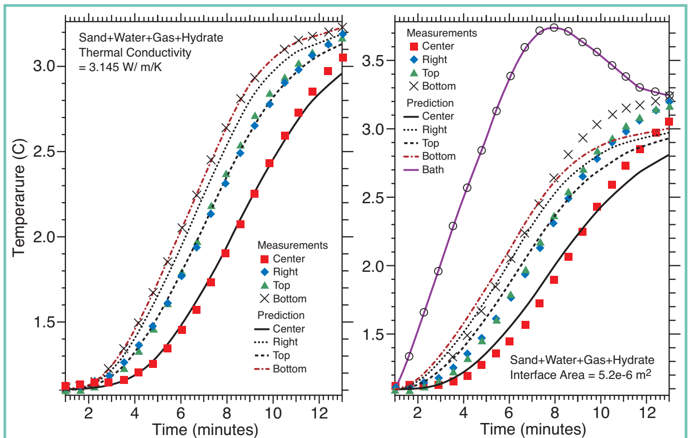

Figure 1. Calibration and parameter determination of the hydrate-bearing sand/water/gas/hydrate system (symbols represent measurements, lines represent model predictions)

APPROACH

To estimate thermal conductivity and kinetic parameters, we formed and dissociated methane hydrate in partially water-saturated sand contained in an x-ray-transparent aluminum pressure vessel. The sediment/hydrate sample was subjected to either thermal perturbations within the hydrate stability zone, or thermal or pressure perturbations leading to dissociation. History matching and inverse modeling with iTOUGH2 and TOUGH-Fx/Hydrate were performed to estimate the properties.

New laboratory tests were performed to estimate the relative permeability of hydrate-bearing porous media using a transient technique. Inverse modeling using iTOUGH2 was performed to optimize relative permeability curves, so as to provide saturation profiles that best match the x-ray computed tomography data.

ACCOMPLISHMENTS

Inverse modeling analysis of the experiments has provided needed estimates of the thermal properties and kinetic parameters of hydrate dissociation in porous media. We numerically inverted the thermal response of the system with and without hydrate, and determined the thermal conductivities of the sand/water/gas system and the sand/water/gas/hydrate system. The thermal conductivity of the system with hydrate exceeded that of the same sample prior to hydrate formation, in spite of the similar thermal conductivities of water and hydrate.

Using the thermal conductivities, we determined intrinsic rate constants and the activation energy of methane-hydrate-dissociation reactions by means of inverse modeling. The good agreement between numerical predictions and observations of pressure, temperature, and methane releases validated the parameters determined through the inversion process. Comparison of the results from the hydrate-bearing porous media to pure methane-hydrate samples has provided an initial measure of the effect of porous media on the kinetics of hydrate dissociation. The relative permeability measurements are in progress.

SIGNIFICANCE OF FINDINGS

Because of the strongly endothermic nature of hydrate dissociation and the importance of heat transfer, knowledge of the reaction kinetics and thermal properties of hydrate-bearing geological media is of critical importance to reliably predicting the gas production potential of natural gas hydrate deposits. These measurements and complementary modeling techniques should provide useful clues for understanding how natural gas can be produced from hydrate-bearing reservoirs.

RELATED PUBLICATIONS

Kneafsey, T.J., L. Tomutsa, G.J. Moridis, Y. Seol, B. Freifeld, C.E. Taylor, A. Gupta, Methane hydrate formation and dissociation in a partially saturated sand—Measurement and observations. In: 5th International Conference on Gas Hydrates, Trondheim, Norway, 2005. Berkeley Lab Report LBNL-57300.

Moridis, G.J., Y. Seol, T.J. Kneafsey, Studies of reaction kinetics of methane hydrate dissociation in porous media. In: 5th International Conference on Gas Hydrates, Trondheim, Norway, 2005. Berkeley Lab Report LBNL-57298.

ACKNOWLEDGMENTS

This work was supported by the Assistant Secretary for Fossil Energy, Office of Natural Gas and Petroleum Technology, through the National Energy Technology Laboratory, under the U.S. DOE Contract No. DE-AC03-76SF00098.

A New Analytical Solution for Migration of Sorbing Solute Tracers in Fractured Porous Media

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RESEARCH OBJECTIVES

The transport of chemicals or heat in fractured reservoirs is strongly affected by the fracture-matrix interfacial area. In water-saturated reservoirs, because molecular diffusion is orders of magnitude smaller than that in gas-dominated reservoirs, the tail of a breakthrough curve (BTC) is usually too weak to be practically useful as a characterization tool for determining the interfacial area. However, recent studies suggest that reversibly sorbing solute tracers can generate strong tails in BTCs that may allow a determination of such an area. To theoretically explore such a useful phenomenon, this paper develops an analytical solution for BTCs in slug-tracer tests within a water-saturated fractured reservoir.

APPROACH

We assume that the system has a single set of identical plane, parallel fractures with uniform fracture spacing and aperture, and that solute tracer is uniformly injected into the fractures at constant pore velocity and tracer concentration. Taking advantage of symmetry, we restrict the solution to an elementary part of the system (one-half of a fracture and its adjacent matrix block). The aperture is assumed much smaller than the length of the fracture, and transport in the fracture is assumed to be one-dimensional along the fracture. We ignore any tracer decay and treat the diffusive mass flux across the fracture-matrix interface as a sink/source term in the mass conservation equation for the fracture. We assume that transport in the matrix is only through diffusion (D is the diffusion coefficient) perpendicular to the interface, and that diffusion along the fracture is negligible compared with advection. Reversible sorption in the matrix is accounted for by a retardation factor, R. We derived the analytical solutions for tracer concentrations in the fracture and aperture, using the Laplace transform.

ACCOMPLISHMENTS

The solution reveals that BTCs in the fracture depend on four characteristic times: the tracer injection time, the travel time to the observation point, the across-fracture time (proportional to DR), and the across-matrix time (proportional to D/R). Since the first two times are known in a field test, and the last time only affects BTCs in the fracture for a fracture spacing on the order of centimeters, the across-fracture time is the only control factor on BTCs in most practical cases. This solution theoretically proves the numerical finding that BTCs depend only on the product, DR. A comparison of the analytical solution with the numerical (TOUGH2) solution is given in Figure 1, which shows excellent agreement for three different retardation factors.

SIGNIFICANCE OF FINDINGS

The analytical solution theoretically verifies an important finding, i.e., the retardation factor has the same effect as that of the diffusion coefficient. Although the diffusion coefficient is practically restricted, a wide range of retardation factors is practically available by using different chemical species as solute tracers. This equivalency thus provides the basis for using reversibly sorbing chemicals as tracers to test a fractured reservoir. In addition to its usefulness in verifying numerical codes, the analytical solution can also be useful as a screening tool for selecting solutes with appropriate sorption properties, and analyzing field data under simplified conditions. Such analysis can inversely estimate the two important parameters: the average fracture porosity and fracture spacing, from which the all-important fracture-matrix interfacial area per unit reservoir volume may be obtained.

RELATED PUBLICATION

Shan, C., and K. Pruess, An analytical solution for slug-tracer tests in fractured reservoirs. Water Resour. Res. (in press), 2005. Berkeley Lab Report LBNL-57285.

ACKNOWLEDGMENTS

This work was 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.

Frequency-Dependent Asymptotic Analysis of Seismic Reflection from a Fluid-Saturated Medium

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Contact: Dmitriy Silin, 510/495-2215, dsilin@lbl.gov

RESEARCH OBJECTIVES

In this project, a linear poroelasticity model is reviewed from the point of view of basic principles of flow in porous media. A low-frequency asymptotic analysis of this model is applied to interpreting the frequency-dependent reflection coefficient component at low-frequency ranges.

The developed approach targets frequency-dependent analysis of seismic data from different types of hydrocarbon reservoirs, at both exploration and development stages. A practically important objective of this research is to demonstrate how reservoir flow properties can be mapped using the obtained asymptotic reflectivity model.

APPROACH

We derive wave propagation equations from the basic principles of the theory of filtration, particularly to verify that both the filtration and poroelasticity theories have a common foundation. In addition, such an approach facilitates establishment of a relationship between seismic imaging attributes and hydraulic reservoir parameters.

Over the last fifty years, a significant effort has been spent on investigating the attenuation of Biot's waves. In many cases, the attenuation coefficient can be obtained in an explicit, but quite cumbersome, form. Computation of the reflection coefficient is even more complex. In this study, we obtain a simple asymptotic expression, in which the role of the reservoir fluid mobility is transparent. We focus on the simplest case of p-wave normal reflection. (Solutions for more complex situations are currently under development.)

ACCOMPLISHMENTS

At low seismic frequencies, viscous fluid flow in pore space results in anomalous reflection of the signal. The reflection coefficient has been asymptotically expressed as the sum of constant and frequency-dependent components. The latter is proportional to the square root of the frequency of the signal, with the proportionality coefficient including the reservoir rock and fluid flow properties. The frequency-dependent component also includes a phase shift of the reflected wave.

In addition, we investigated the dependence of scaling on the dynamic Darcy's law relaxation time, which turns out to be linearly related to Biot's tortuosity parameter. This parameter must be very large to enter first-order asymptotic formulae. In addition, previously processed seismic data sets have been reviewed in the context of the results. In particular, 3-D seismic data from the offshore South Marsh Island reservoir have been successfully reevaluated to image hydrocarbon-rich formation layers (Figure 1).

SIGNIFICANCE OF FINDINGS

It has been demonstrated how frequency-dependent analysis can be successfully used for direct hydrocarbon indication and reservoir characterization. The analysis was performed on field seismic data from onshore and offshore hydrocarbon fields, with different properties for the reservoir rocks. Besides its use in imaging, frequency-dependent analysis based on low-frequency asymptotic scaling has great potential for quantitative reservoir characterization.

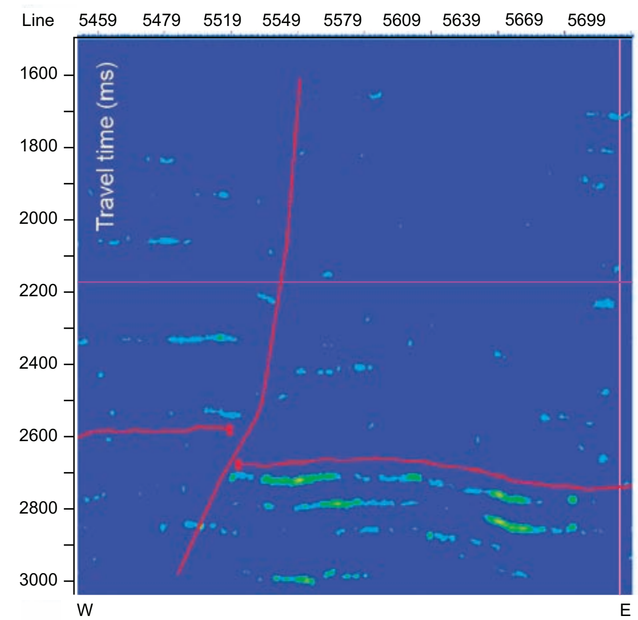

Figure 1. Imaging of the hydrocarbon-bearing zones on South Marsh Island, Gulf of Mexico, based on frequency-dependent analysis of 3-D seismic data. Conventional AVO analysis did not detect the reservoir. Data are courtesy of Fairfield Industries.

RELATED PUBLICATION

Silin, D.B., V.A. Korneev, G.M. Goloshubin, and T.W. Patzek, Low-frequency asymptotic analysis of seismic reflection from a fluid-saturated medium. Transport in Porous Media (in press), 2005. 58213

ACKNOWLEDGMENTS

This work was supported by the Assistant Secretary for Fossil Energy, Office of Oil and Natural Gas, National Energy Technology Laboratory, of the U.S. Department of Energy under Contract No. DE-AC03-76SF00098, Grant No DE-FC26-04NT15503. The industrial partners, Fairfield Industries and Shell International E&P, are gratefully acknowledged for providing field data.

Monitoring Waterflood Operations: Hall Method Revisited

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RESEARCH OBJECTIVES

The principal objective of this research is development of a robust and simple procedure for on-line monitoring of injecting well performance. An important requirement for the method is that it should not require interruption of regular field operations, and should be based on processing data routinely collected in waterflood operations. For example, such data may take the form of injection pressures and injection rates regularly recorded at each individual well as a time series. The results presented here are a part of the field-scale waterflood control system developed jointly by ChevronTexaco, with participation by the University of California, Berkeley, and Berkeley Lab.

APPROACH

Hall's method is a tool for evaluating injecting well performance. It is based on the assumption of radial steady-state flow. However, rigorous implementation of Hall's method requires information about the ambient reservoir pressure. In addition, it is assumed that the radius of influence is constant throughout the observation period. Neither of these parameters can be measured directly.

With this in mind, a series of forward simulations have been combined with analysis of injection pressures/injection rates data acquired from several hundred injection wells used in a waterflood project at the Lost Hills, California, diatomite oil field. The observations have been analyzed and interpreted using the model of steady-state flow. It turns out that inevitable fluctuations of injection pressures and rates can be used for estimation of an effective reservoir pressure, which in turn can be used for rigorous implementation of the Hall's method.

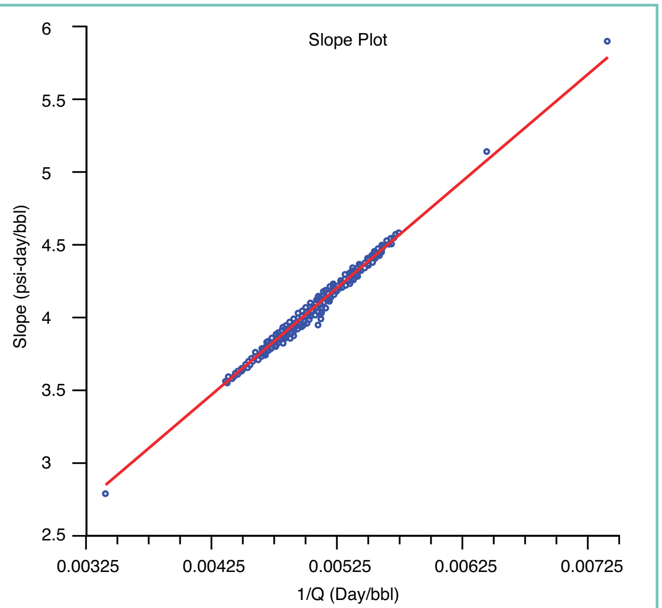

Figure 1. The slope analysis yields the reservoir pressure estimate by fitting injection pressures/injection rates data in special coordinates.

ACCOMPLISHMENTS

A new method called slope analysis has been proposed, based on analysis of Hall plot slope variations. This method produces an estimate of an apparent average reservoir pressure. As input, this method requires only time series of injection pressures and rates, which are routinely collected in the course of a waterflood. An automatic system of data acquisition has been implemented in the field, with measurements sent daily to a computer via the internet. As regular waterflood operations go on, the computer automatically processes the data, using a suite of custom-developed software tools.

The slope method has been verified both on synthetic and field data (Figure 1). It has been demonstrated that using the reservoir pressure estimates obtained by this method leads to correct interpretation of the Hall plot. At the same time, examples show that if such corrections are not done, the interpretation may be incorrect.

SIGNIFICANCE OF FINDINGS

The developed method is based on simple calculations and can be routinely applied for on-line injection-well performance monitoring. It can also be used in the petroleum industry, as well as in underground waste injection projects, where conventional well-performance evaluation procedures require interruption of operations and impose significant costs. The procedure has been incorporated into an injection control loop. Reservoir pressure maps, drawn based on slope analysis at multiple wells, make possible early detection of water breakthrough and reservoir compartmentalization.

RELATED PUBLICATION

Silin, D. B., R. Holtzman, T. W. Patzek, and J. L. Brink, Monitoring waterflood operations: Hall's Method revisited. SPE Paper 93879, Presentation at the 2005 SPE Western Regional Meeting held in Irvine, CA, U.S.A., March 30–April 1, 2005. Berkeley Lab Report LBNL-56928

ACKNOWLEDGMENTS

This work was supported by the Assistant Secretary for Fossil Energy, Office of Oil and Natural Gas, of the U.S. Department of Energy under Contract No. DE-AC03-76SF00098, and Chevron Corporation, through the UCOil consortium, University of California, Berkeley.

Crustal Deformation and Source Models of the Yellowstone Volcanic Field from Geodetic Data

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[2]Department of Geology and Geophysics, University of Utah, Salt Lake City, Utah; [3]UNAVCO, UCAR, Boulder, Colorado
Contact: Don Vasco, 510/486-5206, DWVasco@lbl.gov

RESEARCH OBJECTIVES

The Yellowstone volcanic system is tectonically active, driven by intraplate extension at the eastern edge of the Basin-Range Province. This region has experienced the largest historic earthquake in the Basin and Range province, the M7.5 1959 Hebgen Lake Event. The Yellowstone caldera is the vertex of multiple north- to northwest-trending normal faults, and at this time the extent to which these faults interact with and control the magmatic and hydrothermal system is not known. The rapidly varying and complex deformation of the Yellowstone caldera raises a number of questions: What process drives this deformation? What is the role of pressure change and mass flux? If there is significant mass flux, what is the ratio of partial melt, hydrothermal fluids, and/or gases? What factors control fluid fluxes and pressure changes in the subsurface—magma bodies, caldera structure, geologic boundaries, intersecting faults?

APPROACH

To gain insight into the factors controlling surface deformation, we construct models of subsurface volume change that are compatible with surface deformation data. Our approach, based upon the inversion of multiple types of geodetic data (including interferometric synthetic aperture radar [InSAR—Figure 1a]), is exploratory in nature. That is, we allow for an arbitrary, three-dimensional distribution of subsurface volume change. The resulting pattern of subsurface volume change and source geometry can provide clues to the factors controlling observed surface deformation. With an improved understanding of the nature of the controlling features, we may then go on to construct more detailed and prescribed models for the sources of deformation.

ACCOMPLISHMENTS

The primary accomplishment is a model of subsurface volume change that may be interpreted in terms of subsurface fluid migration [Figure 1b]. The picture that emerges is of subsurface volume change that correlates with the resurgent domes, the Elephant Back fault zone, a north-trending fault zone related to the volcanic vents, and the extensive magma body beneath the caldera. These correlations suggests that such features control or at least influence deformation within the caldera, either as zones of mechanical weakness or as pathways for fluid flow, or both. There is evidence to support the role of both the Elephant Back fault zone and a north-trending central caldera fault zone in both internal deformation and fluid flow. We thus hypothesize that the observed surface deformation within and adjacent to the Yellowstone caldera results from the interaction of an underlying, large-scale, crystallizing magmatic system and zones of weakness associated with crustal faults. In particular, large-scale pressure and mass changes within the magma body are focused into faults that act as narrow conduits or pathways for flow. It is the focused flow and pressure changes that give rise to the observed surface deformation.

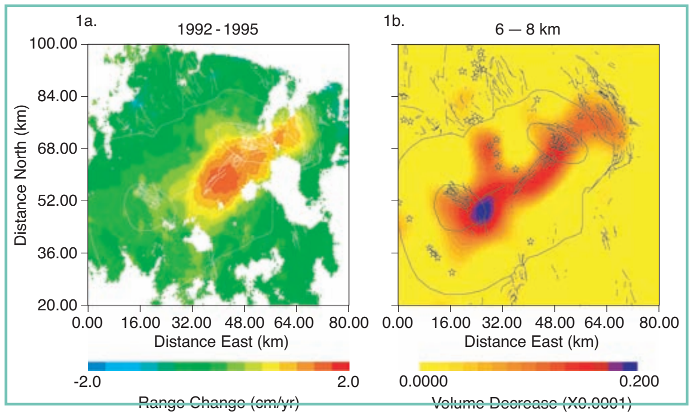

Figure 1a. Range change for the time interval 1992 to 1995. The color scale indicates the change in distance between the observation point in space and the surface of the Earth. Figure 1b. Volume change in the depth range is 6 to 8 km which is compatible with the observed range change.

SIGNIFICANCE OF FINDINGS

The findings are important because they further our understanding of how fluids interact with fault and fracture zones. Such interactions are critical to understanding hazards associated with volcanic regions and processes at work in geothermal fields. To date, little observational data are available on the interaction of fluids and faults/fractures in the earth. Most data are from idealized laboratory experiments or are interpreted using simple models. This work is the first step in an exploration of how geothermal fluids interact and influence faults and fracture zones. Understanding such interactions will help in finding new sources of geothermal energy.

ACKNOWLEDGMENTS

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

Numerical Simulation of Injectivity Effects of Mineral Scaling and Clay Swelling in a Fractured Geothermal Reservoir

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RESEARCH OBJECTIVES

A major concern in the development of hot dry rock (HDR) and hot fractured rock (HFR) reservoirs is achieving and maintaining adequate injectivity, while avoiding the development of preferential short-circuiting flow paths. Rock-fluid interactions and associated mineral dissolution and precipitation effects could have a major impact on the long-term performance of these reservoirs.

APPROACH

We used recent European studies as a starting point to explore the chemically induced effects of fluid circulation in geothermal systems. We performed coupled thermal-hydrologic-chemical simulations in which the fractured medium was represented by a one-dimensional MINC model (multiple interacting continua). The non-isothermal multiphase reactive geochemical transport code TOUGHREACT was used for these simulations.

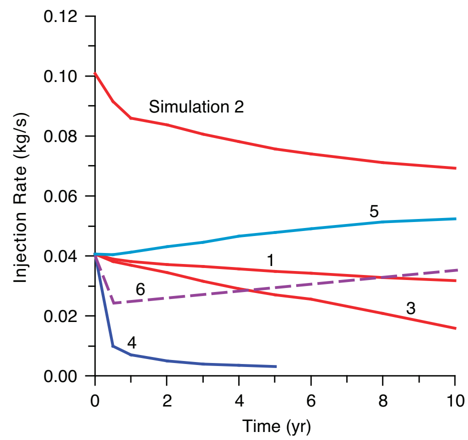

Figure 1. Injection rate of the fracture-matrix column with an area of 1 m^2. Simulation 1—base case; 2—over-pressure; 3—Verma-Pruess; 4—swelling; 5—pH 7; 6—mixing.

ACCOMPLISHMENTS

Injecting produced geothermal brines directly back into the reservoir results in mineral scaling. The reinjected, highly concentrated water from the geothermal reservoir can maintain clay density without swelling, but this limits the availability of water for injection. Mixing the produced geothermal water with large amounts of fresh water (1:4) can cause serious clay swelling when it is reinjected. However, modifying the injection water could avoid mineral scaling and enhance injectivity. Mitigating injection water chemistry could be an efficient way to achieve this objective. In this work, we added alkali to maintain a higher pH and let minerals (mainly calcite and quartz) precipitate out prior to reinjection. Using this modified injection water results in the injection rate gradually increasing, because of continual calcite and quartz dissolution. By mixing the reservoir water with appropriate amounts of fresh water (1:1), together with adding alkali to let minerals precipitate out, we can reduce clay swelling and maintain injectivity. The well configuration and data for mineralogical composition in this study were taken from the European HDR research site, but the results and conclusions should be useful for other HFR reservoirs, because calcite and quartz are commonly present in geothermal systems.

SIGNIFICANCE OF FINDINGS

A detailed, quantitative understanding of processes and mechanisms, as presented in this research, is needed to develop reservoir management tools based on geochemistry. Such a novel approach should result in improvements in reservoir performance.

RELATED PUBLICATIONS

Xu, T, G. Zhang, and K. Pruess, Use of TOUGHREACT to simulate effects of fluid chemistry on injectivity in fractured geothermal reservoirs with high ionic strength fluids. In: Proceedings of the 30th Workshop on Geothermal Reservoir Engineering, Stanford University, California, January 31–February 2, 2005. Berkeley Lab Report LBNL-56532.

Xu, T, and K. Pruess, Numerical simulation of injectivity effects of mineral scaling and clay swelling in a fractured geothermal reservoir. Proceedings of Geothermal Resources Council 2004 Annual Meeting, Palm Springs, California, August 29–September 1, 2004. Berkeley Lab Report LBNL-55113.

ACKNOWLEDGMENTS

This work was 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.

Injection of CO_2 with H_2S and SO_2 and Subsequent Mineral Trapping in a Sandstone-Shale Formation

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RESEARCH OBJECTIVES

Carbon dioxide (CO_2) injection into deep geologic formations can potentially reduce atmospheric emissions of greenhouse gases. Sequestering less-pure CO_2 waste streams (containing H_2S and/or SO_2) would require less energy than separating CO_2 from flue gas. The long-term interaction of these injected acid gases with shale-confining layers of a sandstone injection zone has not been well investigated. We therefore have developed a conceptual model of CO_2 injection with H_2S and/or SO_2 into a sandstone-shale sequence, using hydrogeologic properties and mineral compositions commonly encountered in Gulf Coast sediments of the United States.

APPROACH

We have performed numerical simulations of a 1-D radial well region considering sandstone alone, and a 2-D model using a sandstone-shale sequence under acid-gas injection conditions. The reactive fluid flow and geochemical transport simulator TOUGHREACT was used for these simulations. We considered the presence of organic matter, the kinetics of chemical interactions between the host rock minerals and the aqueous phase, and CO_2 solubility dependence on pressure, temperature, and salinity of the system.

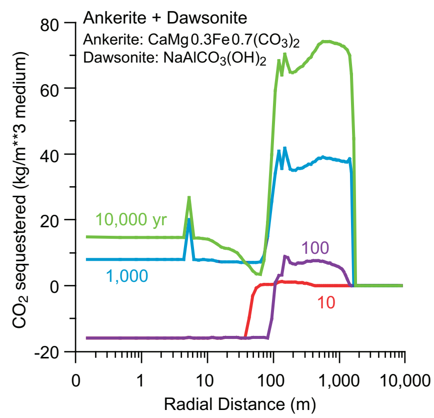

Figure 1. Cumulative CO_2 sequestered by carbonate mineral precipitation at different times

ACCOMPLISHMENTS

The co-injection of H_2S, compared to injection CO_2 alone, does not significantly affect pH distribution and the mineral alteration pattern. The co-injection of SO_2 results in a different pH distribution and mineral alteration pattern. A zonal distribution of mineral alteration and formation of CO_2 and sulfur-bearing minerals has been observed in the simulations, which reflects the pH distribution. Co-injection of SO_2 results in a larger and stronger acidified zone (as low as a pH of 0.6). Corrosion and well abandonment problems will be a very significant issue for SO_2 injection. Most CO_2 is trapped by precipitation of ankerite and dawsonite, with some in siderite. Using conditions and parameters presented in Xu et al. (2005), a CO_2 mineral trapping capability after 10,000 years can reach about 80 kg per cubic meter of medium. The CO_2 trapping capability depends on the primary mineral composition. For example, precipitation of siderite and ankerite requires Fe^{2+} supplied by the dissolution of primary iron-bearing minerals. Most of the sulfur is trapped by alunite precipitation, some by anhydrite, and some still smaller amount by pyrite. Precipitation of these sulfur-bearing minerals occurs primarily during the injection operation period, because the SO_2 inventory is very small (1 wt.% of CO_2 injected in the simulations). Adding acid gases leads to increases in porosity close to the well, caused by mineral dissolution, and decreases at distances, resulting from CO_2 trapping. The simulated mineral alteration pattern is generally consistent with available field observations of natural CO_2 reservoirs.

SIGNIFICANCE OF FINDINGS

The effects of co-injection of H_2S and SO_2 on CO_2 geological sequestration is evaluated, and CO_2 mineral trapping capability is estimated. The "numerical experiments" give a detailed understanding of the acid gas injection system.

RELATED PUBLICATION

Xu, T, J. A. Apps, K. Pruess, and H. Yamamoto, Injection of CO_2 with H_2S and SO_2 and subsequent mineral trapping in sandstone-shale formation. Berkeley Lab Report LBNL-57426, 2005.

ACKNOWLEDGMENTS

This work was supported by the Director, Office of Science, Office of Basic Energy Sciences, of the U.S. Department of Energy, under Contract No. DE-AC03-76SF00098 with Lawrence Berkeley National Laboratory.

TOUGHREACT
A Comprehensive Numerical Simulator for Chemically Reactive Flows

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RESEARCH OBJECTIVES

Reactive chemical transport occurs in many geologic systems and environmental problems, including geothermal systems, diagenetic and weathering processes, subsurface waste disposal, acid mine drainage remediation, contaminant transport, and groundwater quality. The objective of this work was to develop a publicly available comprehensive simulation tool for these processes.

APPROACH

The reactive transport simulator TOUGHREACT (Xu et al., 2004) has been developed by introducing reactive geochemistry into the existing framework of a nonisothermal, multicomponent fluid and heat flow simulator TOUGH2. Our modeling of flow and transport in geologic media is based on space discretization by means of integral finite differences (IFD). The IFD method yields a flexible discretization for geologic media, one that allows use of irregular grids. This is well suited for simulation of flow, transport, and fluid-rock interaction in multiregion heterogeneous and fractured rock systems. An implicit time-weighting scheme is used for the individual components of the model, consisting of flow, transport, and kinetic geochemical reactions. TOUGHREACT uses a sequential iteration approach. Chemical transport is solved on a component basis, with the resulting concentrations obtained from the transport substituted into the chemical reaction model. The system of chemical reaction equations is solved on a gridblock basis by a Newton-Raphson iteration. The chemical transport and reaction equations are iteratively solved until convergence.

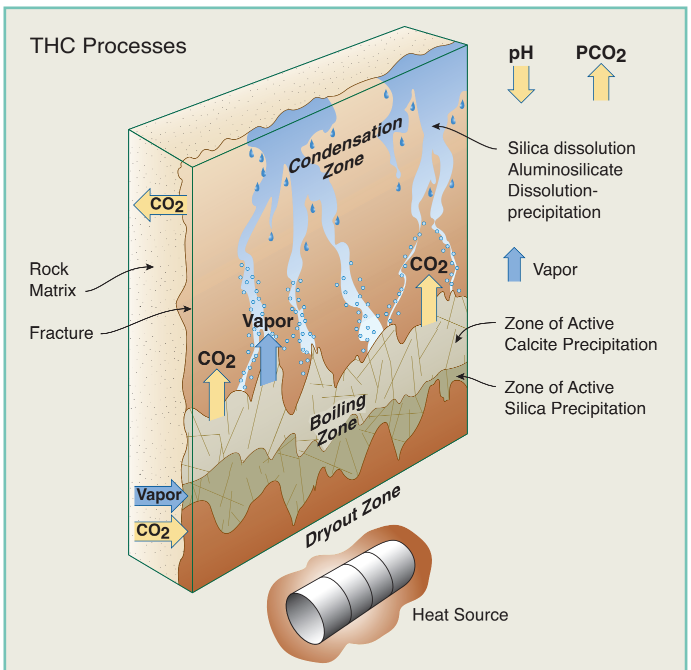

Figure 1. A schematic representation of a coupled thermal-hydro-chemical problem solved by TOUGHREACT

ACCOMPLISHMENTS

TOUGHREACT considers a wide variety of subsurface thermal-physical-chemical processes under various conditions of pressure, temperature, water saturation, ionic strength, and pH and Eh. It can be applied to one-, two-, or three-dimensional porous and fractured media with physical and chemical heterogeneity. The code can accommodate any number of chemical species present in liquid, gas, and solid phases. A variety of equilibrium chemical reactions are considered, such as aqueous complexation, gas dissolution/exsolution, cation exchange, and surface complexation. Mineral dissolution/precipitation can be simulated subject to either local equilibrium or kinetic controls, with coupling to changes in porosity and permeability. Chemical components can also undergo linear adsorption and radioactive decay. TOUGHREACT has been applied to a broad range of chemically reactive flow problems related to geothermal reservoir processes, groundwater protection, nuclear waste disposal, geologic storage of CO_2, and mining engineering. This software was released to the public through the DOE Energy Science and Technology Software Center in November 2004.

SIGNIFICANCE OF FINDINGS

TOUGHREACT is a very versatile simulator that can be applied to a broad range of environmental and resource problems of interest to DOE and industry.

RELATED PUBLICATION

Xu, T., E.L. Sonnenthal, N. Spycher, and K. Pruess, TOUGHREACT User's Guide: A simulation program for non-isothermal multiphase reactive geochemical transport in variable saturated geologic media. Berkeley Lab Report LBNL-55460, 2004.

ACKNOWLEDGMENTS

The development of TOUGHREACT was initially funded by the Laboratory Directed Research and Development Program. Subsequent development was supported by the Assistant Secretary for Energy Efficiency and Renewable Energy, Office of Geothermal Technologies; by the Director, Office of Science, Office of Basic Energy Sciences; and by the Director, Office of Civilian Radioactive Waste Management, of the U.S. Department of Energy, under Contract No. DE-AC03-76SF00098.

Research Program

Environmental Remediation

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The key driver for the Environmental Remediation Program (ERP) within ESD is to provide the scientific foundation needed for environmental remediation and water resources management. Over the last decade, it has become increasingly clear that if we are to face the environmental and water challenges of the future, we must view the system as a complex entity that includes the hydrosphere, geosphere, and biosphere. It has also become clear that these components are coupled and highly dynamic over various spatial and temporal scales. Since the U.S. Department of Energy (DOE) is responsible for the environmental health of over 140 contaminated waste sites across the United States, understanding the complexity of such natural systems is a prerequisite to successful stewardship of the DOE waste sites. As such, the majority of the enviromental research projects within the ERP focus on problems that are critical to the DOE waste sites. However, since many of the contaminants or closely related compounds found at these sites are also dominant at industrial waste sites, much of this research is also applicable to problems faced by the private sector and other government agencies. Because water resources and quality are particularly important for the vitality of water-stressed regions such as California, much of the water resources research performed in the ERP focuses on development of tools and techniques that will lead to better management of California water resources. A brief description of the environmental remediation and water resources programmatic areas of the ERP is given below.

ENVIRONMENTAL REMEDIATION

ESD scientists participating in the ERP conduct multidisciplinary environmental research using theoretical, characterization, modeling, and experimental approaches that range from the molecular to the field scale. The synergy offered by the ensemble of competencies within the ESD facilitates investigation of complex natural systems. Many of the projects within the ERP are associated with one of the following five themes:

- Development of advanced tools and approaches for characterizing biological, hydrological, and geochemical properties and processes at the molecular to field scale
- Development of tools to detect unexploded ordnance (UXOs)
- Improved understanding of complex natural systems and the impact of system complexity on contaminant distribution and remediation efficacy
- Improved ability to predict reactive contaminant transport in the subsurface
- Development of biological or chemical techniques capable of removing or sequestering contaminants

ESD scientists within the ERP program have developed many novel tools and techniques over the past few years that can be used to characterize properties and processes, and to monitor how they change in response to environmental perturbations. The newly developed Virtual Institute of Microbial Stress and Survival (VIMSS), based at Berkeley Lab, seeks to identify stress-response pathways of microbes important for environmental remediation. ERP scientists associated with VIMSS have determined the signature genes for sulfate-reducing bacteria, developed techniques for large-scale biomass production needed for cell analysis, and have developed a community resource for comparative microbial genomics. ERP scientists associated with VIMSS have also successfully used microarray techniques to characterize the phenotype of bacterial strains important for environmental remediation and have used PLFA techniques to determine the phenotypic response of cells to environmental stressors. High-density DNA microarray technologies were used by ERP researchers to detect large numbers of microorganisms within complex environmental environments, and to accurately monitor changes in the composition of microbial populations during laboratory- and field-scale studies of uranium (U) bioremediation.

Collectively, these studies improve our understanding of microbiological properties and processes, which is critical for designing sustainable contaminant bioremediation treatments.

ERP scientists are also involved in the Center for Environmental Kinetics Analysis, a collaborative effort exploring what molecular approaches and insights can be developed to extrapolate rates of environmentally important reactions across a variety of scales. In particular, ERP scientists are investigating the rates of formation and the topology of oxyhydroxide and silicate precipitates from the molecular to the nanoscale using synchrotron techniques, with a goal of understanding precipitate formation and reactivity. Scientists involved in this Center are also investigating mineral dissolution and precipitation rates under biotic and abiotic conditions via synchrotron-based experiments, using microfluidic reactive flow devices and x-ray spectroscopy methods.

Many advances have recently been achieved by ERP scientists in the use of high-resolution geophysical data for characterizing and monitoring subsurface systems. Stochastic joint inversion techniques were developed to combine geophysical and hydrological data for the estimation of hydrological properties at the Hanford Site in Washington, and to estimate fracture zonation at the Oak Ridge National Laboratory in Tennessee. During the past two years, ERP scientists have discovered that noninvasive geophysical techniques could be used at the laboratory scale to monitor biomineralization and gas production associated with bioremediation processes. In related studies, surface geophysical data were used to indicate the change in clay mineralogy caused by bioremediation at the field scale, and tomographic geophysical data were used to monitor amendment distribution associated with a Cr(VI) bioreduction study at the Hanford Site. These studies reveal the potential of high-resolution geophysical data sets for providing the hydrogeological characterization information that is important for predicting contaminant transport, or for noninvasively monitoring system transformations during remedial processes.

Significant advances have also recently been made by ERP scientists in the development of geophysical tools that can detect and extract essential information about buried metallic objects—information that is essential for identification and discrimination of unexploded ordnance (UXO). Through research that received the Strategic Environmental Research and Development Program (SERDP) Project of the Year Award, ERP scientists have developed an active electromagnetic (AEM) field prototype system that can obtain estimates of the location, size, shape, and metal content of a buried metallic object in the presence of other metallic clutter.

Novel isotopic approaches were successfully developed and applied by ERP scientists to identify the source of contaminants at DOE waste sites. Precise U isotopic approaches were used to analyze the pore water of subsurface sediment samples at the T-Waste Management Area (WMA) of the Hanford Site in Washington, and to unravel the history of U contamination there. Isotopic analysis of U and strontium isotopes were used to trace the source of U from the site to the Hanford Reach of the Columbia River, and to monitor how the flux varies with seasons. ERP scientists have streamlined a nitrate isotopic analysis technique and used the technique to study the nitrate distribution and origin at several Hanford vadose zone and groundwater sites. Such novel isotopic approaches are critical to establishing both an understanding of complex transport in natural systems and for establishing remediation strategies and responsibilities.

Laboratory studies conducted by ERP scientists have revealed phenomena that have significant implications for designing and sustaining environmental remediation approaches at the Hanford site. Column studies, designed to mimic the leakage of highly saline and alkaline radioactive waste solutions from Hanford storage tanks into sediments, revealed a significant pH reduction and colloid formation at the plume front. These observations suggest the importance of considering plume-front phenomena for predicting the behavior of contaminants in the Hanford subsurface. Column studies were also used to investigate the conditions that control long-term stability of bioreduced U. These studies indicated that at 100 to 500 days after U reduction, U was reoxidized and solubilized even in the presence of a microbial community capable of reducing U(VI). This study suggests that *in situ* U remediation using organic carbon-based reductive precipitation can be problematic in sediments when uranyl carbonates are stable.

ERP scientists have recently assessed the potential for immobilizing and detoxifying chromium (Cr)-contaminated groundwater at the Hanford 100H site using lactate-stimulated bioreduction. Microbial, geophysical, and geochemical analysis of groundwater, coupled with stable isotope monitoring, permitted accurate tracking of microbial processes during this field treatabilty study, and confirmed that Cr(VI) was successfully removed from groundwater at the Hanford 100H Site. Such studies reveal the benefits of interdisciplinary approaches for investigating and manipulating complex earth systems.

WATER RESOURCES AND QUALITY

To optimally manage our water resources, ERP scientists are developing tools and approaches that can be used to measure, understand, and predict the flow, transport, and residence times of water, nutrients, and contaminants through natural water systems. With a population of over 30 million people, an agricultural economy based on intensive irrigation, and large urban industrial areas, California is highly dependent on water for its vitality and productivity. Consequently, much of the water research within the ERP is focused on problems important to this state.

ERP scientists have developed a variety of tools to characterize hydrological, geochemical, and biological properties and processes needed for managing water resources. Motivated by the concern about endocrine-disrupting compounds in recycled water, ERP scientists have developed a prototype biosensor capable of assessing estrogenic compounds. These scientists have successfully used the biosensor to assess water from various wastewater treatment and natural systems. Several logging tools have also been developed by the ERP this year and applied to watershed studies, including the electrical conductivity sensors used to identify high-salinity zones in agricultural areas, and heat-based sensors used to indicate flow velocities.

System-level studies are being carried out to understand complex hydrological and ecological phenomena. ERP scientists are investigating the San Joaquin River in the Central Valley of California to examine how non-point-source pollution discharge associated with agricultural activities impacts water quality. Their investigations involve field measurements to determine mass balance of algae and nutrients within the system. Understanding the conditions that give rise to unsaturated flow below a streambed in Sonoma County, California, and the impact that this may have on well operations in the area, is being investigated by ERP scientists using advanced measurement and modeling techniques. ERP scientists are also actively investigating water-balance and water-quality issues within several California counties, including Merced County. Remediation approaches have also been recently developed by ERP scientists working on water resources projects. Our scientists developed an algal-bacterial selenium removal process deployed within the agricultural drainage area of the western San Joaquin Valley to remove nitrate and selenium from irrigation drainage. An important component of many of the water resource projects is the development of computer-based decision support systems to enhance environmental monitoring and management of water systems.

ERP PROGRAM MANAGEMENT AND TECHNICAL ASSISTANCE

ERP continues to be the Natural and Accelerated Bioremediation Research (NABIR) Program Office for the Office of Science. The NABIR Program Office maintains the dynamic NABIR Web home page (www.lbl.gov/NABIR/) with links to investigators, program element managers, science team leaders, recent publications, annual meeting registration, calls for proposals, review documents, and other Web sites. In addition, the NABIR Program Office also organizes the NABIR annual investigators meeting, with more than 150 participants and sessions for posters, presentations, and breakout sessions.

ERP scientists also manage the Environmental Program at the Advanced Light Source (ALS), as described by http://esd.lbl.gov/ALS_environmental/index.html. This program is designed to assist environmental researchers in gaining familiarity with and access to the ALS, and in assisting with environmental investigations at the ALS. Many of the environmental investigations in this program focus on understanding how and what microbiological and geochemical species are distributed relative to contaminants and within natural geological materials, which processes occur, and the rates at which they occur. The program provides support across four beamlines, enabling a range of measurement support scales from nanometers to centimeters.

ERP scientists provide technical assistance to DOE Environmental Management International projects. The overall objectives of this program are to use foreign sites as analogues to improve the capability of DOE's conceptual and numerical models for predicting radionuclide transport and impact, and to improve DOE remediation technologies. Recent projects have focused on helping in the design of site characterization, radionuclide transport modeling, and remediation technologies at the Kurchatov Institute in Russia, the Chernobyl Exclusion Zone in Ukraine, and the Ezeiza Atomic Center in Argentina.

PARTNERS AND FUNDING

ERP receives much of its support for environmental research from DOE programs in the Office of Science, Office of Biological and Environmental Research. These programs include the Natural and Accelerated Bioremediation Research (NABIR) and the Environmental Management Science Program (EMSP) of the Environmental Remediation Sciences Division, and from the Genomics: GTL Program. DOE's Office of Environmental Management supports the International Program technical assistance and also supports some of the research performed at the Hanford, Washington, site. Research associated with unexploded ordnance is supported by SERDP. Much of the California water resources and quality projects are supported by the CALFED Bay-Delta Program, Department of Water Resources, and the U.S. Bureau of Reclamation. Support for ERP projects is also provided by NASA, the Department of Defense, the Department of Homeland Security, Cal-EPA, other DOE Labs, the Berkeley Lab LDRD Program, Sonoma County Water Agency, U.S. Army, DHS, UC Berkeley, Panoche Drainage District, and the U.S. Bureau of Land Management.

Real-Time PCR with Reverse Transcription for Quantification of Chlorinated Solvent Degradation

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RESEARCH OBJECTIVES

The purpose of this project is to develop and apply culture-independent molecular approaches for characterizing microbial communities capable of degrading chlorinated solvents in subsurface aquifers.

APPROACH

Our approach is to apply quantitative real-time polymerase chain reactions (qPCR) and reverse transcription to quantify the occurrence and expression of dehalogenating species and genes in laboratory enrichments under varying conditions. Whole-genome microarrays will then be applied to query the transcriptome of *Dehalococcoides* strains.

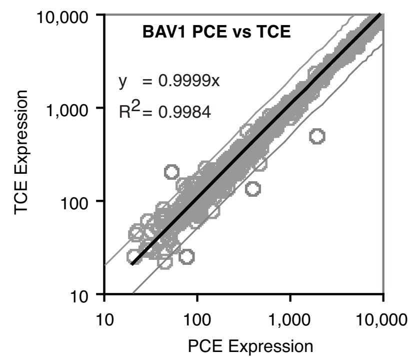

Figure 1. Comparison of microarray fluorescence intensity after 8-hour PCE or TCE exposure for the 618 genes that had significant signal:noise ratios under both conditions. Faint lines indicate 2-fold difference, while the solid line is a linear fit to the data. BAV1 cells were grown on VC and exposed just before exhaustion of VC. BAV1 is a strain of *Dehalococcoides sp.* that utilizes vinyl chloride for growth by means of dehalorespiration.

ACCOMPLISHMENTS

Functional-gene expression analysis using quantitative PCR

By combining qPCR with reverse transcription, we can accurately monitor the expression level, defined as the ratio of mRNA to DNA, of any expressed gene. We have used this technique to study changes in the expression of the *Dehalococcoides* functional reductase gene, *tceA*, within the ANAS mixed community, in response to growth condition perturbations. We found that expression of the *tceA* gene dramatically increases after cells are exposed to trichlorylethylene (TCE) or isomers of dichlorylethylene (DCE), but not perchlorylethylene (PCE) or vinyl chloride (VC). The *tceA* gene expression response did not depend on the sum concentration of TCE and DCE when they were present in environmentally relevant concentrations (≥1.8 μM), nor on the concentration of electron donor above threshold concentrations (≥ 17 nM H_2), or the presence of common microbial electron acceptors (sulfate, sulfite, thiosulfate, nitrate, nitrite, or fumarate). Incubation temperature, however, had a substantial effect on *tceA* expression, with *tceA* expression at 30°C more than 10-fold higher than at 14°C.

Cooperation and interactions between Dehalococcoides strains

We used qPCR to study the *Dehalococcoides* population within an enrichment culture, using primers for three different functional reductase genes and the *Dehalococcoides* 16S rDNA. The data suggest that the enrichment culture contains two cooperating *Dehalococcoides* strains, which in turn contain reductases with different functions in roughly a 1:2 ratio; and that the relative amounts of the two strains can be dramatically altered by adjusting solvent exposure conditions.

Analyzing genomics and transcriptomics using whole-genome microarrays

An Affymetrix whole-genome microarray for *D. ethenogenes* 195 was designed in collaboration with Gary Anderson of Berkeley Lab and Professor Stephen Zinder of Cornell University. The queried transcriptome produced statistically significant hybridization signal on roughly 40% of the 1,600-gene chip: 725 genes showed expression after either PCE or TCE exposure, and 618 genes showed expression under both conditions. The reproducibility between TCE- and PCE-exposed cells was excellent (Figure 1), with an R-2 value of 0.9984.

RELATED PUBLICATIONS

Johnson, D.R., P.K.H. Lee., V.F. Holmes, and L. Alvarez-Cohen. An internal reference technique for quantifying specific mRNAs by real-time PCR with application to the *tceA* reductive dechlorination gene. Applied and Environmental Microbiology (in press), 2005.

Johnson, D.R., P.K.H. Lee, V.F. Holmes, and L. Alvarez-Cohen. Environmental factors affecting the expression of the *tceA* reductive dechlorination gene in an anaerobic microbial enrichment culture. Applied and Environmental Microbiology (submitted), 2005.

ACKNOWLEDGMENTS

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

Whole Genome Transcriptional Analysis of Toxic Metal Stresses in *Caulobacter Crescentus*

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RESEARCH OBJECTIVES

Caulobacter crescentus is an extremely ubiquitous organism with a distinctive ability to survive in low nutrient environments. In this study, we exposed the *Caulobacter crescentus* cells to five heavy metals (chromium, cadmium, selenium, lead, and uranium) and analyzed genome-wide transcriptional activities. The understanding of resistance pathways can provide important insight and knowledge for environmental restoration.

APPROACH

Transcriptional regulation was measured using a *Caulobacter* Affymetrix GeneChip array custom designed by the McAdams Lab (Stanford, California). In addition to the multiple probes for all predicted coding regions, probes were tiled for both strands, encoding all hypothetical proteins plus all intergenic regions. This feature makes it possible to detect all transcripts without prior knowledge and bias, including untranslated regulatory RNAs and antisense transcripts (transcripts from the opposite strand of a predicted open reading frame).

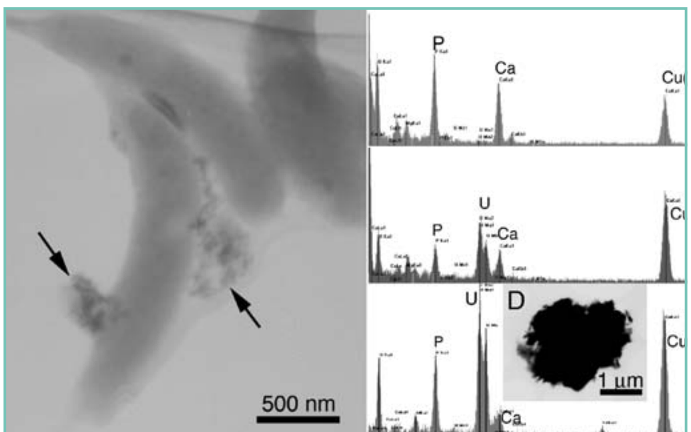

Figure 1. Extracellular uranium-bearing precipitates. The EDX showed the precipitates contained uranium, phosphate, and calcium.

We have also used electron microscopy (EM) to visualize *Caulobacter crescentus* cells under 200 µM uranium stress for 30 minutes and found that uranium was associated with cells extracellularly. Energy Dispersive X-ray (EDX) analysis was carried out to determine elemental compositions of uranium-bearing solid phases associated with cells.

RESULTS

In addition to the unexpected finding that *C. crescentus* CB15N is tolerant to high levels of uranium, our studies—combining physiology observation, transcriptional measurement, and imaging analysis—clearly showed that *Caulobacter* formed a calcium-uranium-phosphate precipitate extracellularly (Figure 1). This observation was consistent with a limited response to oxidative stress such as that seen with other metals and also with the up-regulation of a secreted calcium-dependent phytase domain protein, which may serve as a nucleation site for uranium precipitation. The strategy of lowering intracellular metal concentration was also present in cadmium and chromium response. Efflux pumps were up-regulated under cadmium stress. *C. crescentus* does not seem to have a specific extrusion mechanism for chromium; however, the cells down-regulated a sulfate transporter, which may reduce the uptake of chromate.

Our data have also clearly demonstrated the importance of interrogating the whole genome on both strands. We have identified at least six antisense transcripts that are differentially regulated specific to metals, which, as either proteins or RNAs, may play an import part in the response model. Using knockout mutants, we also confirmed regulatory roles played by a pair of two-component signal transduction proteins under uranium stress.

SIGNIFICANCE OF FINDINGS

The principal response to most metals was protection against oxidative stress (up-regulation of manganese-dependent superoxide dismutase, *sod*A), while glutathione S-transferase, thioredoxin, glutaredoxins and DNA repair enzymes responded specifically to cadmium and chromate. Cadmium and chromium stress response also focused on reducing the intracellular metal concentration, with multiple efflux pumps being employed to remove cadmium while a sulfate transporter was down-regulated to reduce nonspecific uptake of chromium. The function of a two-component signal transduction system involved in uranium response was confirmed by knockout mutants. In addition, several differentially regulated transcripts from regions previously not known to encode proteins were identified, demonstrating the importance of evaluating the transcriptome using the whole genome.

RELATED PUBLICATION

Hu, P., E.L. Brodie, Y. Suzuki, H.H. McAdams, and G.L. Andersen, Whole-genome transcriptional analysis of heavy metal stresses in *Caulobacter crescentus*. Journal of Bacteriology, 187(24), 8437-49, December 2005. Berkeley Lab Report LBNL-59011.

ACKNOWLEDGMENTS

This study was funded by *Department of Energy, Genomes to Life: Microbial Cell Program*. This work was performed under the auspices of the U.S. Department of Energy by the University of California, Lawrence Berkeley National Laboratory, under Contract No. DE-AC03-76SF00098.

16S rDNA Microarray for Microbial Community Analyses in Air, Soil, and Water

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RESEARCH OBJECTIVES

Knowledge of the microbial community structure, including the predominant species composition and shifts in population dynamics, is necessary for understanding the effect of any perturbation on a natural ecosystem. The resulting mixed amplicons can be quickly, but coarsely, typed into anonymous groups using molecular techniques such as restriction fragment length polymorphism. Subsequent sequencing allows application of taxonomic nomenclature to the groups, but requires additional labor to physically isolate each 16S rDNA type and does not scale well for large studies. Instead, hybridizing polymerase chain reaction (PCR) products to a high-density universal 16S rDNA microarray allows rapid taxonomic classification of community members. In this study, we asked, “Which method is more comprehensive in cataloging an environmental prokaryotic 16S amplicon community, clone-and-sequencing or microarray?”

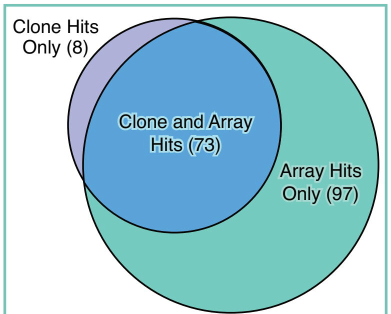

Figure 1. Comparison of bacterial groups detected by either 16S Microarray or 16S Clone Library

APPROACH

Molecular approaches aimed at broad prokaryotic environmental detection routinely rely upon classifying heterogeneous nucleic acids amplified by universal 16S rDNA PCR. Cloning-and-sequencing the PCR products has been the general method of sampling the DNA types, but does not scale well for large studies. Instead, hybridizing PCR products to a universal 16S rDNA microarray allows a more rapid evaluation. We have developed a high-density microarray system to accurately measure the key microbial components in air, water, and soil environments. Unique regions of DNA within gene sequences of a 16S ribosomal RNA small subunit are used to identify specific organisms. A minimum of 11 oligonucleotide probes (25-mers) are used in combination to identify, in parallel, any of over 9,000 distinctive species or taxa on a 500,000-probe, high-density microarray. The combinatorial approach of multiple probes has clear advantages over a single probe for the identification of a target sequence. Broad-range bacterial and archaeal 16S primers that target conserved areas at the 5′ and 3′ ends of the 16S rRNA gene are used to amplify 1,400–1,500-bp fragments for analysis. This 16S microarray system was used to measure the microbial diversity of aerosols collected from a biosurveillance network—subsurface sediment contaminated with uranium and deep subsurface water from a South African gold mine.

RESULTS

In each sample, the array revealed a greater number of taxonomic groups of bacteria than the corresponding clone library. This result was expected, since nonasymptotic rarefaction curves demonstrated that the clone libraries were only a partial sample of the total sequence diversity. To validate the presence of the bacterial groups, which were detected only by the array, taxon-specific primers were created for the aerosol sample. The resulting sequences verified the array detection of probe-sets corresponding to specific bacterial groups. Entire phyla, including *Nitrospira* and *Spirochaetes,* would have been overlooked if the clone library were the sole source of taxonomic sampling. In addition, sample-to-sample variation in probe hybridization intensity of a previously identified airborne organism, *Pseudomonas oleovorans*, was independently confirmed by quantitative, real-time PCR amplification, with species-specific primers using the genomic DNA from the concentrated aerosol samples.

SIGNIFICANCE OF FINDINGS

A hybridization-based approach using oligonucleotide microarrays can be applied for the fast and parallel detection of large numbers of microorganisms from complex environmental samples. Constrained by the numbers of different oligonucleotide probes that can be spotted within a given area, most arrays have been designed to measure a selected subgroup of organisms that have been hypothesized to play critical roles within a larger community. We developed an approach to leverage the vast amount of 16S sequence data available in public databases and search for unique sequences that can be used for identification. Compared with sequencing a 16S rDNA clone library, the microarray was unable to recognize novel prokaryotic families, but could identify greater diversity from organisms with similarity to existing sequence (Figure 1).

ACKNOWLEDGMENTS

This work was performed under the auspices of the U.S. Department of Energy by the University of California, Lawrence Berkeley National Laboratory under Contract No. DE-AC03-76SF00098, and was funded in part by the Department of Homeland Security under Grant No. HSSCHQ04X00037.

Development of Environmental Biosensors for Endocrine Disrupters

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RESEARCH OBJECTIVES

Water recycling is an important strategy for management of this scarce resource, but concerns about residual contamination in recycled water remain a limiting barrier in implementing water conservation through water recycling. Concerns have developed around endocrine disrupting compounds (EDCs) in recycled water because of their ability to mimic hormones involved in many biological processes, including immune function, reproduction, growth, and control of other hormones. EDCs are hormonally active at small concentrations (parts per billion or trillion). The list of EDCs found in water is steadily growing and includes many common agricultural, industrial, and household chemicals and their degradation products. Significant sources of EDCs include both synthetic chemicals like pesticides and those produced naturally by plants and animals. The objective of this work is to develop analytical capabilities to characterize the diverse sources of EDCs in urban and agricultural sources to evaluate the connection between EDCs and pesticides, and to develop biosensors to detect EDC activity in natural sources.

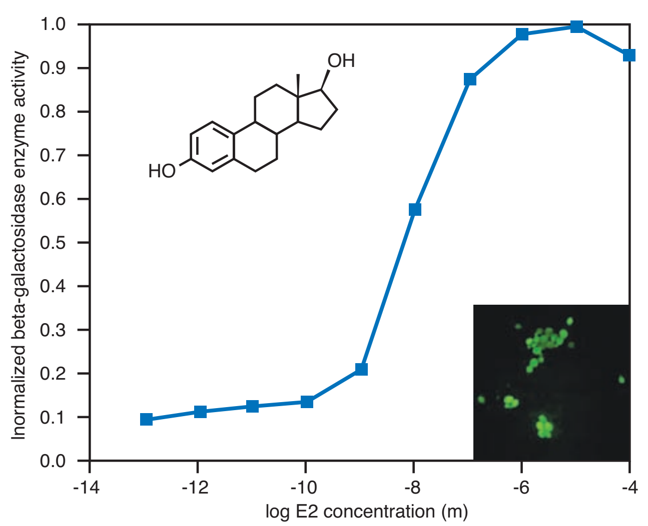

Figure 1. Dose-response of β-galactosidase enzyme production when the estrogen-responsive yeast strain RMY/ER-ERE is exposed to the hormonal estrogen 17β-estradiol (E2). Inset is the chemical structure of E2 and the fluorescent response of live yeast cells to E2. Other estrogenic compounds, including some EDCs, may behave in a similar manner, eliciting a similar response.

APPROACH

Traditional analytical techniques (gas chromatography, gas chromatography/mass spectrometry, high-pressure liquid chromatography) were used for calibration and verification of bioassays. Analytic capabilities were developed for hormones in both sediment and water to improve sensitivity and modify the techniques for use in an automated system. Enzyme-linked immunosorbent assay (ELISA) kits were used for analysis of estrogenic chemicals in water, wastewater, wastewater solids, and sediment. Chromogenic and fluorescent bioassays were developed to monitor estrogenic activity in water samples, and the response was studied using microscopy and spectroscopy to evaluate cell structural changes, viability, and response (Figure 1).

ACCOMPLISHMENTS

A prototype biosensor system was developed to measure the cellular response of luminescent microbes, providing the hardware necessary to use a luminescent EDC biosensor using fluorescence. Extensive bioassay development was performed on time-lapsed EDC activity response in live estrogen-sensitive yeast cells. This fluorescence assay was used in conjunction with Fourier-transform infrared (FTIR) spectromicroscopy, a noninvasive technique used for collecting real-time data on live cells. Employing these methods, we collected dose-response and abundant complementary data on multiple intercellular mechanisms (Figure 1).

SIGNIFICANCE OF FINDINGS

The biosensors developed provide a novel tool for assessing estrogenic compounds and surfactants. We have applied the biosensors to waters from agricultural systems and will apply them to water from the San Joaquin River Basin, and various wastewater treatment systems. Additionally, the sensors will be applied in wastewater treatment plants to demonstrate their usefulness for management of EDC degradation in wastewater treatment processes.

RELATED PUBLICATIONS

Campbell, C.G., S.E. Borglin, W.T. Stringfellow, F.B.Green, and A. Grayson, Review of bioassays for monitoring fate and transport of estrogenic endocrine disrupting compounds in water. Critical Reviews in Environmental Science and Technology (submitted), 2005.

Campbell, C.G., S.E. Borglin, W.T. Stringfellow, F.B.Green, and A. Grayson, Biologically based sensors for endocrine disrupting compounds in water. Conference Paper, American Society of Civil Engineers, Alaska, May 15–20, 2005.

ACKNOWLEDGMENTS

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

Environmental Lipidomics of Microbial Community Structure and Function

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RESEARCH OBJECTIVES

Phospholipid Fatty Acid (PLFA) analysis has become an interesting and valuable tool for determining the microbial community structure in soils, water, and other environmental samples with complex microbial communities. During PLFA analysis, phospholipids from cell membranes of microorganisms are extracted and used in determining the predominant types of microorganisms in the system, give indications of the physiological status of the microbial community, and also provide a means for estimating the microbial biomass. This type of information is valuable in evaluating changes in community structure and status during remediation or treatment activities, and can also be useful in evaluating the microbial status of natural systems. Our research focuses not only on identifying microbial community structure in the environment, but also applying this technique to look at stress response of pure cultures of metal-reducing bacteria. These bacteria are exposed to stressors in the environment that affect viability as well as the efficiency of metal reduction during the bioremediation processes. Because phospholipids are part of the cell membrane, changes in lipid composition are one of the first phenotypic responses to stress and give insight into cell response and survival mechanisms.

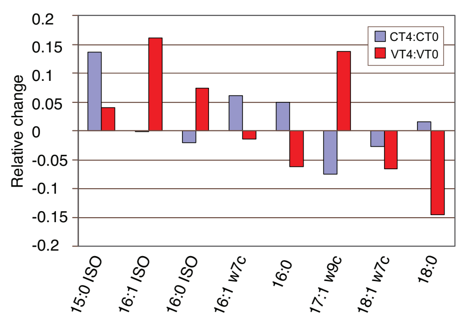

Figure 1. Relative changes in the 8 major types of PLFA after NaCl stress

APPROACH

To determine the lipid response to stress, we grew both *Desulfovibrio vulgaris* and *Shewenella oneidensis* in batch culture and exposed them to a variety of stressors, including cold, heat, pH, salt, nitrate, and oxygen. The phospholipids were extracted from the cultures at different time points to determine how the cell membrane responded to stress and to determine if specific fatty acid patterns can be used as an indicator of phenotypic response to stress analysis.

ACCOMPLISHMENTS

To date, approximately 40 *Desulfovibrio vulgaris* and 5 *Shewenella oneidensis* stress experiments have been completed. The results show that the lipid response is varied and highly dependent on stress conditions and organism type. For example, during salt stress, *Desulfovibrio vulgaris* increases its amount of lipid per cell, and at the same time increases its proportion of saturated lipids (see Figure 1). During oxygen stress of *D. vulgaris*, no growth occurs in the cells, but the PLFA analysis shows also that no significant death occurs, and there is little or no change in the lipid patterns or total amount of lipids in the culture. For *Shewenella oneidensis*, many genes involved in production of saturated and/or branched-chain fatty acids are affected by both temperature and salinity. During salt stress, the cells adapt their membrane fluidity to external conditions by increasing the proportion of unsaturated lipids and decreasing the relative amount of unsaturated lipids.

SIGNIFICANCE OF FINDINGS

This research documents the phenotypic response of cells to environmental stressors. Continued work will be focused on linking the PLFA phenotypic responses to genetic pathways. This research is expected to increase the ability to identify stress responses in environmental samples.

RELATED PUBLICATION

Borglin, S., T. Hazen, D. Joyner, R. Huang, N. Katz, E. Alm, and A. Kazakov, Phospholipid fatty acid analysis as phenotypic indicators of common stress response pathways in *Desulfovibrio vulgaris* and *Shewanella oneidensis*. ASM General Meeting, Atlanta, Georgia, June 8, 2005.

ACKNOWLEDGMENTS

This work was part of the Virtual Institute for Microbial Stress and Survival supported by the U. S. Department of Energy, Office of Science, Office of Biological and Environmental Research, Genomics Program: Genomes to Life (GTL) through Contract No. DE-AC03-76SF00098 between Berkeley Lab and the U.S. Department of Energy.

Phenotypic Microarray Analysis for Phenomics and Pathway Analyses in Anaerobes

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RESEARCH OBJECTIVES

Phenotypic Microarray™ analysis is a recently developed analytical tool to determine the phenotype of an organism. This technique can be useful in understanding the growth changes of an organism when changing medium, temperature, or adding a stressor, or when testing mutant strains. The tool, which is commercially available from Biolog™ (Hayward, CA), consists of an array of 20 plates. The first eight plates test a variety of metabolic agents, including electron donors, acceptors, and amino acids. Plates 9 and 10 cover pH and osmotic stressors, while plates 11–20 contain a variety of inhibitors, including toxic agents and antibiotics. In total, the plates simultaneous test nearly 2,000 independent conditions on a single bacteria culture.

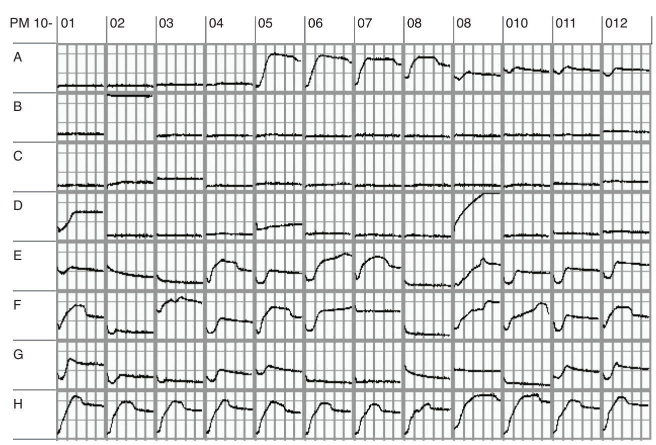

Figure 1. Growth of *Desulfovibrio vulgaris* in phenotypic microarray plate 10 (PM10). This plate measures the effect of pH on growth. Each plot represents growth in a different pH condition, the horizontal axis representing time (7 days), the vertical axis representing increase in turbidity, which is correlated with growth.

APPROACH

Techniques have been developed at Berkeley Lab for using these plates under anaerobic condition, to enable culturing of an obligate anaerobe, *Desulfovibrio vulgaris*. To accomplish this task, plates were set up in an anaerobic chamber and heat-sealed in polyethylene bags containing an anaerobic sachet. This technique permitted maintenance of anaerobic conditions in the plates for up to a week. Growth of the cells was measured by the increase in turbidity of the cells, which was correlated with both optical densities at 600 nm and total cell counts. Preconditioning of the cells and specialized media preparation are required for the different types of plates to obtain a valid phenotype.

ACCOMPLISHMENTS

The plates have been successfully used to characterize the phenotype of the *Desulfovibrio vulgaris* American Type Culture Collection (ATCC) strain (see Figure 1). The plates are currently being applied to mutant strains to provide rapid screening of mutant phenotypic changes needed for rapid pathway analyses and modeling. Several method-development obstacles have been overcome, including optimization of the plate-sealing technique, density of the inoculated organisms, and false positive and negative results from either excess or deficient inoculum.

SIGNIFICANCE OF FINDINGS

This technique will allow the production of high-volume and high-quality data related to the effect of targeted mutations and environmental stressors on bacterial cultures. This array, which will provide a unique tool for the study of bacterial stress and survival, is currently being applied to metal-reducing bacteria in soil.

RELATED PUBLICATION

S. Borglin, T. Hazen, J. Carlson, J. Wall, D. Joyner. Phenotypic microarray analysis of *Desulfovibrio vulgaris*. ASM General Meeting, Atlanta, Georgia, June 8, 2005.

ACKNOWLEDGMENTS

This work was part of the Virtual Institute for Microbial Stress and Survival supported by the U.S. Department of Energy, Office of Science, Office of Biological and Environmental Research, Genomics Program: Genomes to Life (GTL) through Contract No. DE-AC03-76SF00098 between Lawrence Berkeley National Laboratory and the U.S. Department of Energy.

Bioreoxidation of Uranium from the Oak Ridge Y-12 Site: Microbial Community Structure and Function

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RESEARCH OBJECTIVES

Uranium contamination is an unwanted legacy of the Cold War era. When uranium mining and processing for nuclear weapons and fuel were at their peak, uranium-containing wastes accumulated, resulting in a multitude of contaminated sites around the world. Uranium remediation strategies in recent years have focused on containment, minimizing migration of uranium in groundwater to prevent infiltration into surrounding water courses and potable water supplies.

One promising approach to minimizing uranium migration is to catalyze the reduction of soluble U(VI) to the less soluble U(IV). This process can be accelerated by the action of indigenous microorganisms fuelled through addition of exogenous carbon. Organic carbon addition stimulates biomass and microbial activity in these typically nutrient-poor environments, and has a profound impact on microbial community composition. The focus of our work is to use novel high-density DNA microarray technology to accurately monitor changes in composition of microbial populations during lab and field-scale studies of uranium bioreduction and observed reoxidation/remobilization.

APPROACH

To determine if the remobilization of U(VI) was associated with alterations in microbial populations, we have used a novel high-density oligonucleotide-microarray-based approach, which permits simultaneous monitoring of the dynamics of over 9,000 distinguishable prokaryotic taxa/units (OTUs) (Figure 1). To identify dynamic groups of organisms during biostimulation, we have applied hierarchical clustering methods combined with global graphical representation methods. To validate the high-density array approach, we analyzed identical samples, using a more common clone-library approach in addition to confirmatory tests using quantitative polymerase chain reactions (PCR). This is the first application of high-density array technology in profiling complex microbial communities such as those in soils or sediments.

ACCOMPLISHMENTS

Array analysis of the contaminated sediment confirmed the presence of most clone sequence types detected using conventional methodology. In addition, array analysis also indicated the presence of many bacterial families not detected by cloning, including those of importance for uranium reduction (e.g., *Geobacteraceae*). PCR with primers specific for *Geobacteraceae* confirmed this finding. Array analysis of bacterial communities during a laboratory-scale remediation simulation permitted time- and cost-effective monitoring of the dynamics of over 9,000 groups of bacteria. By using hierarchical clustering and principal component analysis, it was possible to readily identify those organisms responding with treatment or over time.

Lactate infusion into columns resulted in a significant change in bacterial populations, and following an initial period of successful uranium immobilization/reduction, we observed a remobilization of uranium, despite an adequate supply of lactate and suitable redox conditions. However, array data demonstrated that bacteria capable of uranium reduction had not decreased in quantity; therefore, a loss of this functional group was not considered the primary reason for the remobilization of uranium.

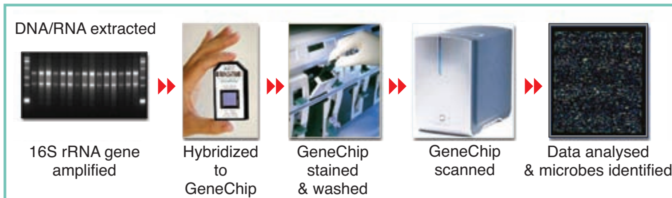

Figure 1. Flow schematic for high-density DNA microarray analysis of environmental microbial communities

SIGNIFICANCE OF FINDINGS

This is the first application of high-density microarrays in analysis of complex microbial communities. We have also demonstrated the ability to accurately track complete populations of bacteria using this array and have shown that loss of microbial functional groups was not a primary cause of uranium remobilization. Bacterially mediated carbonate accumulation has been identified as a possible driver of uranium remobilization, and we are currently investigating further biological and geochemical explanations for this significant observation.

PUBLICATIONS

Wan, J., T.K. Tokunaga, E.L. Brodie, Z. Wang, Z. Zheng, D. Herman, T.C. Hazen, M.K. Firestone, and S.R. Sutton, Reoxidation of bioreduced uranium under reducing conditions. Environmental Science and Technology, 39, 6162-6169, 2005.

ACKNOWLEDGMENTS

This work was supported by the Director, Office of Science, Office of Biological and Environmental Research, Environmental Remediation Sciences Division, Natural and Accelerated Bioremediation Research (NABIR) Program; and the Office of Basic Energy Sciences, Division of Chemical Sciences, Geosciences, and Biosciences, of the U.S. Department of Energy under Contract No. DE-AC03-76SF00098. Support was also provided by GeoSoilEnviroCARS, Advanced Photon Source (APS), Argonne National Laboratory.

Ecogenomic Analysis of Very Deep Subsurface Environments as Analogues to Life on Mars

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[1]Pacific Northwest National Laboratory, [2]Princeton University, [3]Indiana University
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RESEARCH OBJECTIVES

Terrestrial subsurface ecosystems have been proposed as analogues to life on other planets. Subsurface environments may provide habitable niches, protecting microorganisms from surface-related stress such as ultraviolet radiation, although at a cost. These environments are typically isolated from standard terrestrial energy economies (i.e., those revolving around solar energy): temperatures in the deep subsurface can reach 60°C. As such, microbes inhabiting these deep-subsurface ecosystems must adapt to such harsh conditions and be capable of obtaining energy by other means. By studying such isolated ecosystems, we hope to better understand the thresholds of life and determine the feasibility of life, past and present, on other planets in our solar system.

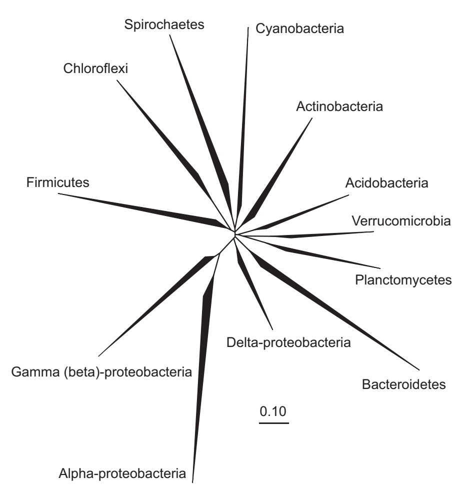

Figure 1. Phylogenetic tree showing phyla detected in deep-subsurface goldmine fracture-water samples by clone and high-density array analysis

APPROACH

We have obtained fracture water samples from 2–3 km below ground level from multiple gold mines of the Witwatersrand Basin in South Africa. These water samples have been dated by isotopic methods as being 14 Kyr to 20 Myr old, with an energy system that appears to be sulfate-and hydrogen-based. To identify the microbial populations in the fracture water, we used a standard clone-library approach and a novel high-density microarray approach. Metagenomic analyses of extracted DNA were carried out at the DOE Joint Genome Institute and at Berkeley Lab to investigate the physiological capabilities of the dominant organism(s).

ACCOMPLISHMENTS

A deep-branching clade of nearly identical *Desulfotomaculum*-like, 16S rDNA sequences (>99% homology) was identified as the dominant microorganism in the planktonic phase of the deepest (2–3 km depth), most saline fracture water. The closest cultured relative is *Desulfotomaculum kuznetsovii* (90% similarity). Further sequences detected by clone library and high-density-array analysis included relatively abundant Firmicutes (*Bacillus*) and less abundant Alpha-, Beta-, Gamma and Delta-proteobacteria, *Cyanobacteria, Chloroflexi, Acidobacteria, Bacteroidetes, Actinobacteria, Spirochaetes, Verrucomicrobia* and *Planctomycetes*. For metagenome analyses, 2.3 Mb of DNA was assembled into 53 scaffolds, and 2,140 likely protein coding genes were identified. Preliminary analyses indicate that the dominant *Desulfotomaculum*-like organism (DLO) represents a new family of organisms and is almost certainly a SO_4 reducer, based on its genomic content. The gene repertoire used for SO_4 reduction is largely the same described for other sulfate-reducing bacteria (SRB), including both delta-proteobacteria and the archeon *Archeoglobus fulgidis*. Although it is a gram-positive organism, it shares a surprising number of its closest homologs with a diverse set of SRB, including *Desulfovibrio vulgaris, D. alaskensis* G20, *D. psychrophila*, and *A. fulgidis*. A number of close homologs were also observed to related organisms such as the S-reducing *Geobacter* and *Desulfuromonas* spp., and the SO_4 oxidizing *Chlorobium tepidum*. This dominant DLO most likely has flagellar motility controlled by a relatively small set of methyl-accepting chemotaxis proteins.

SIGNIFICANCE OF FINDINGS

Clone libraries and high-density microarrays allowed us to profile both the dominant and nondominant fraction of the microbial community in this sulfate/hydrogen-driven subsurface ecosystem. Through metagenome sequencing, we are able to gain insight into the growth strategy of the dominant *Desulfotomaculum*-like organism, which appears capable of sulfate reduction linked to either hydrogen or formate oxidation, in addition to chemotactic motility. This data will enable a better understanding of adaptation and survival of microorganisms in isolated deep-subsurface systems.

RELATED PUBLICATIONS

Brockman, F., D. Moser, T. Gihring, D. Culley, E. Brodie, G. Andersen, T.C. Hazen, P. Richardson, L. Pratt, and T.C. Onstott, Inferred bioenergetics of an uncultured bacterium common in fracture fluids of South African deep mines. NASA Astrobiology Institute (submitted abstract), Biennial Meeting, Boulder, Colorado, 2005.

ACKNOWLEDGMENTS

Funding for this project was provided by the NASA Astrobiology Institute (NAI) and the NSF LExEn (Life in Extreme Environments) Program. We thank the team members of the Witwatersrand Microbiology Project and geologists at the Mponeng Mine for their assistance in field sampling and coordination of logistic supply.

Characterization of Fracture Zonation Using Seismic Data and MCMC Methods

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RESEARCH OBJECTIVES

Our goal in this study is to delineate fracture zonation in order to understand field-scale bioremediation experiments carried out at the DOE Field Research Center (FRC) in Oak Ridge, Tennessee, using crosswell seismic-travel-time and borehole-flowmeter-test data. Our focus is on the development of an effective joint inversion model for combining the crosswell geophysical data with the borehole measurements to characterize fracture zonation in high resolution. The joint inversion approach was developed to minimize problems sometimes encountered with sequential two-step hydrogeophysical estimation approaches, which entails initial inversion of the geophysical dataset, followed by the use of that dataset to estimate hydrogeological parameters. In this example, seismic anisotropy and discrepancies between the borehole and crosshole measurement support scales prohibited the meaningful use of the conventional two-step hydrogeophysical inversion approach for identifying the spatial distribution of fracture zones.

APPROACH

We developed a true joint inversion approach for estimating fracture zonation by combining crosswell seismic travel-time and borehole-flowmeter-test data using a Bayesian framework. First, we transferred the continuous values of hydraulic conductivity data, obtained from borehole flowmeter test data, into indicator values (1 = high conductivity, 0 = low conductivity), using the median of hydraulic conductivity as the cutoff value. Then, we created a Bayesian model to estimate the probability of being within the high-conductivity fracture zone at each pixel in space, by conditioning crosswell travel-time data and indicator values of borehole flowmeter test data. In the model, the prior probability of being within the high conductivity zone at each pixel was determined using an indicator kriging method. The likelihood function, which links seismic slowness (the inverse of seismic velocity) and hydraulic conductivity, was determined from cross-correlation analysis. Finally, we used Markov chain Monte Carlo methods (MCMC) to draw many samples of the indicator values at each pixel in space. Through statistical analysis of those samples, we obtained the probability of being within the high-conductivity fracture zone at each pixel.

ACCOMPLISHMENTS

Figure 1 illustrates the probability of being within the high-conductivity fracture zone along three vertical cross sections at the FRC site, obtained using the developed joint stochastic inversion approach. The cross sections illustrate the value of the developed procedure for such investigations: in some cases, interpolation of borehole data might be sufficient for representing the connectivity of the fracture zone, while in other cases, such interpolation could lead to incorrect assumptions about fracture zone connectivity. Our fracture zonation estimates were corroborated using other types of information, such as field tracer breakthrough data and bioremediation results.

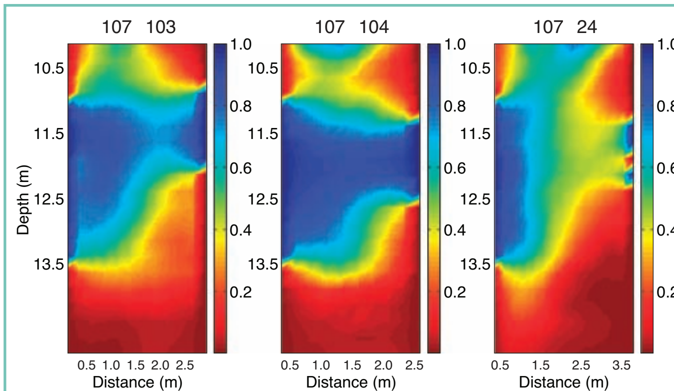

Figure 1. Estimated probability of being within the high-conductivity fracture zones along three transects at the DOE NABIR Field Research Center in Oak Ridge, Tennessee. The blue color represents high probability, the red color represents low probability.

SIGNIFICANCE OF FINDINGS

We have found that the developed stochastic MCMC model is effective for combining seismic travel-time and borehole-flowmeter-test data. This is one of the first examples of true joint inversion of geophysical and hydrological information for hydrogeologic investigations. The study also illustrates the value of using joint inversion methods for subsurface characterization, especially in "challenging" subsurface environments (such as the FRC), where conventional hydrogeophysical approaches fail to provide quantitative property estimates.

RELATED PUBLICATIONS

Chen, J., and S. Hubbard, Development of a joint hydrogeophysical inversion approach and application to a fractured aquifer. Water Resour. Res. (in preparation), 2005.

ACKNOWLEDGMENTS

This work was supported by the Director, Office of Science, Office of Biological and Environmental Research, Environmental Remediation Sciences Division, Natural and Accelerated Bioremediation Research (NABIR) Program, of the U.S. Department of Energy under Contract No. DE-AC03-76SF00098.

Unraveling the History of Uranium Contamination to the Vadose Zone in the T-WMA, Hanford Site, Washington

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RESEARCH OBJECTIVES

For decades, the Hanford, Washington, site was used to process nuclear fuels for the production of plutonium. These past industrial-scale activities resulted in local contamination of the vadose zone and groundwater. An important consideration in the process of cleanup is the source and fate of such contaminants as uranium (U). Our previous work in the B-BX-BY waste management area demonstrated the power of high-precision U isotopic measurements in providing practical constraints on the sources of U contamination, as well as on the behavior and transport of U in the vadose zone. Here we extend this work to two cores that sampled contaminated vadose zone sediments in the T and TX waste management areas (WMAs), laying the groundwork to trace the source of recently recognized ^{99}Tc groundwater contamination in the vicinity of the T-WMA.

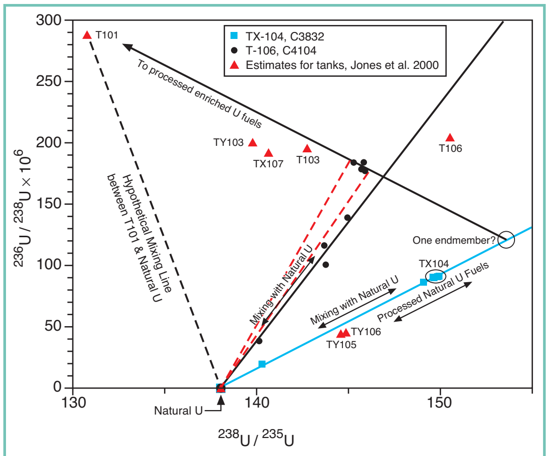

Figure 1. Plot of $^{238}U/^{235}U$ vs. $^{236}U/^{238}U \times 10^6$. Black circles are analyses of U from pore water from core C4104 near T-106, blue squares are analyses of pore water from core C3832, near TX-104. Also shown are estimates of tank waste compositions for the T-TX-TY WMAs at their declared leak dates.

APPROACH

The isotopic composition of natural U contrasts with the variable isotopic composition of U from processed fuel rods. This variation can be used as a tracer and fingerprint of contamination. Samples were analyzed for U isotopic composition from two cores (C4104 and C3832) near two single-shelled tanks, T-106 and TX-104, respectively. Uranium from pore waters in the sediment samples were separated and analyzed for isotopic composition by a multiple-collector inductively-coupled-plasma-source mass spectrometer (MC-ICPMS). The results of the isotopic analyses were evaluated and compared to each other to identify sources and the extent of mixing with background U. The isotopic data were also compared to models of the U fuel processing history to provide some temporal constraints.

ACCOMPLISHMENTS

The U isotopic analyses for Core C4104 near Tank T-106, known to have leaked over a six-week period in 1973, indicate that the contaminant U introduced to the vadose zone at this location had a component of processed enriched U fuel, along with a component of processed natural U fuel (Figure 1), at most about 20% and at least 80%, respectively. Moreover, consideration of $^{234}U/^{238}U$ data (not shown here) constrains the composition of the processed natural U fuel end member. The proportion of processed enriched U decreases down core, until the U isotopic compositions fall along a mixing array with background natural U. In the case of the U isotopic analyses for Core C3832 near Tank TX-104, most of the data form a tight cluster on the array, representing natural U fuels.

SIGNIFICANCE OF FINDINGS

For vadose zone U contamination associated with tanks BX-102 (BX WMA, 200 East Area) and TX-104 (TX WMA, 200 West Area), we found that the contaminant U isotopic composition was highly homogeneous. In contrast, the core near T-106 shows a more complex history, involving mixtures of natural U fuel and enriched fuel, with variable proportions apparently through time. It appears either that contamination was decanted from a tank stratified in U isotopic composition, or that the vadose zone contamination represents mixing with near-contemporaneous contamination from nearby Tank T-103. In either case, the down-core mixing array with background U suggests that the earlier contamination had a lower proportion of processed enriched fuel, providing a basis for modeling the mobility of U in the vadose zone. The data for C4104 also establishes the U isotopic signatures of the waste leak associated with T-106, providing an important part of the isotopic context needed to evaluate the source of ^{99}Tc groundwater contamination in the vicinity of the T-WMA.

RELATED PUBLICATION

Christensen, J.N., P.E. Dresel, M.E. Conrad, K. Maher, and D.J. DePaolo, Identifying the sources of subsurface contamination at the Hanford Site in Washington, using high-precision uranium isotopic measurements. Environ. Sci. Technol., 38 (12), 3330–3337, 2004. Berkeley Lab Report LBNL-54979.

ACKNOWLEDGMENTS

This work was supported by the Assistant Secretary of the Office of Environmental Management, Office of Science and Technology, Environmental Management Science Program, of the U.S. Department of Energy, under Contract No. DE-AC03-76SF00098 to LBNL and Contract No. DE-AC06-76RL01830 to PNNL.

Tracing Sources of Uranium to the Hanford Reach of the Columbia River

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RESEARCH OBJECTIVES

As part of the World War II-era Manhattan Project, the Hanford Site was established along the Columbia River to take advantage of local hydroelectric power and ample water supply for cooling of a series of nuclear reactors. Decades of nuclear-related activities have left significant local contamination (e.g., nitrate, uranium (U), tritium, Cr^{6+}, ^{99}Tc) in the vadose zone and groundwater within the site. Some of this contamination has reached the Columbia River, and there remains the potential for further contaminant migration to the river. We collected and analyzed samples of Columbia River water for U and strontium (Sr) isotopes in coordination with the ongoing sampling and monitoring of the river. The U and Sr isotopic data allow us to evaluate sources of U (e.g., natural background, Hanford related, agricultural runoff) and their relative contributions to the river's U budget. The data also provide constraints on the flux and sources of contaminant U from the Hanford Site to the river.

APPROACH

We analyzed three sample traverses across the Columbia, one near the Vernita Bridge, upstream from Hanford Site contamination, a second just downriver of the 300 Area, and a third about 5 km downstream of the Hanford Site, adjacent to the town of Richland. Additional samples were collected up to 350 km downstream. Sampling was conducted in fall 2003, spring 2004, and fall 2004. Filtered (0.45 micron) water samples were analyzed for U isotopic composition (including ^{236}U, one marker of spent U fuel) and U concentration, as well as ^{87}Sr/^{86}Sr and Sr concentration. Uranium isotopes were measured by multiple-collector-inductively-coupled-plasma source mass spectrometer (MC-ICPMS), and Sr isotopes by thermal ionization mass spectrometry (TIMS).

ACCOMPLISHMENTS

The samples from the upstream traverse had no detectible ^{236}U (^{236}U/^{238}U $< 2 \times 10^{-8}$), natural ^{238}U/^{235}U, uniform ^{234}U/^{238}U, ^{87}Sr/^{86}Sr, or U and Sr concentrations. In contrast, the downstream traverses showed variation in all of these parameters. As an example, ^{236}U/^{238}U data are shown in Figure 1a for the fall 2003 and spring 2004 Richland traverses. The ^{236}U/^{238}U highlight a plume of U contamination coming from the Hanford Site. Correlation of ^{236}U/^{238}U with ^{238}U/^{235}U is consistent with a component of 2nd cycle enriched U fuels. For the river water sample with the highest ^{236}U/^{238}U, about 30% of the total U comes from Hanford contamination. For the eastern portion of the traverse, no detectable ^{236}U was found (Figure 1a). However, ^{234}U/^{238}U and ^{87}Sr/^{86}Sr (not shown) indicate significant contributions from agricultural return canals about 6 km upstream of the traverse. Measurable ^{236}U/^{238}U, though small, was observed in all the downstream samples (Figure 1b), and together with ^{238}U/^{235}U was consistent with a Hanford Site source.

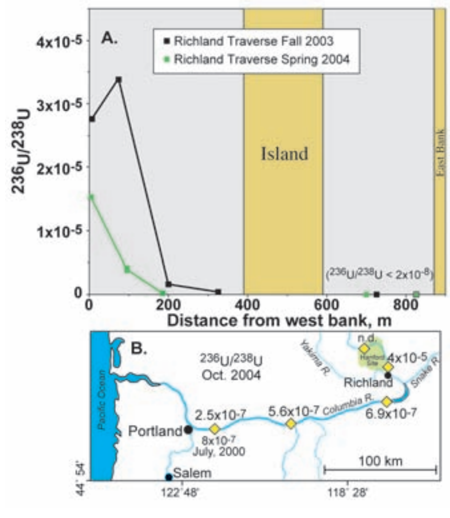

Figure 1. (a) River sampling traverse across the Columbia River at the Richland pump house, about 5 km downstream of the Hanford Site 300 Area. Shown are ^{236}U/^{238}U data for sampling in fall 2003 and spring 2004. The sampling traverse is divided by an island. (b) Map showing locations of the Hanford Site and downstream sampling sites along the Columbia River, with indicated ^{236}U/^{238}U. N.D. = not detected.

SIGNIFICANCE OF FINDINGS

The isotopic compositions of the U-contaminated river samples are consistent with a U-contaminated groundwater source in the 300 Area, where fuel elements (both 2nd cycle enriched and natural U) were fabricated. In fact, particular 300 Area groundwater and seep samples are matched as sources, pointing to particular points along the shore.

Both U concentrations and ^{236}U/^{238}U decrease downstream (Figure 1b), indicating not only progressive dilution of the Hanford U signature, but also suggesting that at the same time U was being lost from solution (in this case, the <0.45 mm fraction) to particulates. Comparing fall 2003 and spring 2004 Richland traverses, we have found that the flux and apparent source of Hanford U changes with season, with higher relative flux in the fall.

RELATED PUBLICATION

Christensen, J.N., P.E. Dresel, M.E. Conrad, G.W. Patton, and D.J. DePaolo, Tracing and apportioning sources of uranium to the Hanford reach of the Columbia River using uranium isotopes. Eos Trans. AGU, 85(47), F858, 2004.

ACKNOWLEDGMENTS

This work was supported by the Assistant Secretary of the Office of Environmental Management, Office of Science and Technology, Environmental Management Science Program, of the U.S. Department of Energy under Contract No. DE-AC03-76SF00098 to LBNL and Contract No. DE-AC06-76RL01830 to PNNL.

Nanotechnology and Environmental Policy: Analysis of Funding and Outcomes

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RESEARCH OBJECTIVES

Nanotechnology and nanoscience can lead to great advances in many fields, and the potential revolutions they may bring to medicine, energy systems, and information technology have been widely publicized. However, the potential societal and environmental implications are a growing concern. There have been a few recent reports that initiate the discussion of environmental impact, but these are not yet comprehensive or conclusive. This work analyzes the National Nanotechnology Initiative (NNI) funding related to the environmental impact of nanotechnology and the research outcomes in this area.

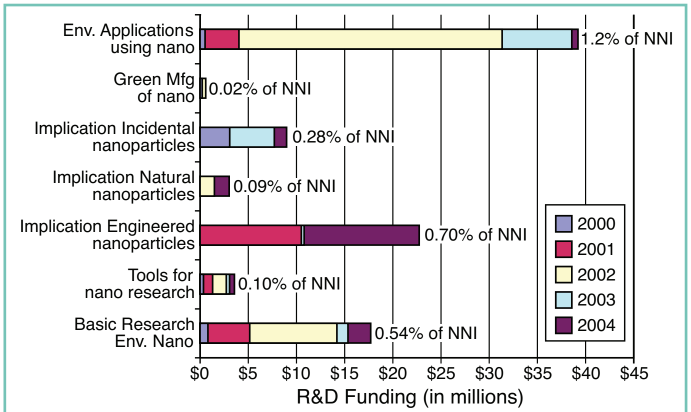

Figure 1. Estimated NNI environmental research, 2000–2004. These preliminary results include an overestimate of funding in the "implication of engineered nanoparticles" area.

APPROACH

We use an ecosystem approach to define "environmental impact" such that it encompasses positive, negative, and neutral effects on soil, air, water, plants, animals (including humans), and other organisms. We obtained data from several sources: agency websites, interviews with agency representatives, and the NNI website. All funding data were assigned a coded category, shown in Figure 1. To code funding data, we reviewed the available title, abstract, and progress-report data on individual grants, and categorized these grants by research topic. In some instances, the principal investigators of the grants were contacted to identify the distribution of the awards by category.

ACCOMPLISHMENTS

We analyzed the NNI funding data for nanotechnology and the environment from 2000–2004 cumulatively, as well as by year and agency, as shown in Figure 1. Preliminary estimates indicate that funding to date in all environmental nanotechnology studies is only 2.9% of the $3.26 billion of federal grant money coordinated by the NNI in this period. This environmental nanotechnology funding is heavily weighted towards "environmental applications of nanotechnology," or the positive environmental uses of nanotechnology. "Implication of engineered nanoparticles" received a little over half of the overall funding for positive environmental applications, but includes a significant funding increase in 2004.

We also analyzed the published research on environmental implications of nanotechnology. Toxicity of nanosized aerosol particles and carbon fullerenes has been discussed in the literature for a number of years prior to the establishment of the NNI. Recent studies on nanotechnology impact are limited, and focus on the toxicity of nanoparticles such as cadmium selenide, carbon nanotubes, and fullerenes. Limited studies on nanoparticle exposure and transport of nanoparticles also have been published. Many of the studies cite enhanced toxicity or anomalous behavior at the nanoscale, reinforcing the need to investigate the unique impact of nanosized particles on all aspects of the environment.

SIGNIFICANCE OF FINDINGS

Funding priorities for environmental nanotechnology do not yet appear to have stabilized. This situation is likely to be the result of shifting "top-down" considerations of the environmental issues related to nanotechnology by government officials. It is important, however, to consider the influence that "bottom-up" factors have had on this result, because the ultimate distribution of funds according to topic area must reflect the proposed research of scientists applying for NNI environmental grants. The limited published studies on the overall environmental impact of nanotechnology demonstrate that there are many interesting and vital studies to be conducted in this area.

RELATED PUBLICATIONS

Banfield, J.F., and H. Zhang, Nanoparticles in the environment. In: Nanoparticles and The Environment: Reviews in Mineralogy and Geochemistry, J.F. Banfield and A. Navrotsky, eds., 44, 1–59, 2001.

Taylor, M.R., E.S. Rubin, and D.A. Hounshell, Stimulating environmental technological innovation: Government actions and SO_2 control technology. Technological Forecasting and Social Change, November 2004.

ACKNOWLEDGMENTS

This work was supported by a President's Postdoctoral Fellowship, provided by the Executive Director, President's Postdoctoral Fellowship Program, Department of Academic Advancement, Division of Academic Affairs, of the University of California Office of the President. This work was also partially supported by the Assistant Director, Directorate of Geosciences, Division of Earth Sciences, Nanoscale Interdisciplinary Research Team Program, of the National Science Foundation under Contract No. EAR0123967.

DOE Environmental Management International Projects Highlights

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RESEARCH OBJECTIVES

Berkeley Lab provides technical assistance to the U.S. Department of Energy (DOE) Environmental Management (EM) Office in conducting projects with Russia, Ukraine, and Argentina. The overall objective of these EM international projects is to use foreign sites as analogs for DOE contaminated sites, to:

- Improve the capability of DOE's conceptual and numerical models for predicting radionuclide transport through unsaturated and saturated subsurface media.
- Predict the future environmental and human impact of radioactive contaminant releases.
- Assist DOE sites in designing effective remediation technologies and long-term stewardship programs.

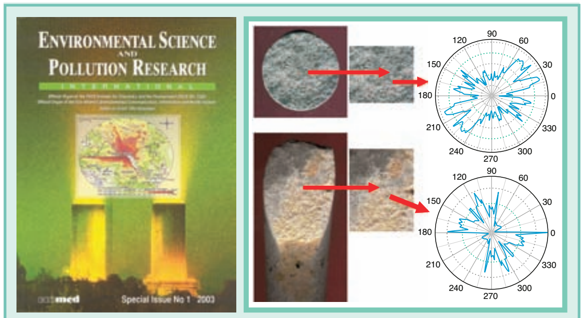

Figure 1. *Environmental Science and Pollution Research Journal* cover page (left), and photographs of basalt core and RIMAPS results (right)

APPROACH AND ACCOMPLISHMENTS

In 2004–2005, Berkeley Lab assisted DOE-EM in designing site characterization, radionuclide transport modeling, and selecting soil and groundwater remediation technologies at the Russian Research Center "Kurchatov Institute" (RRC KI). Information about the radionuclides leaking from individual waste disposal facilities, and the field observations of radionuclide distribution in groundwater at the RRC KI site, can be used to validate the source-term assessment approaches being used at nuclear waste disposal sites in the U.S.

The results from investigations conducted within the Chernobyl Exclusion Zone, established after the Chernobyl Nuclear Power Plant Accident of 1986, suggest several important potential areas of collaboration between DOE and the International Radioecology Laboratory (Slavutych, Ukraine). These collaborative possibilities include the development and testing of models for radionuclide migration through the chain of "fallout-soils-plants-animals-humans"; radionuclide transport in soils and groundwater; bioremediation, natural attenuation, and deactivation of radioactive contaminants; colloidal transport; nondestructive determination of Pu, Am, and Sr in hot particles, water, and soil samples (using alpha-, beta-, and gamma spectrometers as well as a fluid scintillation spectrometer); and resuspension of radionuclides as a result of wind and soil erosion.

The projects with Argentina consisted of two components: (1) numerical modeling and characterization of groundwater flow and contaminant transport at the Ezeiza Atomic Center, and recommendations for source containment and groundwater remediation; and (2) investigations of the physics of liquid flow and transport through partially saturated fractures. Within the scope of the second task, Argentine scientists developed a new technique, rotated imaging with a maximum average power spectrum (RIMAPS). This technique is used for the digital characterization of a fracture-surface topography, which is then applied to assess the main flow paths along the fracture surface. The RIMAPS technique was tested at Comisíon Nacional de Energía Atómica using (a) digital images of the fracture pattern and flow paths from fracture model flow experiments conducted at Berkeley Lab and (b) a fractured basalt core collected at the Box Canyon site in Idaho (Figure 1). The application of this technique will allow researchers to predict the water flow parameters from the analysis of fracture surfaces.

SIGNIFICANCE OF FINDINGS

It was determined that the international sites chosen could be used as analogs for some DOE contaminated sites. DOE would likely benefit from access to long-term and detailed monitoring of contaminant transport in the variety of contaminant, climatic, and geological settings provided by these analogous sites. These projects will allow DOE researchers, engineers, and managers to use international scientific resources to test and build confidence in DOE's fate and contaminant transport models and remediation technologies, which will allow DOE to reduce costs, improve remedy and mitigation reliability, and increase the effectiveness of remediation technologies during long-term stewardship of DOE sites.

RELEVANT PUBLICATION

Fuentes, N.O., and B.A. Faybishenko, RIMAPS and variogram characterization of water flow paths on a fractured surface. In: Proceedings of the Second International Symposium on Dynamics of Fluids in Fractured Rock, pp. 120–123, Berkeley, CA, 2004.

ACKNOWLEDGMENTS

This work is supported by the Assistant Secretary of the Office of Environmental Management, Office of Science and Technology, Environmental Management Science Program, of the U.S. Department of Energy under Contract No. DE-AC03-76SF00098. The above-mentioned projects are managed by the DOE Environmental Management Office (project manager Kurt Gerdes), and the Institute for International Cooperative Environmental Research of Florida State University (Associate Director John Moerlius). DOE supported publication of a special issue of the *International Journal Environmental Science and Pollution Research* devoted to Chernobyl problems (Figure 1).

Biological Treatment of Irrigation Drainage for Selenium Removal

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RESEARCH OBJECTIVES

Much of the subsurface agricultural drainage in the western San Joaquin Valley (SJV) is contaminated with selenate (50–1,200 mg/L as Se) and nitrate (20–120 mg/L as N), in addition to high total dissolved solids (TDS) and boron. This water is currently either discharged to sloughs that drain into the San Joaquin River and then to the San Joaquin Delta, or it is evaporated in terminal ponds. These means of disposal are problematic because selenium is a teratogen that bioaccumulates in the aquatic food web, and because nitrate contaminates groundwater supplies and promotes eutrophication of surface waters. Nitrate also interferes with the reduction and removal of selenate, SeO_4^{-2}, the most abundant form of selenium found in western SJV drainage. Our objective is to develop reliable and economical treatment methods to remove these contaminants.

APPROACH

From Pilot Plant to Prototype Facility

We have developed the algal-bacterial selenium removal (ABSR) process to remove nitrate and selenium from irrigation drainage. A 75 m^3/day pilot-scale ABSR Facility has been used to study the mechanisms and rates of selenium and nitrate removal. Based on the success of the pilot facility, a 10-fold scale-up intermediate-scale ABSR Facility may be implemented. In the ABSR process, subsurface drainage is dosed with a carbonaceous energy source for bacteria (usually animal feed-grade molasses) and then injected into a baffled and covered anoxic reduction pond. In the reduction pond, bacteria denitrify nitrate and reduce selenate to selenite, elemental selenium, and bacterial-associated organic selenium. Much of the reduced selenium settles in the pond. Settled bacterial biomass in the reduction pond undergoes anaerobic decomposition, so the volume of solid residues increases very slowly. Removal of the selenium-containing solids should not be required for many years, possibly decades. The effluent water from the reduction pond is coagulated, clarified, and filtered to remove suspended bacteria and selenium-containing suspended solids.

ACCOMPLISHMENTS

Selenium Removal

Over two years, the pilot-scale ABSR Facility at the Panoche Drainage District has removed 95% of the influent nitrate-nitrogen load and 80% of the influent soluble selenium load. Addition of physical-chemical treatment processes, including dissolved air flotation and filtration processes to remove particulate selenium, has increased total selenium removal to 87%. Dozens of bacterial species have been isolated from the ABSR Facility and identified by 16S rRNA sequencing, including the prevalent *Acinetobacter Johnson*II/genospecies 7, *Pseudomonas mendocina*, and *Xanthomonas maltophilia*. Pure cultures of several of these bacteria have been proven to reduce selenite in the laboratory.

Brine Treatment

Planned "zero discharge" drainage management in the SJV will create brines that require treatment. The high salt concentration of brines may inhibit bacterial selenium reduction, thereby increasing the cost of irrigation drainage treatment. We have found that denitrification and selenate reduction are unaffected by NaCl concentrations augmented up to 22 g/L. Above 22 g/L, however, reduction is substantially inhibited. This information is important in the planning and design of proposed integrated-reverse-osmosis and biological-drainage treatment processes.

SIGNIFICANCE OF FINDINGS

With the ABSR Facility at the Panoche Drainage District, we have demonstrated a promising, cost-effective process that will be used in planning full-scale facilities to remove nitrate and selenium from irrigation drainage.

RELATED PUBLICATIONS

Green, F.B., T.J. Lundquist, N.W.T. Quinn, M.A. Zárate, I.X. Zubieta, and W.J. Oswald, Selenium and nitrate removal from agricultural drainage using the AIWPS® Technology. Water Science and Technology, 48 (2): 299–305, 2003. Berkeley Lab Report LBNL-55205.

Sudame A., S. Lee, H. Lee, T. Lundquist, P. Muller, K. Hida, H. Ng, P. F. Strom, and T. Leighton, Selenite-reducing bacteria of Panoche Algal Bacterial Selenium Removal (ABSR) Facility, California. In: Proceedings of 34th Mid-Atlantic Industrial and Hazardous Waste Conference, 159–172, September 2002.

Quinn, N.W.T., T.J. Lundquist, F.B. Green, M.A. Zárate, W.J. Oswald, and T.J. Leighton, Algal-bacterial treatment facility removes selenium from drainage water, California Agriculture, 54 (6), 50–56, 2000. Berkeley Lab Report LBNL-50318.

ACKNOWLEDGMENTS

We are grateful to the U.S. Bureau of Reclamation, the CALFED Bay-Delta Program, Department of Water Resources, and the Panoche Drainage District for their support.

Field Investigations of Lactate-Stimulated Bioreduction of Cr(VI) to Cr(III) at the Hanford 100H Area

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RESEARCH OBJECTIVES

Field investigations have been performed to assess the potential for immobilizing and detoxifying chromium-contaminated groundwater, using lactate-stimulated bioreduction of Cr(VI) to Cr(III), at the Hanford Site's 100H Area.

APPROACH AND METHODS

Lactate (Hydrogen Release Compound—HRC^{TM}) injection into chromium-contaminated groundwater is expected to cause indirect or direct bioreduction of chromate, Cr(VI), and precipitation of insoluble species of Cr(III). At Hanford 100H, two new wells were completed using a newly developed assembly with inflatable (argon gas) rubber packers, groundwater samplers, and an inner geophysical access tube. Pre-HRC injection and post-HRC injection geophysical (seismic and radar) cross-borehole measurements were performed (see a summary by Hubbard et al., 2005 [this volume]). Forty pounds of ^{13}C-labeled HRC were injected into Well 699-96-45 (44–50 ft within the Hanford formation) on August 3, 2004, immediately followed by pumping (which continued until August 30) from the Monitoring Well 699-96-44.

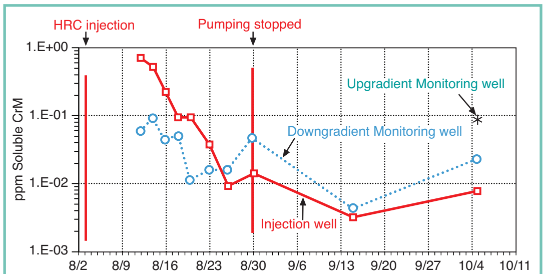

Figure 1. Changes of Cr(VI) concentration in injection and monitoring well resulting from HRC groundwater biostimulation

Groundwater analyses included: Acridine orange direct counts and molecular analyses—PLFA, 16S GeneChip, clone library, qPCR, bromide (tracer added to the injection well), chloride and phosphate (added to HRC), acetate (byproduct of HRC microbial metabolism), nitrate and sulfate (present in background groundwater), Cr(VI), total Cr, and Fe(II), total Fe, carbon, nitrate, and oxygen isotopic compositions.

ACCOMPLISHMENTS

Groundwater biostimulation caused microbial cell counts to increase from a background of $\sim 10^5$ cells g^{-1} to reach a maximum of 2×10^7 cells g^{-1} 13 to 17 days after the injection. This maximum lasted for 2 months and then decreased to values even less than those under pre-HRC-injection conditions. Biostimulation also generated highly reducing conditions: DO dropped from 8.2 to 0 mg/L, redox potential from 240 to -130 mV, and pH from 8.9 to 6.5. After pumping stopped and the system returned to natural regional groundwater flow, DO, redox, and pH began to recover to background values. PLFA and direct counts both indicated similar biomass changes. Carbon isotope ratios of DIC decreased, but remained for 6 months above background in Well 699-96-44 and within the injection interval in Well 699-96-45—until December 2004. The $\delta^{13}C$ ratios in dissolved inorganic carbon confirmed microbial metabolism of HRC. Geophysical investigations show that HRC products (such as lactic acids) injected into groundwater can be detected using radar and seismic survey, and that even small variations in hydrogeological heterogeneity may influence the distribution of the amendment and its products.

Hydrogen sulfide production was first observed after about 20 days post-injection, which corresponds with the enrichment of a *Desulfovibrio* species (sulfate reducer) identified using 16S rDNA microarray and monitored by direct fluorescent antibodies. DO and nitrate began to return to background concentrations two months after HRC injection, despite groundwater bacteria densities remaining high (>10^7 cells/mL).

As a result of groundwater biostimulation, Cr(VI) concentrations in the monitoring and pumping wells decreased below drinking water minimum-contaminant limits and remained below upgradient concentrations, even after 6 months (Figure 1), when redox conditions and microbial densities had returned to background levels.

SIGNIFICANCE OF FINDINGS

Microbial, geophysical, and geochemical analyses of groundwater, coupled with stable isotope monitoring, allowed for accurate tracking of microbial processes during this field treatability study, and confirmed that Cr(VI) was successfully removed from groundwater at a contaminated site using HRC as an electron donor and carbon source.

PROJECT WEBSITE

http://www-esd.lbl.gov/ERT/hanford100h/index.html

RELATED PUBLICATIONS

Hubbard, S., K. Williams, J. Peterson, J. Chen, B. Faybishenko, and T. Hazen, Geophysical monitoring of HRC distribution in groundwater during a Cr(VI) bioreduction experiment at the Hanford 100H site. This Volume, 2005.

ACKNOWLEDGMENTS

This work was supported by the Director, Office of Science, Office of Biological and Environmental Research, Environmental Remediation Sciences Division, Natural and Accelerated Bioremediation Research (NABIR) Program, of the U.S. Department of Energy under Contract No. DE-AC03-76SF00098. The work was conducted jointly by Berkeley Lab, Pacific Northwest National Laboratory, and Regenesis, Ltd.

VIMSS: Large-Scale Biomass Production of Obligate Anaerobes for Simultaneous Transcriptomics, Proteomics, Metabolomics, and Lipidomics Analysis

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RESEARCH OBJECTIVES

The Virtual Institute for Microbial Stress and Survival (VIMSS) at Lawrence Berkeley National Laboratory (Berkeley Lab) seeks to identify stress-response pathways of *Desulfovibrio vulgaris* induced by various environmental factors, by combining multiple simultaneous analyses in an effort to conceptualize these pathways. The Applied Environmental Microbiology core at Berkeley Lab is responsible for producing large quantities of *D. vulgaris* biomass for different research laboratories, to accomodate simultaneous analyses on cells with the same growth condition and stress level. Biomass production at Berkeley Lab involves the production of nonstressed and stressed *D. vulgaris* culture at various time points during the growth phase, which is a four-month process with two major stages. During Stage 1, Berkeley Lab determines the stressor and the dosage, as well as designing and carrying out a multi-time point experiment for Oak Ridge National Laboratory's transcriptome analysis. During Stage 2, Berkeley Lab will produce 12 to 30 liters of biomass for all the VIMSS laboratories, based on the results of transcriptomics. Berkeley Lab is also responsible for all QA/QC verifications, all sample shipments, the uploading of data, and analysis for all experiments.

APPROACH

To rapidly determine induced-stress-response pathways in anaerobic microorganisms, we need to produce biomass for simultaneous analyses, using the latest techniques in transcriptomics, proteomics, metabolomics, and lipidomics. To accomplish this, batch cultures of 30 liters of stressed versus nonstressed *D. vulgaris*, as biological replicates in triplicates, are needed to ensure that all the analyses will be performed on cells of the same condition. Various technical improvements and adaptations were made for the large-scale production and distribution of biomass exposed to a variety of stressors, such as oxygen, salt, nitrate, nitrite, and temperature. Because of the rapidly changing nature of DNA and the short half-life of mRNA, *D. vulgaris* cultures needed to be immediately cooled to 5°C during biomass sampling. As a result, a fast sample-cooling system was developed to chill biomass from 30°C to 5°C in less than 30 seconds. Because of the concomitant analysis by several laboratories, rigorous quality control measures were used to ensure the quality and sterility of biomass from each time point in a production run (e.g., direct cell counts, optical density, pH, plate streaks, phospholipid fatty acid [PLFA] analysis, and protein assays). In addition, advanced Fourier Transform Infrared (FTIR) spectromicroscopy profiling was used to study gross bimolecular changes and to determine optimal sampling times. QA/QC procedures were developed and documented to track every step in production, from experiment inception to final analyses, including all chemicals, procedures, and technicians. Data are immediately uploaded to a database shared by all investigators (http://vimss.lbl.gov)

ACCOMPLISHMENTS

Over a 20-month period from September 2003 to May 2005, the Applied Environmental Microbiology core at Berkeley Lab conducted over 40 large-scale *D. vulgaris* biomass production experiments and countless small-scale experiments. During this time, the group developed various techniques and made numerous improvements to VIMSS biomass production, such as in media composition, anaerobic sampling, and biomass harvesting. Direct filtration and tangential flow filtration were studied as viable cell harvesting alternatives to centrifugation. However, studies showed that centrifuging *D. vulgaris* cells was the best option in terms of time, cost, efficiency, and quality control. The consistency of growth determined by the comparison data allows a set biomass production schedule and sampling time, which minimize variability between experiments.

SIGNIFICANCE OF FINDINGS

- Biomass production of batch cultures in biological replicates demonstrated a reliable and carefully controlled method to inoculate, grow, stress, and sample *D. vulgaris* cultures.
- QA/QC verifications at every stage of biomass production insure maximum reproducibility between biomass production experiments.
- Centrifugation and the fast chilling system appropriately prepared replicate samples simultaneously for transcriptomics, proteomics, metabolomics, and lipidomics processing.
- The large-scale biomass production of *Desulfovibrio vulgaris* for stress response studies can be used as a model for the large-scale production of other obligate anaerobes in the future.

RELATED WEB SITE

http://vimss.lbl.gov

ACKNOWLEDGMENTS

This work was part of the Virtual Institute for Microbial Stress and Survival supported by the U. S. Department of Energy, Office of Science, Office of Biological and Environmental Research, Genomics Program: Genomes To Life (GTL) through Contract No. DE-AC03-76SF00098 between Berkeley Lab and the U. S. Department of Energy.

Geophysical Monitoring of Amendment Distribution and Reactivity During a Cr(VI) Bioreduction Experiment at the Hanford 100-H Site

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RESEARCH OBJECTIVES

The efficacy of *in situ* contaminated-groundwater remediation, using the injection of chemical or biological amendments, depends on the ability to control their distribution within contaminated heterogeneous media. However, understanding how amendments are distributed in natural subsurface systems is difficult to ascertain using conventional (wellbore) characterization techniques, which often sample only a very localized area. In this study, we explore the use of time-lapse geophysical data for imaging amendment distribution as a function of time and heterogeneity. The geophysical research was performed as part of a Cr(VI) bioreduction experiment at the Hanford 100H Site in Washington, where Hydrogen Release Compound (HRC^{TM}; a slow-release polylactate amendment, is being used to reduce Cr(VI) into insoluble Cr(III) complexes. Hazen, et al. (2005; this volume) provide more details on the Cr(VI) bioreduction study.

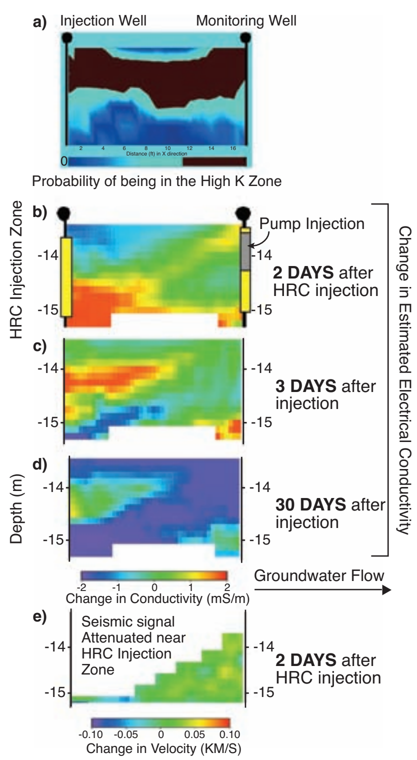

Figure 1. Estimates obtained using geophysical tomographic data: (a) probability of being in a high conductivity zone where black indicates higher hydraulic conductivity; changes in electrical conductivity, (b) 2 days after HRC injection, (c) 3 days after injection, and (d) 30 days after injection; (d) changes in seismic velocity 2 days after HRC injection.

APPROACH

These estimates were determined using seismic and radar crosshole data sets (collected before the injection experiment) with wellbore flowmeter data in a discriminant analysis technique. In August 2004, HRC was injected through the injection well into a Hanford sand/gravel saturated aquifer. Pumping was initiated simultaneously to "pull" the HRC products towards the downgradient monitoring well. Cross-borehole field seismic and radar tomographic data were collected during and subsequent to amendment injection, and were then compared with those data acquired prior to the injection. Geophysical data were also compared with the results of analytical analyses of water samples collected from both wells. Because the HRC and its byproducts are likely to change the electrical conductivity of porous solution, radar tomographic amplitude and velocity data were used to estimate the electrical conductivity changes between the injection and pumping wells.

ACCOMPLISHMENTS

Figure 1a depicts the zonation of hydraulic conductivity of the Hanford formation. Figure 1b indicates the initial increase in the estimated electrical conductivity near the base of the injection interval, which was likely caused by the release of the lactic acid upon hydration of the HRC in groundwater. Figure 1c demonstrates that after 3 days, the effect of pumping from the monitoring well pulled the lactic acid into the higher hydraulic conductivity zone. After 30 days, while the electrical conductivity remained practically the same near the injection well, it decreased (blue areas in Figure 1d) downgradient from the injection well. We hypothesize that this change is likely associated with formation of precipitates. HRC injection caused the seismic response to completely attenuate immediately after the HRC injection (Figure 1e). The field-scale geophysical responses to the HRC injection agree with the results of observations conducted during a series of laboratory controlled HRC-injection and geophysical monitoring experiments.

SIGNIFICANCE OF FINDINGS

The high-resolution, field-scale, cross-borehole geophysical (seismic and radar) measurements hold significant potential for imaging the spatial distribution of lactate-based amendments in heterogeneous sediments, and may be useful for detecting chemical transformations (such as precipitates) of metals. These results also indicate the importance of heterogeneity in controlling amendment distribution. Continuation of this research is necessary to further explore the concept of using geophysical techniques for assessing the remediation efficacy of contaminated sites.

RELATED WEBSITE

http://esd.lbl.gov/ERT/hanford100h/

ACKNOWLEDGMENTS

This work was supported by the NABIR Program, Office of Science, Environmental Remediation Sciences Division of DOE's BER Program under Contract No. DE-AC03-76SF00098. All computations were carried out at the Center for Computational Seismology supported by DOE's Basic Energy Science Program.

Groundwater Flow Monitoring and Plume Evolution

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RESEARCH OBJECTIVES

In the mid-1990s, investigators observed transgradient expansion of the groundwater plume of halogenated, aliphatic volatile organic compounds (VOCs) at Operational Unit 1 (OU-1) of the former Fort Ord Army Base in Monterey, California. Additionally, the plume was found to extend considerably farther in a downgradient direction than determined in the initial characterization performed during the late 1980s. A possible second contaminant release site was posited to explain this latter observation. The objective of this project was to use advanced flow and analyte monitoring instrumentation, efficient data management and analysis, and numerical modeling to understand the evolution of the OU-1 plume.

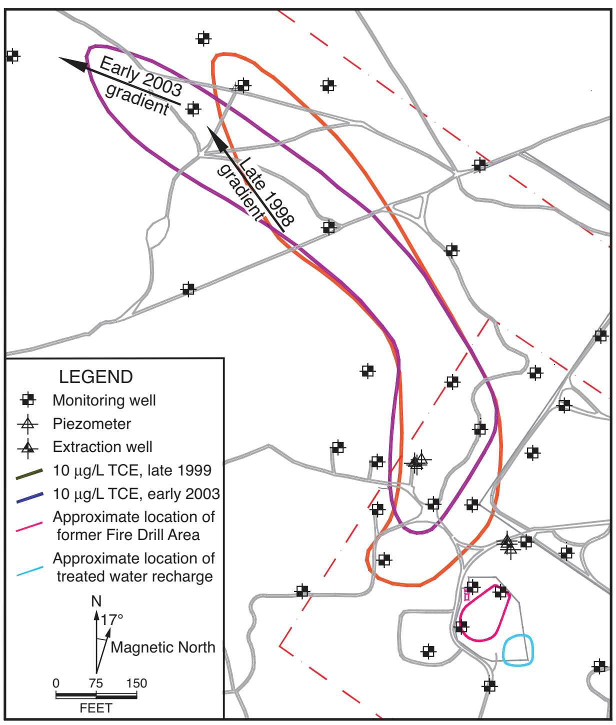

Figure 1. Gradient rotation and extent of trichloroethylene (TCE) plume greater than 10 µg/L after historically intense precipitation in early 1998 at OU-1, Former Fort Ord Army Base

APPROACH

Well-log, water-level, and chemistry data were provided by the groundwater monitoring contractor for OU 1, MacTec Engineering and Consulting, Inc. Treatment system totalizer data were provided by the remedial contractor, AHTNA Government Services, Inc. To improve analysis efficiency, and therefore insight, water-level and chemistry data were loaded into the environmental information management system software (EIMS) GIS\Key (produced by GIS Solutions, Inc.), which integrates data management with graphing and mapping. Precipitation data for the area were obtained from the National Oceanic and Atmospheric Administration (NOAA) National Data Center and incorporated into the analysis. We installed five Hydrotechnics heat-based *in situ* flow sensors to measure well-scale groundwater flow velocities (magnitude and direction). In addition, we carried out short-duration pump tests to measure hydraulic conductivity.

The data set aggregated from the above activities was analyzed to determine the hydrogeologic structure, precipitation recharge rates, hydraulic gradient, contaminant concentrations, porosity, and hydraulic conductivity distribution, orientation, and scaling. A conceptual model of the relationship between these parameters was tested through numerical modeling.

ACCOMPLISHMENTS

The hydraulic conductivity of the aquifer materials was found to be remarkably uniform across scales, orientations, and locations. The numerical modeling demonstrated that the entire OU-1 plume evolved from one contaminant release site. Concentration trend analysis indicated that treated water recharge occurred within the plume area and therefore caused transgradient expansion of the plume. Water-level analysis revealed that gradients in the distal portion of the plume rotated counterclockwise upwards of 30° in response to historically intense precipitation in early 1998 (see Figure 1). Concentration trend analysis further revealed advection of the distal portion of the plume oblique to the plume axis, as expected because of the plume rotation.

SIGNIFICANCE OF FINDING

The rotation of the plume at OU 1 has profound implications. One implication is the need for a significantly expanded well field to monitor and remediate the plume over time as it rotates. These results demonstrate the value of an integrated approach to plume monitoring that includes flow sensors for local groundwater velocity measurement, increased efficiency of data analysis provided by an EIMS, and numerical simulation.

RELATED PUBLICATIONS

Jordan, P.D., C.M. Oldenburg, and G.W. Su, Analysis of aquifer response, groundwater flow, and plume evolution at Site OU 1, former Fort Ord, California. Berkeley Lab Report LBNL-57251, February 2005.

ACKNOWLEDGMENTS

This work was supported by University of California Santa Cruz through the U.S. Army Construction Engineering Research Laboratories under Contract No. DACA42-02-2-0056, and by the U.S. Department of Energy under Contract DE-AC03-76-SF00098.

Joint Inversion of Ground-Penetrating Radar and Hydrological Measurements

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RESEARCH OBJECTIVES

Ground-penetrating radar (GPR) measurements are not directly related to soil hydraulic parameters (e.g., permeability and the parameters of the capillary pressure and relative permeability functions). However, GPR measurements are highly sensitive to fluid distribution (and to transients therein) and are thus potentially useful for inferring soil hydraulic parameters in the vadose zone, especially when combined with additional data types. The objective of this study is to develop a method that jointly uses cross-borehole GPR measurements and hydrological measurements to provide quantitative estimates of field-scale soil hydraulic parameters.

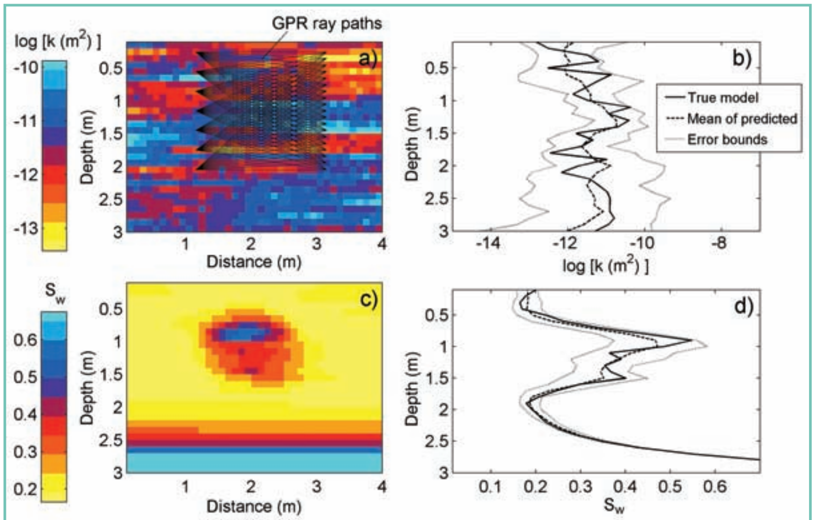

Figure 1. A heterogeneous permeability model (a) is used to simulate a water injection experiment. Joint inversion of synthetic GPR and neutron probe data allow for accurate estimates of permeability (b), which can be used to predict flow phenomena, such as the water saturation profile at a given time (c–d). Vertical cross sections through the two-dimensional models of (a) and (c) are shown in (b) and (d), respectively.

APPROACH

How a hydrological system responds to external stimuli, such as the injection of water, is influenced by the soil hydraulic parameters and their variations in space. Corresponding GPR measurements of the same system also depend on the soil hydraulic functions—although indirectly—since the soil hydraulic functions influence the water distribution, which in turn influences the GPR measurements. Our approach allows for the estimation of soil hydraulic parameters through the coupled simulation (and inversion) of multiple-offset cross-borehole GPR travel times and hydrological measurements collected during transient flow experiments. Joint inversion proceeds by perturbing the unknown hydraulic parameters—which alters the simulated water distributions and subsequent geophysical observations—until a good match is achieved between the simulated and measured (geophysical and hydrological) observations.

BERKELEY LAB
http://www-esd.lbl.gov/

ACCOMPLISHMENTS

Within the context of water injection experiments, we tested the approach with synthetic examples and also applied it to field data. The synthetic examples show that while realistic errors in the petrophysical function (the function that relates soil porosity and water saturation to the effective dielectric constant) cause substantial errors in the soil hydraulic parameter estimates, simultaneously estimating petrophysical parameters and soil hydraulic parameters allows for these errors to be minimized. Additionally, inaccuracy in the GPR simulator can cause systematic error (bias) in the simulated travel times, making necessary the simultaneous estimation of a correction parameter. After demonstrating the usefulness of the method with synthetic examples (Figure 1), we applied it in a three-dimensional field setting to field data (GPR and neutron probe data) collected during an infiltration experiment at the U.S. Department of Energy (DOE) Hanford site in Washington. We find that inclusion of GPR data in the inversion procedure provides hydrological models that predict water-content distributions better than models obtained using neutron probe data alone.

SIGNIFICANCE OF FINDINGS

GPR and other geophysical methods offer high resolution and minimally invasive information that has traditionally been difficult to relate to hydrological properties. Our joint inversion approach provides a way to incorporate geophysical data into hydrological investigations in a meaningful and quantitative way. The flexible framework we have developed should prove useful for inclusion of additional geophysical data types, such as from seismic and electrical methods.

RELATED PUBLICATIONS

Kowalsky, M.B., S. Finsterle, and Y. Rubin, Estimating flow parameter distributions using ground-penetrating radar and hydrological measurements during transient flow in the vadose zone. Advances in Water Resources, 27 (6), 583–599, 2004. Berkeley Lab Report LBNL-53786.

Kowalsky, M.B., S. Finsterle, J. Peterson, S. Hubbard, Y. Rubin, E. Majer, A. Ward, and G. Gee, Estimation of field-scale soil hydraulic and dielectric parameters through joint inversion of GPR and hydrological data. Water Resources Research (in press), 2005. Berkeley Lab Report LBNL-57560.

ACKNOWLEDGMENTS

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

A Multisensor System for Detection and Characterization of UXO

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RESEARCH OBJECTIVES

The objective of this field demonstration project is to show that a multisensor active electromagnetic (AEM) system can be built to detect and extract essential information about a metallic object in the ground, so as to discriminate unexploded ordnance (UXO)-like bodies from non-UXO scrap. Further, we hope to demonstrate that the system can perform target characterization from a single position of the sensor platform above a target. This system will equal or exceed the detection capabilities of existing systems, but with the important advantage of being able to quantitatively determine size and principal polarizabilities of the target. The cart-based system is designed to detect and characterize UXO in the 20 mm to 150 mm size range.

APPROACH

Drawing on the experience gained in the completion of Strategic Environmental Research and Development Program (SERDP) Project UX-1225 (Detection and Classification of Buried Metallic Objects), we are building an optimally designed field prototype system. The system employs two orthogonal vertical loop transmitters and a pair of horizontal loop transmitters vertically spaced 0.7 m apart. Eight vertical field detectors are deployed in the plane of each of the horizontal loops and are arranged to measure the offset vertical gradients of the fields. The system employs a bipolar half-sine pulse-train current waveform, and the detectors are dB/dt induction coils designed to minimize the transient response of the primary field pulse. The sensor coil pairs are located on symmetry lines through the center of the system, so that they detect identical primary fields (for all three transmitters) during the on-time of the pulse. These coil pairs are wired in opposition to produce a null output. Secondary fields from the target have a large gradient that is easily measured in the differenced output. Field prototype sensors are critically damped and resonant at about 20 kHz, and resonant frequency allows a 270 Hz waveform repetition rate and a duty factor of about 20%. The location and orientation of the three principal polarizabilities of a target can be recovered from a single position of the transmitter-receiver system. Further characterization of the target is obtained from the broadband response.

ACCOMPLISHMENTS

We have developed a field-prototype active EM system that can extract from the measurements the best possible estimates of the location, size, shape, and metal content of a buried metallic object, in the presence of an interfering response from the ground and/or non-UXO metallic objects. The prototype system has been tested in the laboratory with very encouraging results. This project received the SERDP Project of the Year award in the UXO Field at the Partners in Environmental Technology Symposium in Washington on December 2, 2004. A rigorous field test is under way and will be followed by a demonstration survey at an Environmental Security Technology Certification Program (ESTCP) standard test site.

RELATED PUBLICATIONS

Smith, J.T., H.F. Morrison, and A. Becker, Parametric forms and the inductive response of a permeable conducting sphere. Journal of Env. and Engin. Geophysics, 9, 213–216, 2004a. Berkeley Lab Report LBNL-54621.

Smith, J.T., H.F. Morrison, and A. Becker, Resolution depths for some transmitter-receiver configurations. IEEE Trans. Geosci. Remote Sensing, 42, 1215–1221, 2004b. Berkeley Lab Report LBNL-51574.

Smith, J.T., H.F. Morrison, and A. Becker, Optimizing receiver configurations for resolution of equivalent dipole polarizabilities *in situ*. IEEE Trans. Geosci. Remote Sensing (submitted), 2005. Berkeley Lab Report LBNL-54585.

ACKNOWLEDGMENTS

This work was supported by the Office of Management, Budget, and Evaluation, of the U.S. Department of Energy under Contract No. DE-AC03-76SF00098, and the U.S. Department of Defense under Strategic Environmental Research and Development Program Project No. UX-1225 and Contract No. W74RDV30452524.

Remote-Sensing Techniques for Assessing Impacts of Wetland Real-Time Water Quality Management on Wetland Seasonal Habitat

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RESEARCH OBJECTIVES

The U.S. Bureau of Reclamation has recently announced its intention to require wetlands in the western U.S. to develop best management practices (BMP's). The formulation of BMP's requires detailed knowledge of current practices, together with accurate water balances and estimates of evapotranspiration, to allow assessment of water-use efficiency. The Bureau of Reclamation has entered into a collaboration with Berkeley Lab to develop remote - sensing tools to improve estimates of evapotranspiration and to assess habitat value based on quantitative estimates of moist soil plants. Recent advances in available image data and processing techniques have increased the scope for success in discriminating between moist soil plants found in managed wetlands in California's Central Valley. Models such as SEBAL and METRIC use thermal infrared data, in combination with visible and near-infrared data, to estimate evapotranspiration. Vegetation mapping can help extrapolate these estimates to the entire wetland resource area. This study explored the development of an accurate, consistent, and efficient methodology for mapping land cover and vegetation through remote-sensing technology.

APPROACH

Multispectral satellite imagery was used to map vegetation and other land cover in Central Valley wetlands. The imagery displayed reflected light in blue, green, red, and near-infrared wavelengths. High-resolution image data enabled mapping of small and irregularly shaped vegetation communities. An integrated GPS/field computer permitted rapid collection of consistent ground-truth data. The protocol for describing vegetation communities was based on the California Native Plant Society's Rapid Assessment Protocol, and a comprehensive field guide was developed for identification of plant species. Image data were processed using the software packages ERDAS Imagine and Definiens eCognition. Spectral signatures were developed using field data to guide the selection of representative pixels. A maximum likelihood algorithm was used to classify each pixel according to its statistical similarity to defined classes.

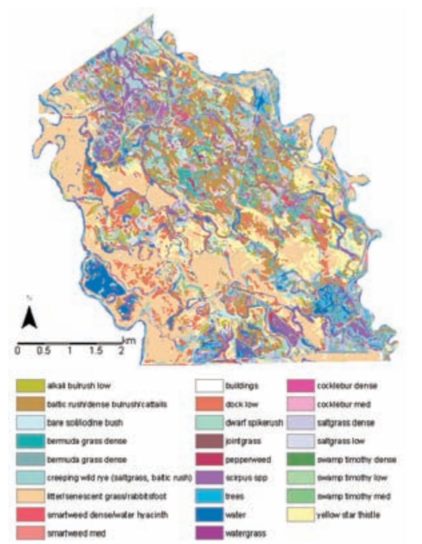

Figure 1. Map of land-cover classes derived from satellite image data using statistically based image processing. Image classification is an efficient process, using a few thousand known pixels to classify an entire image comprised of tens of millions of pixels.

ACCOMPLISHMENTS

A land-cover map was produced for an area of Central Valley wetlands covering 160 km^2. Figure 1 shows a map of land-cover classes represented in the San Luis National Wildlife Refuge. Most important vegetation communities, including those dominated by alkali bulrush, baltic rush, cocklebur, and swamp timothy, were represented with greater than 75% accuracy. Other classes, such as bermuda grass, smartweed, and watergrass, were classified with lesser accuracy. Overall, the remote-sensing methodology mapped a large area, using minimal field data, with a high degree of accuracy.

SIGNIFICANCE OF FINDINGS

Central Valley wetlands are significant water users and compete with agriculture for an adequate water supply. Effluent impacts water quality in the San Joaquin River, and real-time management of drainage may be incorporated into BMP's for these wetlands. Management decisions regarding water should be evaluated with respect to habitat health. A remote-sensing mapping methodology can provide an accurate and consistent means to track changes in habitat. Accurate land-cover maps also provide the basis for water-needs analyses through quantitative assessment of evapotranspiration from open water, bare soil, and vegetation communities.

RELATED PUBLICATION

Quinn, N.W.T, W.M. Hanna, J.S.Hanlon, J.R. Burns, C.M. Taylor, D. Marciochi, S. Lower, V. Woodruff, D. Wright, and T. Poole, Real-time water quality management in the grassland water district. Berkeley Lab Report LBNL-56825, 2004.

ACKNOWLEDGMENTS

This work was supported by CALFED Ecosystems Restoration Program administered by the U.S. Bureau of Reclamation under the U.S. Department of Interior Interagency Agreement N.3-AA-20-1097, through the U.S. Department of Energy under Contract No. DE-AC03-76SF00098.

Fluid Logging Experiments to Determine Depth Distribution of Salts Beneath Seasonally Flooded Wetlands

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RESEARCH OBJECTIVES

Groundwater conjunctive use in California is being promoted by the State and Federal water resource agencies as a means of alleviating over-allocated water supply, especially in the western San Joaquin Valley. The U.S. Bureau of Reclamation, having recently undertaken a study of water banking in the aquifers that underlie seasonally flooded wetlands, has partnered with Berkeley Lab to assess the potential impact of long-term pumping strategies on the quality of the water produced by these wells. Tsang and Doughty (2003) have shown how the flowing-fluid-electric-conductivity (FEC) logging method can be used to yield a profile of water quality along the length of the screened interval in the well. This current research extends this analysis in a very practical way, allowing the technique to be deployed in some nonideal situations, in particular at sites where the motor and well pump could not be removed to access the well casing.

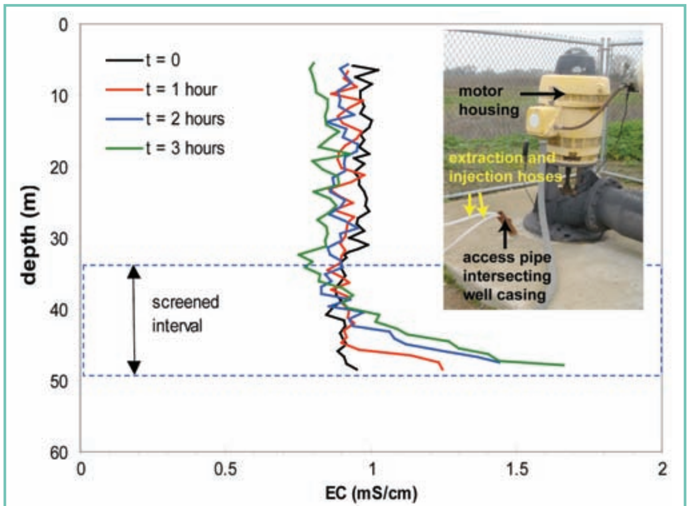

Figure 1. Electrical conductivity profiles measured over time in a well in the San Joaquin Valley as water is extracted at a constant rate of 0.7 m^3/hr. Photograph of a well with limited access is shown in the upper right-hand corner.

APPROACH

FEC logging has been conducted in wells around the wetlands in the San Joaquin Valley. This technique involves replacing the wellbore water with deionized or low-salinity water while the wellbore water is simultaneously extracted. After the wellbore water is replaced by low-salinity water, the change in the electrical conductivity (EC) profile in the well is recorded over time as the water is extracted at a constant rate (Figure 1). The FEC logging technique had previously been performed only in vertical wells with diameters typically ranging between 5 to 15 cm. The wells at our study site had very limited access through a 3.8 cm diameter pipe that intersected the wellbore at a 45º angle (Figure 1). We modified the FEC logging technique such that this method could be used in these wells.

ACCOMPLISHMENTS

The typical EC probe used to log vertical wells has a diameter of 3.8 cm and a length of 1.8 m; such a probe could not fit into the access pipe intersecting our study wells. Instead, we successfully deployed a small EC probe manufactured by Campbell Scientific up to depths of 90 m. The probe has a cross-sectional dimension of 2.5 × 1.9 cm and is 8.9 cm long. To inject and extract the water simultaneously through the access pipe, we used small-diameter (1.9 cm) hoses. Because we were limited to using such a small hose, we developed and tested a new technique of injecting water uniformly over the well length by inserting pressure-compensating emitters along the length of the hose. This new technique replaces the more time-consuming, traditional approach of injecting low-salinity water only at the well bottom.

SIGNIFICANCE OF FINDINGS

We successfully conducted FEC logging in wells with limited access and obtained transient measurements of the electrical conductivity with depth (Figure 1). Over time the EC increases faster towards the bottom of the well than at the top of the screened interval, indicating that the formation at the bottom of the screened interval is more permeable or the EC of the water at the bottom of the well is higher. Obtaining data on the depth distribution of salts and identifying high salinity zones in the aquifers in the San Joaquin Valley is critical for evaluating the potential of groundwater for conjunctive water use.

RELATED PUBLICATION

Tsang, C.-F. and C. Doughty, Multi-rate flowing fluid electric conductivity method. Water Resour. Res., 39(12), 1354, doi:10.1029/2003WR002308, 2003. Berkeley Lab Report LBNL-52518.

ACKNOWLEDGMENTS

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

Impact of Agricultural Non-Point-Source Pollution on Water Quality

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RESEARCH OBJECTIVES

Non-point-source (NPS) water pollution is now recognized as the most significant remaining source of water quality impairment in the United States. NPS pollution is a worldwide problem and impacts drinking water and quality of life in both industrial and nonindustrial societies. NPS pollution, unlike pollution from industrial or sewage treatment plants, comes from diffuse sources that are hard to identify and are poorly understood and characterized. Agriculture is a major source of NPS pollution, but the nature, character, and impact of this pollution is largely unknown.

We are currently conducting an ecosystem-level study on the San Joaquin River in the Central Valley of California, examining how NPS discharge impacts water quality. The primary objective is to understand how nutrient and sediment-laden drainage from agriculture influences primary productivity (algal growth) in the river, and how algal growth produces secondary impacts on water quality and fish habitats in the river and connecting delta ecosystem. We are also examining how changing agricultural practices, referred to as best management practices (BMPs), will influence productivity and water quality in riverine ecosystems.

APPROACH

To understand the interaction between NPS pollution, algae growth rate, and algae biomass carrying capacity, we are measuring a complete mass balance on algae and nutrients over a 110 mile reach of the San Joaquin River. Simultaneous collection of water quality and biological data at 21 sites in the watershed develops an instantaneous "snapshot" or profile of algae and nutrients in the river. Seasonal and diurnal changes in algal productivity are studied, using continuously deployed chlorophyll measuring devices and field experiments in which individual algal blooms are tracked and characterized. Specific tributaries and "hot spots" for algal growth are subject to focused studies to answer basic scientific and engineering questions concerning environmental conditions limiting algal growth. The installation and operation of a network of 51 stations, for the continuous measurement of flow and salt concentration in the main stem of the river and the tributaries, provides the final piece of the puzzle that allows us to develop a complete mass balance on algae and nutrients in this ecosystem.

ACCOMPLISHMENTS

This year is the first of a three-year study. Collection of water quality and biological data has begun. The continuous-flow and water-quality monitoring network is almost complete. Studies of bloom dynamics and individual tributaries are in progress.

SIGNIFICANCE OF FINDINGS

Initial studies have already contributed to our understanding of NPS pollution in the San Joaquin Valley. Studies of algal growth and water quality at previously uncharacterized tributaries have raised new questions concerning our understanding of algal growth dynamics in this river. Such studies have challenged assumptions included in water quality models used by state agencies to manage water quality in this severely impacted water body.

RELATED PUBLICATIONS

Stringfellow, W.T., and N.W.T. Quinn, Discriminating between west-side sources of nutrients and organic carbon contributing to algal growth and oxygen demand in the San Joaquin River. CALFED Bay-Delta Program, Sacramento, California; Berkeley Lab Report LBNL-51166, 2002.

ACKNOWLEDGMENTS

This research is supported by funding from the California Bay-Delta Authority Ecosystem Restoration and Drinking Water Quality Programs, the State Water Resources Control Board, the Center for Science and Engineering Education, and the University of the Pacific Environmental Engineering Research Program.

Development of an Unsaturated Region Below a Perennial River

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RESEARCH OBJECTIVES

Field observations along the Russian River in Sonoma County, California, indicate that an unsaturated region exists below the streambed near two adjacent collector wells located along the riverbank. Understanding the conditions that give rise to unsaturated flow below the streambed is critical for improving and optimizing riverbank well-pumping operations. A three-dimensional model was developed using TOUGH2 to investigate the conditions under which an unsaturated region develops below a perennial river when the collector wells were pumping.

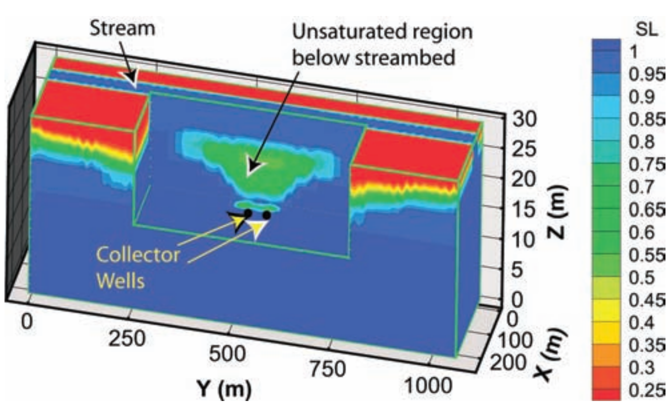

Figure 1. Simulated water saturation (SL) below the streambed after the two collector wells had pumped continuously for seven days at 1,600 m^3/hr. The aquifer permeability is 2.4×10^{-10} m^2 and the streambed permeability is 7.4×10^{-13} m^2.

APPROACH

The numerical model was based on the region near two collector wells in the Russian River Bank Filtration Facility. These wells consist of nine perforated pipes that are projected horizontally into the aquifer at a depth of approximately 20 m below the land surface. A grid was developed that was highly refined near the wells, so that the individual pipes could be represented. The two collector wells each pumped continuously at a rate of 1,600 m^3/hr.

ACCOMPLISHMENTS

The aquifer below the streambed remained saturated when the aquifer and streambed permeability were the same (both 2.4×10^{-10} m^2), and when the streambed permeability was one order of magnitude smaller than the aquifer permeability. When the streambed permeability was 2.4×10^{-12} m^2, which was two orders of magnitude smaller than the aquifer permeability, an unsaturated region developed below the streambed that was approximately 25 m wide, 130 m long, and 3 m deep. When the streambed permeability was 7.4×10^{-13} m^2, which was 2.5 orders of magnitude less than the aquifer permeability, a large unsaturated region formed below the river that extended across the entire river width (60 m), was over 350 m long, and up to 10 m deep. Under these conditions, the simulated unsaturated region that developed near the streambed after seven days of continuous pumping is shown in Figure 1.

SIGNIFICANCE OF FINDINGS

As the permeability of the streambed decreased relative to the aquifer permeability, the extent of the unsaturated region below the streambed increased. The results of the numerical simulations have important implications for well operation. During the summer and fall months, when the inflatable dam is raised at the Russian River Bank Filtration Facility and the streambed permeability decreases over time, well operation may have to be altered if the permeability decreases to a value such that a large unsaturated region forms below the streambed.

RELATED PUBLICATION

Su, G.W., J. Jasperse, D. Seymour, and J. Constantz, Estimation of hydraulic conductivity in an alluvial system using temperatures. Ground Water, 42(6), 890–901, 2004. Berkeley Lab Report LBNL-53167.

ACKNOWLEDGEMENTS

This work was supported by the Sonoma County Water Agency (SCWA), through U.S. Department of Energy Contract No. DE-AC03-76SF00098.

Interpretation of Groundwater Velocities from Heat-Based Flow Sensors

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RESEARCH OBJECTIVES

Heterogeneities in formation properties around an *in situ* heat-based flow sensor may lead to incorrect interpretations of groundwater flow velocities. The flow sensor operates by constant heating of a 0.75 m long, 5 cm diameter cylindrical probe, which contains 30 thermistors in contact with the formation. The temperature evolution at each thermistor is inverted to obtain an estimate of the groundwater flow velocity vector, based on the assumption that the formation is homogeneous. Analysis of data from three heat-based flow sensors installed in a shallow sand aquifer at the Former Fort Ord Army Base near Monterey, California, suggested a strong and unexpected component of downward flow. Three-dimensional TOUGH2 simulations were conducted to investigate how differences in the thermal conductivity and permeability around the instrument may lead to inaccurate indications of downward flow velocities.

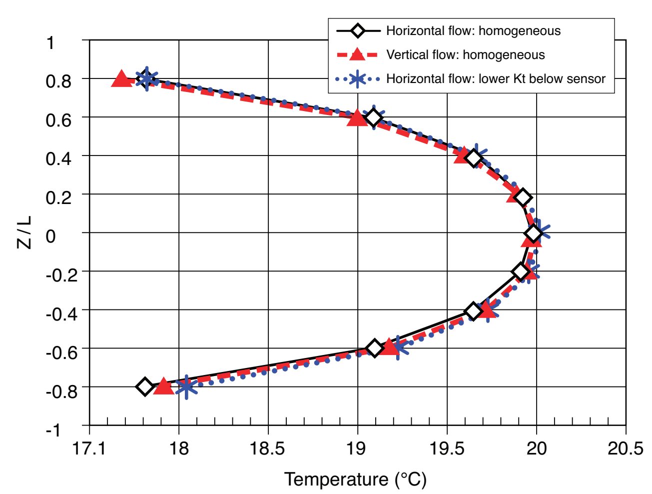

Figure 1. Simulated temperature profiles along the sensor for horizontal and vertical flow in a homogeneous formation, and for horizontal flow when K_t below the sensor is lower than K_t along the sensor

APPROACH

Conformal mapping was used to generate a discretization highly refined near the cylindrical instrument body to use for simulating flow and heat transport near the sensor. A 17-layer model was used in the 3-D simulations, with the heated portion of the flow sensor represented by the nine center layers. Horizontal flow was imposed across the domain in all the simulations, except for one where vertical flow was imposed. Heterogeneity was assumed only in the vertical direction, resulting in a "layer-cake" type stratigraphy.

ACCOMPLISHMENTS

Simulated temperature profiles on the downstream side of the flow sensor are plotted as a function of depth in Figure 1. In a homogeneous formation, the temperature profile is symmetric for horizontal flow, while higher temperatures are observed along the bottom half of the sensor relative to the top half for vertical (downward) flow. When the thermal conductivity (K_t) of the formation is lower below the sensor compared to the thermal conductivity along the length of the sensor (2.1 versus 1.8 W/m°C), the temperature profile becomes shifted in such a manner that it could be interpreted as resulting from downward flow, even though flow is actually horizontal. A decrease in the permeability towards the bottom of the sensor relative to the top can also result in a temperature profile that could be interpreted as having a downward flow component, although the effect tends to be smaller.

SIGNIFICANCE OF FINDINGS

The simulations demonstrate that the temperatures recorded by heat-based flow sensors are sensitive to differences in the thermal and hydraulic properties of the formation. Under conditions of strictly horizontal flow, the temperature profile along the length of the sensor can be perturbed by changes in the thermal conductivity and permeability, such that analysis of the data assuming homogeneous formation properties could result in interpreting the temperature shift as the result of downward flow.

RELATED PUBLICATIONS

Su, G.W., B.M. Freifeld, C.M. Oldenburg, P.D. Jordan, and P.F. Daley, Simulation of *in situ* permeable flow sensors for measuring groundwater velocity. Ground Water (in review), 2005. Berkeley Lab Report LBNL-57084.

Jordan, P.D., C.M. Oldenburg, and G.W. Su, Analysis of aquifer response, groundwater flow, and plume evolution at Site OU1, Former Fort Ord, California. Berkeley Lab Report LBNL-57251, 2005.

ACKNOWLEDGMENTS

This work was supported by U.C. Santa Cruz (UCSC) through the U.S. Army Construction Engineering Research Laboratories (US ACERL), and by the U.S. Department of Energy under Contract No. DE-AC03-76SF00098.

Use of Biomarker Sequences for the Identification and Phylogenic Analysis of Filamentous Fungi Isolated from Extreme Environments

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RESEARCH OBJECTIVES

Fungi play complex and diverse roles in ecosystems. Their importance to biotechnology and bioprospecting is enhanced by the vast diversity of extant fungi. The search for novel capabilities and useful new genetic traits most often targets microorganisms that live under extreme environmental conditions, such as high temperature, extreme pH, salinity, and radiation. Scientists at Berkeley Lab's Center for Environmental Biotechnology have been bioprospecting for many years at contaminated sites and closed military bases, in deserts and forests in the USA, in Lake Baikal sediments and at geothermal and hydrothermal sites on the Kamchatka peninsula in Russia, and at the failed nuclear power plant and within the surrounding 30 km "Exclusion Zone" in Chernobyl, Ukraine. Their work focuses on filamentous fungi that often possess the ability to produce unique secondary metabolites with potential commercial value. These natural products are advantageous to the organism in their respective environment as chemical defense against predators, pathogens, or competitors. Identification of these microorganisms provides a better understanding of their ecological function. The overall goal of this project is the taxonomic characterization of thousands of fungal cultures in a way that is amenable to a much wider range of laboratories.

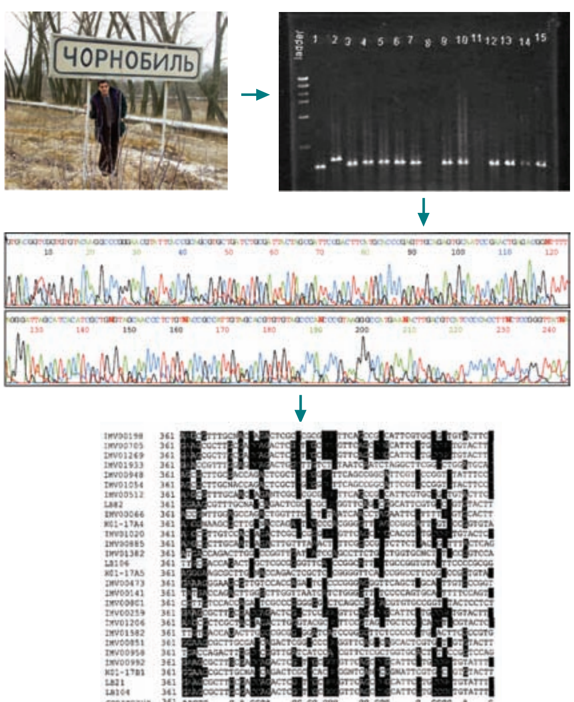

Figure 1. Flow diagram of the sequence-based identification (from environmental sample to the consensus of aligned sequences)

APPROACH

Procedures traditionally used for fungal identification rely on colony-and cell morphology and other distinctive biochemical reactions. Recently, molecular-level protocols have been increasingly used for fungal identification. Here, we applied a polymerase chain reaction (PCR) combined with amplicon sequencing and comparative sequence analysis of biomarker genes. DNA sequencing was done at the University of California-Berkeley DNA Sequencing Facility. Raw sequences were edited and aligned using online multiple sequence aligner subroutines. Aligned sequences were further analyzed for consensus and finally queried against the National Center for Biotechnology Information database for species determination (Figure 1).

ACCOMPLISHMENTS

The main objective of this study was to test an alternative method of fungal identification. Though the number of strains/species/genera included in this study was biased by the extreme environmental habitats, most of over 100 species tested so far were identified correctly, in agreement between classical and molecular-level identification. More definite results will be available when the sequence-based identification of the over 2,000 filamentous fungi isolated from extreme environmental samples is completed.

SIGNIFICANCE OF FINDINGS

Taxonomic identification and detailed characterization of extremophillic microorganisms provides a greater understanding of their diversity, unique metabolism, and ecological function. Here, fungal organisms were characterized successfully by comparing classical techniques and sequence-based phylogenetic differentiation. Because we consider filamentous fungi major sources of novel biotechnology and biomedical applications, a future goal is to design an Affymetrix-type microarray to aid in better understanding of fungal phylogenetic relatedness and diversity.

RELATED PUBLICATIONS

Torok, T., N. Zhdanova, M. Kuchuk, G. Dahlbacka, Amaku, G. Andersen, and J. Hunter-Cevera, Characterization of filamentous fungi isolated from extreme environments. Proceedings of the Fifth International Conference on Extremophiles ("Extremophiles 2004"), p. 86, Cambridge, Maryland, September 19–23, 2004.

ACKNOWLEDGMENTS

We wish to express our deepest appreciation for the support we have received from the U.S. Department of Energy Office of Science and the National Science Foundation. The DOE-supported Initiatives for Proliferation Prevention (IPP) program, and the DOE-NSF jointly sponsored Faculty and Student Training (FaST) program, made progress possible. Special thanks are due to friends and peers.

Enhanced Bioremediation of Contaminated Groundwater at Berkeley Lab, Using Hydrogen-Release Compound®

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RESEARCH OBJECTIVES

The U.S. Department of Energy is actively pursuing innovative, cost-effective methods of remediating contaminated groundwater at its facilities, including Berkeley Lab. The accidental release of solvents used at Berkeley Lab decades ago resulted in contamination of underlying groundwater at several onsite locations. Several groundwater cleanup technologies have been deployed to address the contamination, including conventional groundwater extraction and treatment, soil washing, chemical oxidation, thermally enhanced dual vapor and groundwater extraction, natural attenuation, and enhanced bioremediation. Among these, enhanced bioremediation is a particularly promising, innovative cleanup technology that reduces contaminant levels below regulatory standards in a relatively short period of time.

APPROACH

Indigenous bacteria found in groundwater are known to biodegrade chlorinated solvents, leading to the natural attenuation of groundwater contaminant plumes. Unfortunately, natural attenuation can be a relatively slow process, potentially taking decades to reduce contaminant levels below cleanup requirements. Therefore, supplements that promote bacteria growth can be added to the groundwater to help enhance natural bioremediation and expedite cleanup. This technique is referred to as enhanced bioremediation.

An *in situ* pilot study performed at Berkeley Lab's Building 71B successfully demonstrated rapid biodegradation of chlorinated solvents, within nine months of injecting concentrated glycerol tripolylactate ester into contaminated groundwater. Gycerol tripolylactate (sold under the trade name Hydrogen Release Compound, HRC®) is a commercially available, dense, viscous liquid that is highly soluble in water. Full-scale treatment of the contaminated area, located beneath and downgradient of the building, is currently under way using dilute HRC®. Groundwater is mixed with HRC® and heated in an aboveground bioreactor to stimulate quick bacterial growth, then injected into a drainfield located within the footprint of the building at the source. An existing groundwater pump and treat system, located downgradient from the source, hydraulically controls the plume and supplies water to the drainfield, thus distributing HRC® throughout the contaminated area.

ACCOMPLISHMENTS

Dissolved oxygen and oxidation-reduction potentials rapidly decreased in groundwater within three weeks of HRC® injection. This rapid decrease indicates that reducing conditions favoring anaerobic biodegradation of solvents quickly developed after introducing HRC®. More importantly, total contaminant levels in groundwater decreased throughout the winter months, in contrast to normal trends when concentrations increased because of winter recharge and rising water table conditions (Figure 1).

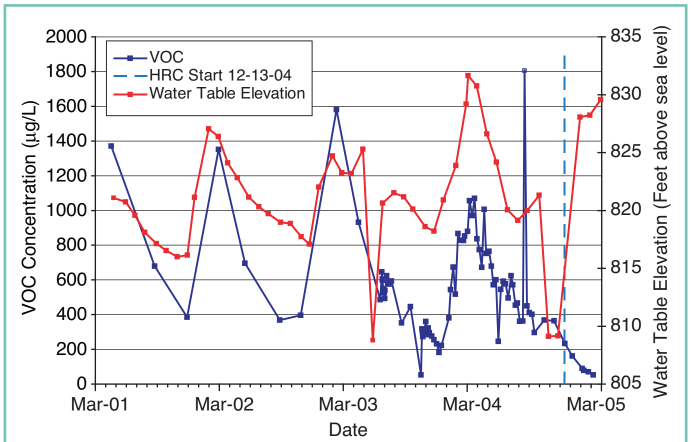

Figure 1. Total volatile-organic compound concentrations increase every year when the water table beneath Building 71B rises because of winter rains. This trend ended after injecting HRC®.

SIGNIFICANCE OF FINDINGS

HRC® is typically applied by direct injection of the concentrated product into the subsurface, using a dense network of direct push or conventionally drilled borings. The size and depth of the plume, which controls the number of borings and amount of HRC® applied, can have a significant impact on remediation costs. Our study shows that HRC® can be successfully incorporated into an existing conventional groundwater extraction system by injecting it into the subsurface in its dilute form. Additional time is needed to study our approach to assess whether biofouling by bacteria will reduce the permeability of the drainfield, production well, or porous material, rendering our approach ineffective. However, few viable alternatives are available that can be used to treat contaminated soils beneath an existing structure, as with HRC®.

ACKNOWLEDGMENTS

This work was performed by the Berkeley Lab's Environmental Restoration Program, which is operated by the University of California for the U.S. Department of Energy under Contract No. DE-AC03-76-SF00098.

Reoxidation of Bioreduced Uranium Under Reducing Conditions

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RESEARCH OBJECTIVES

Interest in the biogeochemical cycle of uranium (U) is growing, especially for remediating contaminated environments. The mobility of U depends strongly on its oxidation state, with U(IV) being much less soluble than U(VI). Therefore, some strategies under development for immobilizing U in contaminated sediments are aimed at promoting precipitation of U(IV) minerals, typically by injecting organic carbon (OC) into sediments to stimulate microbial U(VI) reduction. Previously, observations of OC-stimulated U reduction have only reported fairly short-term results. Our studies are directed at understanding the conditions controlling longer-term stability of bioreduced U.

APPROACH

Columns packed with a U contaminated (206 mg kg^{-1}) sediment obtained from the Natural and Accelerated Bioremediation (NABIR) Program's Field Research Center in Oak Ridge National Laboratory were supplied with sodium lactate (32 mM OC) solutions, and effluent solution chemistry was monitored. U oxidation states were determined nondestructively in soil columns at the Advanced Photon Source, GSECARS beamline, by micro-X-ray absorption spectroscopy (micro-XAS). Fluorescence spectroscopic measurements were conducted to determine the U species in effluents. Microbial communities within sediment columns were characterized by high-density oligonucleotide array analyses and real-time quantitative polymerase chain reaction methods..

ACCOMPLISHMENTS

Our 17-month study showed that bioreduction of U was transient, even under sustained reducing conditions. Micro-XAS showed that U was reduced during the first 80 days, but later (100 to 500 days) reoxidized and solubilized (Figure 1), although a microbial community capable of reducing U(VI) was maintained. OC-stimulated microbial respiration caused increases in (bi)carbonate concentrations and formation of uranyl carbonate complexes, thereby increasing the favorability of U(IV) oxidation. Fluorescence spectroscopy showed that U(VI) in effluents occurred primarily as uranyl tricarbonate and dicalcium uranyl tricarbonate. We hypothesize that kinetic limitations allowed Fe(III) to persist as terminal electron acceptors for U reoxidation.

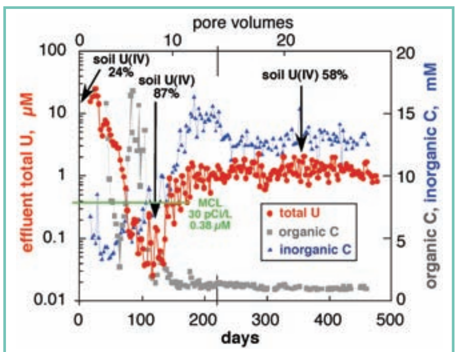

Figure 1. Concentrations of U, OC, and bicarbonate concentrations in effluents from columns supplied with 32 mM OC. Micro- XAS showed that the soil U was initially oxidizing (24% U(IV)), then largely reduced (87% U(IV)), and later reoxidized (58% U(IV)).

SIGNIFICANCE OF FINDINGS

These results show that *in situ* U remediation by OC-based reductive precipitation can be problematic in sediments when uranyl carbonates are stable, and that OC concentrations in remedial solutions need to be carefully considered to minimize carbonate-enhancement of U(VI) solubility. This work also demonstrates the need for long-term experiments to evaluate remediation strategies that rely on transforming actinides and metals to low-solubility products. In considering much longer time scales set by the half-life of ^{238}U, the practicality of reduction-based immobilization strategies in regionally oxidizing sediments needs to be carefully reevaluated.

RELATED PUBLICATIONS

Tokunaga, T.K., J. Wan, J. Pena, E. Brodie, M.K. Firestone, T.C. Hazen, S.R. Sutton, A. Lanzirotti, and M. Newville. Uranium reduction in sediments under diffusion-limited transport of organic carbon. Environ. Sci. Technol. (in final review), 2005.

Wan, J., T.K. Tokunaga, E. Brodie, Z. Wang, Z. Zheng, D. Herman, T.C. Hazen, M.K. Firestone, and S.R. Sutton. Reoxidation of bioreduced uranium under reducing conditions. Environ. Sci. Technol., 39 (in press), 2005. Berkeley Lab Report LBNL-56058.

ACKNOWLEDGMENTS

This project is supported by the Director, Office of Science, Office of Biological and Environmental Research, NABIR Program, and Office of Basic Energy Sciences, Division of Chemical Sciences, Geosciences, and Biosciences, of the U.S. Department of Energy under Contract No. DE-AC03-76-SF00098. Use of the Advanced Photon Source was supported by the DOE, Office of Science, Basic Energy Sciences. Fluorescence spectroscopic measurements were performed at the Environmental Molecular Sciences Laboratory, sponsored by the Office of Biological and Environmental Research. We thank J. Larsen, D. Joyner, S. Baek, J. Pena, and M. Newville for technical assistance.

Geochemical Evolution of Tank Waste Plumes upon Infiltrating into Sediments

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RESEARCH OBJECTIVES

Leakage of highly saline and alkaline radioactive waste solutions from storage tanks into underlying sediments is a serious problem at the Hanford Site in Washington State. Although it was found from field samples that pH values of the initially highly alkaline (pH 14) waste plumes dramatically decreased (to pH 10–7), understanding of the neutralization process was lacking. Since pH is a master geochemical variable, the behavior of waste plume contaminants, including their speciation, sorption, solubility, precipitation, and transport, can be reliably predicted only when the evolution of the pH profile is understood. This study focuses on the geochemical evolution of major geochemical parameters, including pH, and addresses how pH evolved as the plumes propagated.

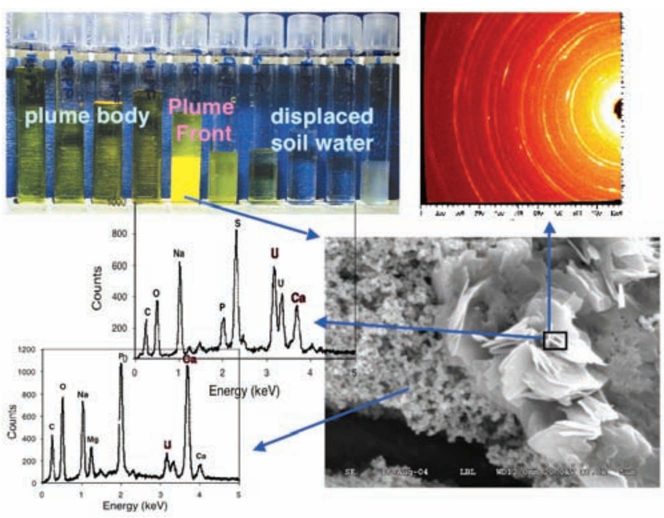

Figure 1. Formation of plume-front colloids from a uranium waste plume. The upper-left photograph shows a profile of extracted pore solution from a U plume and the massive colloid formation at the plume front. The lower-right SEM image shows morphology of the plume front colloids. The EDS analyses (lower-left) indicate U is a major element in these colloid particles. Synchrotron micro-XRD (upper-right) identified the plate-like phase as sodium-uranyl-carbonate.

APPROACH

A plume-profiling method was designed to obtain spatially and temporally resolved direct measurements of plume geochemistry profiles. To simulate the leakage events, we injected synthetic tank waste solutions into Hanford sediment columns at desired temperatures. Experimental conditions were chosen as close to the field conditions as possible, yet simple enough so that causes and effects could be identified. Geochemical and transport processes were studied simultaneously. Finally, we obtained spatially resolved data of geochemical evolution over different waste plume distances and for different times.

ACCOMPLISHMENTS

This study revealed that: (1) a large (i.e., several-units) pH reduction occurred at the plume fronts, which would have a substantial impact on contaminant fate and transport (as demonstrated for uranium); (2) maximum colloid formation occurred at plume fronts (hundreds to thousands times higher than within the plume bodies or during later leaching); and (3) cation exchange of Na^+ replacing Ca^{2+}/Mg^{2+} from the sediments during flow, and precipitation of Ca^{2+}/Mg^{2+}-bearing solids, were identified as being responsible for these plume-front phenomena.

SIGNIFICANCE OF FINDINGS

These plume-front phenomena were not previously revealed by either geochemical modeling or by laboratory batch experiments. This new understanding obtained through our column-based experiments is important for predicting the behavior of contaminants in waste plumes.

RELATED PUBLICATIONS

Wan, J., T.K. Tokunaga, E. Saiz, J.T. Larsen, Z. Zheng, and R.A. Couture, Colloid formation at waste plume fronts. Environ. Sci. Technol., 38, 6066–6073, 2004. Berkeley Lab Report LBNL-56059.

Wan, J., J.T. Larsen, T.K. Tokunaga, and Z. Zheng, pH neutralization and zonation in alkaline-saline tank waste plumes. Environ. Sci. Technol., 38, 1321–1329, 2004. Berkeley Lab Report LBNL-53646.

Wan, J., T.K. Tokunaga, J.T. Larsen, and R.J. Serne, Geochemical evolution of highly alkaline and saline tank waste plumes during seepage through vadose zone sediments. Geochim. Cosmochim. Acta, 68, 491–502, 2004. Berkeley Lab Report LBNL-55733.

ACKNOWLEDGMENTS

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

Noninvasive Geophysical Monitoring of Clay-Mineral Transformations During Simulated Iron Reduction

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RESEARCH OBJECTIVES

The importance of iron-bearing clay-sized minerals as a source of bioavailable iron is well documented. During biostimulation, reduction of such accessible ferric compounds by iron-reducing microorganisms can occur rapidly and result in the sequestration of soluble contaminants, such as uranium and chromium in insoluble phases. As the clay-sized fraction is exhausted and more recalcitrant forms of ferric iron are accessed, competition by other microbial strains can result in decreased remediation efficacy. Improved diagnostic methods are needed to elucidate the extent of microbe-induced mineral transformations over the large spatial scales encountered during field experiments.

APPROACH

The complex-resistivity method was used to monitor the effect of iron-reduction at both lab- and field-scales. The lab experiments investigated the effect of both chemical and enzymatic reduction of iron-bearing clays and clay-sized minerals on complex-resistivity signals. The field experiment used an analogous methodology to track the extent of iron reduction that occurred following acetate amendment of a shallow alluvial aquifer near Rifle, Colorado, designed to stimulate microorganisms capable of co-metabolic U(VI)-reduction.

ACCOMPLISHMENTS

Alterations in the physiochemical properties of iron-bearing clays and clay-sized minerals, resulting from both abiotic reduction and microbial respiration, led to decreases in the measured values of complex resistivity at the lab scale (Figure 1b). Reduction of structural iron led to an increase in the layer charge of the clay minerals, which resulted in structural collapse and a decrease in the specific surface area. This decrease in surface area was inferred to be the primary cause of the time-varying complex-resistivity signatures. Similar decreases in the phase response of the complex-resistivity signals were observed during the field biostimulation experiment (Figure 1a). The phase decreases corresponded in both space and time to the onset of microbial iron-reduction and reached a maximum following the cessation of active bioreduction. Mineralogical alterations in the clay-sized fraction of the aquifer sediments were believed to be responsible for the observed geophysical anomalies.

SIGNIFICANCE OF FINDINGS

Noninvasive geophysical monitoring methods have shown sensitivity to the mineralogical changes associated with iron reduction and show promise for monitoring the progress of stimulated subsurface bioremediation at field-relevant scales. Time-varying complex-resistivity anomalies correlated with the exhaustion of bioavailable iron, suggesting an approach for monitoring the sustainability of prolonged iron reduction under stimulated conditions.

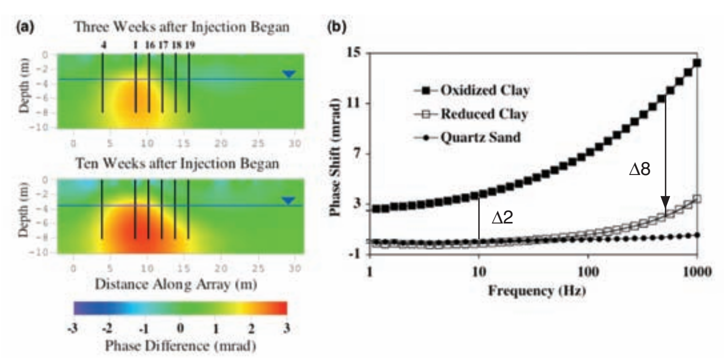

Figure 1. Variations in the complex-resistivity signatures of bioreduced clay minerals resulting from stimulated microbial activity: (a) changes in the phase response measured at the Old Rifle, Colorado, site three and ten weeks after acetate amendment–acetate injection occurred throughout the saturated zone along the location labeled 'I'; and (b) laboratory-derived phase response of oxidized and reduced versions of the same clay mineral as compared to fine quartz sand. The magnitude of the change corresponds to that observed during the field experiments.

RELATED WEBSITE

http://esd.lbl.gov/ERT/sshubbard

ACKNOWLEDGMENTS

This work was supported by the Assistant Secretary of the Office of Environmental Management, Office of Science and Technology, Environmental Management Sciences Program, of the U.S. Department of Energy under Contract No. DE-AC03-76SF00098. The clay-reduction experiments were carried out at the Environmental Molecular Sciences Laboratory, a national scientific user facility sponsored by DOE's Office of Biological and Environmental Research and located at Pacific Northwest National Laboratory, Washington.

SOURCING VADOSE ZONE AND GROUNDWATER NITRATE USING NITRATE ISOTOPES

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RESEARCH OBJECTIVES

Nitrate is one of the of the most widespread groundwater contaminants in the United States. There are a number of potential sources for nitrate contamination, including fertilizers, chemical processing, sewage, and elevated natural backgrounds. Analyses of the nitrogen ($\delta^{15}N$) and oxygen ($\delta^{18}O$) isotope ratios of the nitrate represent a powerful tool for distinguishing between different sources. Methods for analyzing the $\delta^{15}N$ and $\delta^{18}O$ values of dissolved nitrate have historically been unwieldy and time-consuming. However, recent advances using denitrifying bacteria to generate N_2O from nitrate have greatly reduced both the preparation time and sample size requirements.

We have streamlined this denitrification technique and are using it for research on the fate and transport of nitrate in the vadose zone. To date, we have applied this technique to tracking nitrate contamination associated with radioactive waste at the Hanford site in south-central Washington and identifying the sources of nitrate in the Exploratory Studies Facility at Yucca Mountain. Highlights of the work at Hanford are presented below.

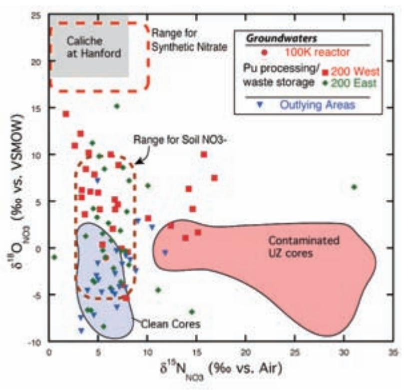

Figure 1. Plot of nitrogen versus oxygen isotope ratios of groundwater nitrate from the Hanford site in south-central Washington. Also shown is the range of values measured for unsaturated zone nitrate from clean and contaminated core samples from Hanford, and the general ranges of isotopic compositions of soil nitrate and synthetic nitric acid.

APPROACH

We modified the existing bacterial technique by increasing initial culture inoculation. We also grow the cultures on the bench top in vials used for our automated headspace sampler and reduced the venting time of the vials before injecting the sample, to decrease sample-processing time. Groundwater samples from the Hanford site were injected directly into inoculated vials. Vadose zone nitrate was extracted from cores by rinsing dried sediment with de-ionized water. The filtered rinse water, assumed to contain the nitrate originally dissolved in the pore fluids, was then injected into the inoculated vials. The vials are then loaded into the headspace sampler and analyzed using an automated trace gas pre-concentration system interfaced to a continuous-flow isotope-ratio mass spectrometer (CF-IRMS).

ACCOMPLISHMENTS

The modifications to the bacterial nitrate technique have significantly reduced sample preparation time. The use of the automated headspace sampler coupled to the CF-IRMS system has also reduced the amount of nitrate necessary per analysis. Using this method, we are able to analyze samples with nitrate concentrations as low as 0.2 mg/L. The reproducibility of the method is ±0.2‰ for $\delta^{15}N$ and ±0.3‰ for $\delta^{18}O$ (1σ).

The method has been successfully used to identify the sources of vadose zone nitrate at the Hanford site. The relationships between the vadose zone nitrate and nitrate contamination in the groundwater are summarized below.

SIGNIFICANCE OF FINDINGS

The isotopic compositions of nitrate in unsaturated zone (UZ) and groundwater samples from Hanford indicate at least four potential sources of nitrate in the groundwater. Natural sources of nitrate include microbially produced nitrate from the soil column ($\delta^{15}N$ of 4 to 8‰, $\delta^{18}O$ of -9 to 2‰) and nitrate in buried caliche layers ($\delta^{15}N$ of 0 to 8‰, $\delta^{18}O$ of -6 to 42‰). Industrial sources of nitrate include nitric acid in low-level wastewater ($\delta^{15}N$ ~0‰, $\delta^{18}O$ ~23‰) and nitrate in high-level radioactive waste from plutonium processing ($\delta^{15}N$ of 8 to 33‰, $\delta^{18}O$ of -9 to 7‰). The isotopic compositions of nitrate in 97 groundwater wells with nitrate concentrations up to 1,290 mg/L have been analyzed (Figure 1). These data indicate that the primary sources of nitrate in groundwater are nitric acid and natural nitrate flushed out of the UZ during disposal of low-level wastewater. Nitrate associated with high-level radioactive UZ contamination does not appear to be a major source of groundwater nitrate.

RELATED PUBLICATION

Singleton, M.J., K.N. Woods, M.E. Conrad, D.J. DePaolo, and P.E. Dresel, Tracking sources of unsaturated zone and groundwater nitrate contamination using nitrogen and oxygen stable isotopes at the Hanford Site, Washington. Environ. Sci. Technol., 39, 3563–3570, 2005. Berkeley Lab Report LBNL-57044.

ACKNOWLEDGMENTS

Funding for this study was provided by the Department of Energy under Contract DE-AC06-76RL01830, through the Hanford Science and Technology Program, and by the Assistant Secretary for Environmental Management, Office of Science and Technology, under the Environmental Management Science Program of the U.S. Department of Energy under Contract DE-AC03-76SF00098.

Research Program

Climate Change and Carbon Management

Margaret Torn

(With contributions from Sally Benson, James K. Bishop, Inez Fung, Norman L. Miller, Curt Oldenburg, and William J. Riley)

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The Climate Change and Carbon Management (CC&CM) program is a growing interdisciplinary research effort within ESD. The program conducts research to increase the scientific foundation for climate change prediction, impact assessment, and mitigation. In addition, program research on biogeochemical cycles and climate addresses other pressing issues under the purview of DOE and other public agencies, such as stewardship of water resources and the environmental effects of energy and land use. To that end, we have active projects on climate and hydrology, climate change, terrestrial and marine biogeochemistry, and carbon management in geologic, oceanic, and terrestrial systems.

One of CC&CM's strengths is its active partnerships with universities, industry, and other research laboratories. The most important of these is our strong partnership with UC Berkeley, which includes collaboration with faculty, sharing research facilities, teaching, advising and mentoring UC students, and interaction with the Berkeley Atmospheric Sciences Center.

RECENT ACCOMPLISHMENTS

Below we illustrate some of the recent accomplishments of CC&CM in the areas of climate studies, terrestrial carbon cycling, oceanic carbon cycling, and carbon capture and storage in geologic reservoirs.

Coupled Climate Carbon Cycle Modeling

A major concern about future climate forcing is how the current terrestrial and marine carbon sinks will respond as fossil fuel emissions increase and climate changes. ESD scientist Inez Fung and coworkers recently added interactive land and ocean carbon cycles to the global Community Climate Simulation Model (CCSM) to study how diverse features of the environment, including plants, soil, precipitation, microbes, oceans, phytoplankton, clouds, and carbon dioxide emissions interact to affect the strength of carbon sinks. They found an inverse relationship between fossil fuel emission rates and land and ocean carbon sink capacity—the faster the emission, the less effective the carbon sinks. This result implies that carbon storage by the oceans and land will lag further and further behind, and climate warming will accelerate with growing carbon dioxide emissions. Climate warming will increase the amount of carbon dioxide in the atmosphere, which in turn makes the climate even warmer, and so on. This model and nine others in a coupled climate carbon cycle model intercomparison (C4MIP) predicted large decreases in ecosystem carbon uptake (especially in the tropics) with climate change, and consequently an acceleration of warming.

Regional Climate and Water Resources

Climate Change and Carbon Management scientists contributed to the Fourth Assessment Report of the Intergovernmental Panel for Climate Change through the above work and through regional climate analysis. The Fourth Assessment Report includes CC&CM's analyses of regional climate model projections, temperature extremes, and the impacts of snowpack on water resources. CC&CM researchers quantified the range of uncertainty in the hydrologic response, finding that, regardless of emissions scenario, there are likely to be significant decreases in snowpack and available water resources in California. This finding has led CC&CM researchers to develop a new water-energy model with surface water, groundwater, and dynamic vegetation, and to apply this to a multidecade drought study. They have determined new heat extreme likelihoods based on exceedence probability analysis, and determined the intensity and persistence of these heat extremes. Correlating these results with temperature-related energy demand suggests that current energy capacity projections will likely be exceeded. Additional recent activities include a regional climate model intercomparison that evaluated California land-use change between pre-industrial and present time, multidecadal high-resolution simulation of land-surface processes with the development of scaling relationships for soil moisture, an analysis of the impact of China's Three Gorges Dam on the local climate, an analysis of the relationship between atmospheric circulation and snowpack in the western U.S., heat island effects in California's Central Valley, climate change water allocation sensitivities, and new ensemble simulations for the initialization of soil moisture and plant functional types.

Ocean Carbon Cycle

Oceans contain more carbon than any other dynamic reservoir on earth. They pose a great observational challenge because the pulses of biological productivity are episodic and rapid, and the areas are vast. Climate Change and Carbon Management scientists have developed the Carbon Explorer, an autonomous float that uses satellite telemetry to report its observations from distant oceans. Twelve of these low cost robots have achieved the equivalent of 8 years of continuous observations of particulate organic carbon variability in remote and biologically dynamic ocean regions since 2001, a data record that would not have been possible with conventional research ships. Seagoing work to prove and enhance new sensors for the Carbon Explorer is ongoing. CC&CM's new sensor for particulate inorganic carbon was operationally deployed to full ocean depth during pole-to-pole survey transects of the Atlantic Ocean in July 2003 and January 2005. The data it reported allow the first comprehensive examination of the spatial variability of particulate organic and inorganic carbon. CC&CM's optical carbon sedimentation recorder was most recently deployed in Oyshio waters near Japan.

Terrestrial and Atmospheric Carbon Cycle

One of the focal points of carbon cycle research is the vast range of scales—from a single leaf to an entire continent—that must be bridged with measurements and models. The Climate Change and Carbon Management program has implemented a coordinated suite of carbon concentration, isotope, and flux measurements in the Southern Great Plains, as part of the DOE Atmospheric Radiation Measurement (ARM) Program. Simultaneously monitoring from crop fields, tall towers, and aircraft, this facility is one of the best-instrumented site for regional carbon studies in the world. To support the North American Carbon Program, various approaches to estimating regional scale ecosystem CO_2 fluxes are under way.

The second major thrust in this area is determining terrestrial carbon residence times and storage strategies. Soils contain twice as much carbon as the atmosphere and efflux carbon at ten times the rate of fossil fuel emissions. CC&CM scientists are using ecosystem experiments and isotopic analysis to study the rates of C cycling and storage belowground. Results from this work are leading to changes in forest ecosystem models and estimates of the amount of carbon pumped belowground by root growth.

CC&CM has recently begun a new project exploring the impact of climate change on ecosystems: "An Annual Grassland Exploration of Scaling from Genomes to Ecosystem Function." This effort tests whether we can enhance our ability to predict ecosystem response to future environmental conditions by incorporating genomic, transcriptomic, and bioinformatics analysis with traditional biogeochemical and physiology approaches.

Carbon Capture and Storage

Carbon dioxide capture with storage in deep geological formations is one of the most promising options for mitigating CO_2 emissions over the next century. DOE began funding ESD research and development in 2000, to develop greater understanding of storage processes and security through the application of high-resolution monitoring tools to field-scale pilot and industrial scale projects.

CC&CM scientists are playing a leading role in WESTCARB (the West Coast Regional Sequestration Partnership). This is one of seven partnerships recently established by the DOE-Fossil Energy to evaluate CO_2 capture, transport, and sequestration technologies best suited for different regions of the country. A number of major tasks have already been completed within this partnership, including the identification of major CO_2 point sources and transportation options, an assessment of the ability for geologic sinks in the West Coast region to store CO_2, development of monitoring approaches and screening criteria for comparing storage sites, and identification of sites and industry partners for three pilot tests in California and Oregon to be conducted over the next four years.

Also, over the past year, CC&CM scientists have lead the way in designing and monitoring the first U.S. pilot test of CO_2 storage in a deep saline formation on the Texas Gulf Coast. The test involved injecting 1,600 tons of CO_2 into highly permeable sandstone 1,540 m below the ground surface. Combined seismic imaging, pressure monitoring, and fluid sampling successfully tracked migration of the injected CO_2 and demonstrated that its movement was consistent with model predictions. As part of this work, CC&CM researchers developed a novel U-tube sampler for rapid sampling of formation fluids under *in situ* pressure conditions, to monitor CO_2 arrival at the observation well. They also demonstrated the use of crosswell seismic methods to image CO_2 in the subsurface.

In addition, CC&CM began participation in a new research program on geologic CO_2 storage, the Zero-Emission Research and Technology Program (ZERT), which aims to generate the fundamental understanding necessary for predicting long-term performance of geological storage and selecting secure storage sites. For ZERT, CC&CM is developing reliable techniques to predict CO_2 migration and trapping mechanisms, demonstrating storage effectiveness, and quantifying migration out of the storage formation and release rates at the surface. A combination of laboratory, field, theoretical and simulation studies are being used to accomplish these goals.

Funding and Partnerships

The Climate Change and Carbon Management Program is funded by a variety of federal and state agencies, and international collaborations. These include the U.S. Department of Energy's Office of Basic Energy Sciences, Office of Fossil Energy, Office of Geological and Environmental Research, and Office of Biological and Environmental Research; National Aeronautics and Space Administration; National Science Foundation; National Oceanographic and Atmospheric Administration, as well as the California Energy Commission and CAL-FED.

Flow Modeling of Supercritical CO_2 Injection at the Frio Brine Pilot

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RESEARCH OBJECTIVES

Geologic sequestration of CO_2 in brine-bearing formations has been proposed as a means of reducing the atmospheric load of greenhouse gases. Numerous brine-bearing formations have been identified as having potential for geologic sequestration of CO_2. One promising setting is the fluvial/deltaic Frio formation in the upper Texas Gulf Coast, which was the site of a CO_2 sequestration pilot in October 2004. The objective of this research was to investigate the physical processes controlling the behavior of CO_2 in the subsurface during the pilot, by means of numerical modeling. Sensitivity simulations were conducted to help design the pilot, predictive simulations were used to assess our state of understanding of the issues accompanying CO_2 sequestration in brine-bearing formations, and calibration simulation results were compared to results of the pilot to improve that understanding.

APPROACH

The numerical simulator TOUGH2, developed at Berkeley Lab, is used to model the flow and transport processes occurring during the Frio Brine Pilot. TOUGH2 considers all flow and transport processes relevant for a two-phase (liquid-gas), three-component (CO_2, water, dissolved NaCl) system. In the subsurface, supercritical CO_2 forms an immiscible gas-like phase and partially dissolves in the brine. Under the pilot conditions (P = 150 bars, T = 55°C, ~100,000 ppm salinity), supercritical CO_2 is strongly buoyant compared to the native brine.

A three-dimensional numerical model of the pilot site was developed over the months preceding CO_2 injection, beginning with a simple model, and adding more detail and realism as results of site characterization studies became available. The final model consists of 23 m thick brine-saturated sand near the top of the Frio within a 900 m x 900 m partially sealed, dipping fault block. Two wells penetrate the sand, one injection well and one observation well, both of which are perforated over the upper quarter of the sand thickness.

ACCOMPLISHMENTS

Sensitivity modeling helped decide practical questions such as which of several upper Frio sands to inject into, how far apart the injection and observation wells should be (in particular showing that existing wells were too far apart, necessitating the drilling of a new injection well), how much CO_2 to inject and at what rate. Modeling of hydrologic tests helped in the design of pre-injection, site characterization pump and tracer tests to optimize the information gained on formation flow properties, *in situ* phase conditions, and fault-block boundary conditions. Predictive modeling of CO_2 movement between wells (Figure 1 and Table 1) has illustrated the complex interplay between phase interference and buoyancy flow that occurs as CO_2 is injected into a high-permeability, steeply dipping sand layer, and the ability of the model to reproduce it. By running simulations with a range of parameters and comparing model results to field data, we have greatly improved our understanding of these flow processes. Generally good agreement between observed and modeled CO_2 and tracer travel times between injection and observation wells has validated our ability to model CO_2 injection, while minor discrepancies have pointed out areas where future research is needed.

Table 1. Comparison of observed and modeled CO_2 arrivals at the observation well

	Event	Time (days)
Field	Immiscible CO_2 arrival at observation well	2.1
Model	Dissolved CO_2 arrival at observation well	2.8
	Immiscible CO_2 arrival at observation well	3.0

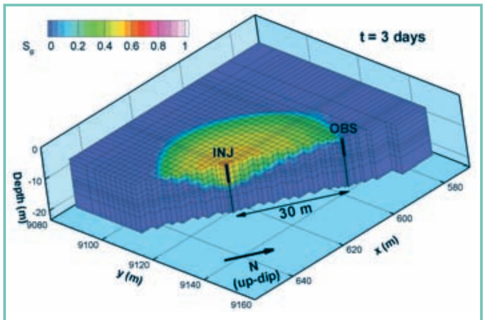

Figure 1. Modeled distribution of CO_2 in the immiscible gas-like phase after 3 days of injection at the Frio Brine Pilot, where CO_2 was injected at an average rate of 180 metric tons per day for nine days. The injection and observation wells are displayed as black lines, with the perforated intervals shown thicker.

SIGNIFICANCE OF FINDINGS

This work has demonstrated that we have a good understanding of the complex multiphase flow processes involved in CO_2 injection, as well as an effective modeling capability for designing future CO_2 injection tests and investigating CO_2 sequestration scenarios.

RELATED PUBLICATION

Doughty, C., and K. Pruess, Modeling supercritical CO_2 injection in heterogeneous porous media. Vadose Zone Journal, 3(3), 837–847, 2004. Berkeley Lab Report LBNL-52527.

RELATED WEBSITE

http://www-esd.lbl.gov/GEOSEQ/index.html

ACKNOWLEDGMENTS

This work is part of the GEO-SEQ project, which is supported by the Assistant Secretary for Fossil Energy, Office of Sequestration, Hydrogen, and Clean Fuels, through the National Energy Technology Laboratory, of the U.S. Department of Energy under Contract No. DE-AC03-76SF00098.

The U-Tube: An Innovative Method for Collecting and Analyzing Deep-Well Samples

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RESEARCH OBJECTIVES

A novel sampling system, called a "U-tube," was deployed at the Frio Project site (Dayton, Texas) to collect and analyze multiphase fluids from a 1.5 km deep well during a CO_2 injection experiment, performed on a brine-saturated reservoir. Collection of representative fluid samples from deep reservoirs is challenging, because samples undergo depressurization and can be contaminated when brought to the land surface, causing changes in fluid chemistry, physical properties, and exsolution of dissolved gases. Project-specific goals also required high-frequency sample collection to capture CO_2 breakthrough and to characterize rapidly changing brine-CO_2 saturations during injection. High-quality samples and fluid saturation measurements provide insight into geochemical and hydrologic processes affecting sequestration of greenhouse gases (including CO_2) in deep geologic formations.

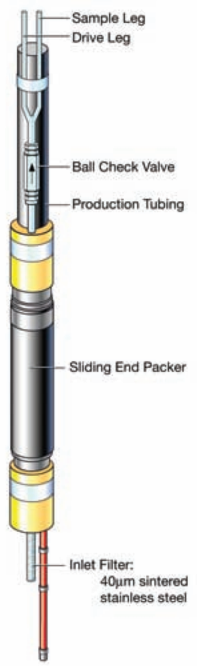

Figure 1. U-Tube sampling system

APPROACH

The U-tube sampling system consists of a continuous loop of steel tubing that starts and ends at land surface and is strapped to the outside of standard oil-field production tubing lowered into the well (Figure 1). The bottom of the U-tube is installed above the perforated production (sampling) interval and an inflatable packer. The packer isolates the interval from the upper part of the well, thus minimizing the volume purged during sample collection. A check valve connected to the bottom of the U, located immediately above the packer, controls the movement of fluid from the production interval into the U-tube. A short tube passing through the packer connects the U-tube through a filter to the production interval. The filter allows formation water to enter the U-tube, but prevents debris from clogging the valve. Operation of the U-tube is relatively simple. Compressed nitrogen gas is injected into the "drive leg" of the U-tube, closing the downhole check valve and forcing a slug of fluid to the surface via the "sample leg."

ACCOMPLISHMENTS

While the basic premise underlying the U-tube is not new, the system is unique because careful attention was given to processing the recovered two-phase samples. Strain gages mounted beneath high-pressure sample vessels at the surface measure the ratio of recovered brine to supercritical CO_2, providing gas-brine densities at reservoir conditions. A quadrupole mass spectrometer provided real-time gas analyses, allowing measurement of CO_2 and tracer breakthrough, and providing information on CO_2 saturations.

SIGNIFICANCE OF FINDINGS

Conventional approaches for deep-well sampling use submersible pumps, gas lift, or surface-based wireline samplers. Submersible pumps and gas-lift techniques can degas and/or contaminate samples, thus compromising fluid chemistry and promoting phase separation. Wireline samplers take small, discrete, infrequent samples that have the potential to miss CO_2 breakthrough. In comparison, the U-tube sampling system can be used to collect frequent, representative samples at reservoir conditions. In addition, it easily incorporates other program elements into its design, including bottomhole pressure and temperature measurements, and wireline logging through the center production tube.

RELATED PUBLICATIONS

Freifeld, B.M., C.A. Doughty, R.C. Trautz, S. Hovorka, L.R. Myer, and S.M. Benson, The Frio Brine Pilot CO_2 Sequestration Test—Comparison of field data and predicted results. Chapman Conference on the Science and Technology of Carbon Sequestration, San Diego, California, January 16–20, 2005. Berkeley Lab Report LBNL-56649.

ACKNOWLEDGMENTS

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

Coupling of CLM3 into MM5 to Improve Snow and Dynamic Vegetation Processes

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RESEARCH OBJECTIVES

The Pennsylvania State University/National Center for Atmospheric Research (Penn State/ NCAR) fifth-generation Mesoscale Model (MM5) has been extensively used for regional weather and climate forecasts as well as research for more than ten years. However, the snow schemes in this model are unable to produce realistic simulations for the winter and spring periods because of oversimplified snow physics (Jin and Miller, 2005a). Additionally, the prescribed vegetation parameters, such as leaf area index, significantly weaken the model's ability to predict future climate and weather. In this study, the advanced NCAR Community Land Model version 3 (CLM3), with its sophisticated snow and dynamic vegetation schemes, is incorporated into MM5 to improve its forecast and simulation capability.

APPROACH

The nonhydrostatic version of MM5 is used in this study, with the Grell convection scheme adopted to parameterize cumulus clouds and the Medium Range Forecast planetary-boundary-layer scheme applied to solve boundary-layer processes. CLM3 physically describes the mass and heat transfer within the snowpack, using five snow layers that include liquid water and solid ice. Interactions among the snow, soil, and vegetation are a function of the CLM3 mass and energy equations. A sophisticated surface albedo scheme is chosen to improve the surface energy-balance simulations. Introduction of a maximum of eight subcells within each CLM3 cell strengthens the description of land-surface heterogeneity. The vegetation is dynamically generated under soil and atmospheric conditions favoring vegetation respiration and photosynthesis processes.

The coupled MM5-CLM3 was used to generate two-way, 60-km-to-20-km-resolution nested simulations. The 20 km simulation is the focus of the present analysis. The National Centers for Environmental Prediction (NCEP) Reanalysis data was used as MM5-CLM3 initial and 6-hourly-updated lateral-boundary conditions for the period of March 1 to May 31, 2002, and the model output was saved every six hours. The MM5-CLM3 performance was evaluated at the Columbia River basin for the cold season, using ground observations from an automated Snowpack Telemetry (SNOTEL) system. The SNOTEL data includes snow-water equivalent and surface air temperature.

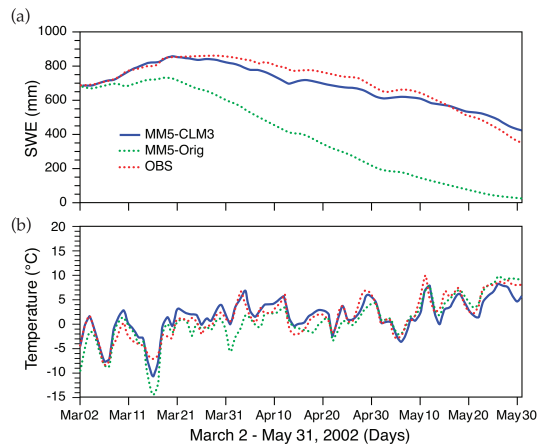

Figure 1. Comparison of simulated and observed (a) SWEs and (b) temperatures averaged over 50 SNOTEL stations in the Columbia River basin for the period of March 2 through May 3, 2002.

ACCOMPLISHMENTS

Compared with the original version of MM5, the coupled MM5-CLM3 significantly improves snow and surface temperature simulations. Figure 1a shows the time series of snow-water equivalent (SWE) averaged over 50 SNOTEL stations in the Columbia River basin. The SWEs produced by MM5-CLM3 are in very good agreement with the observations, as a result of sophisticated snow physics and related model processes, while the SWEs from the original MM5 with simple snow processes are greatly underestimated. The 50-station averaged temperatures from MM5-CLM3 are also consistent with observations, but the original MM5 produces cold biases during the early simulation period, caused by the large amount of energy consumed by the faster snow melt.

SIGNIFICANCE OF FINDINGS

The coupled MM5 and CLM3 model significantly improves snow and surface air-temperature simulations. The evaluation of the dynamic vegetation scheme, using our ensemble techniques, are part of our current work and will be reported in the near future. This coupled model increases the predictability of the regional climate model and provides a reliable tool for regional weather and climate research.

RELATED PUBLICATIONS

Jin, J., and N.L. Miller, An analysis of climate variability and snowmelt mechanisms in mountainous regions. Journal of Hydrometeorology (in press), 2005a. Berkeley Lab Report LBNL-53845.

Jin, J., and N.L. Miller, Coupling of CLM3 into MM5 to improve snow simulation and dynamic vegetation processes. Journal of Hydrometeorology (submitted), 2005b.

ACKNOWLEDGMENTS

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

Relationship Between Atmospheric Circulation and Snowpack in the Western United States

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RESEARCH OBJECTIVES

Snow anomalies in the western United States (WUS) have been widely investigated by many researchers because of their significant impact on water availability. This previous research indicated that the ocean has a dominant effect on snow variation in the WUS and contributes to more than 60% of the variance in snow anomalies. This study investigates those findings, focusing on the snow variations in the WUS resulting from anomalous atmospheric circulation, attributed to both atmospheric internal variability and tropical Pacific sea surface temperature (SST) forcing.

APPROACH

In this study, the observed Snow Water Equivalent (SWE) data in the WUS was obtained from snow course data collected manually by the U.S. Department of Agriculture (USDA) cooperative snow survey program and the California Department of Water Resources. The April 1 SWE maximum for 1950–1997 is the focus of this analysis. The observed tropical Pacific SST was averaged for December to February (DJF) to identify winter season El Niño-Southern Oscillation (ENSO) events. When the average SST is above 1°C, below -1°C, or between -1°C and 1°C, the ENSO event is defined as "warm," "cold," or "neutral," respectively. For 1950–1997, there are 8 warm, 6 cold, and 33 neutral winters. The Pacific/North American (PNA) index indicates the 500 mb geopotential height anomalies. PNA indices for DJF are averaged to identify winter PNA patterns. When the DJF-average PNA index is above 0.5, the corresponding atmospheric pattern is defined as the "positive PNA pattern"; when it is below -0.5, the atmospheric pattern is defined as the "negative PNA pattern." There are 9 positive and 6 negative PNA patterns for the 33 neutral winters.

ACCOMPLISHMENTS

Table 1 provides the quantitative comparison of SWE, temperature, and precipitation anomalies during the ENSO episodes and under the PNA circulation patterns, which represent the ocean and atmospheric internal variability influences, respectively. The numbers for the SWE anomaly in Table 1 are the averages of those SWEs passing the 95% significance test in the northwest and southwest, and the numbers for temperature and precipitation anomalies are the averages over the corresponding snow-course stations in the same regions. Table 1 shows that the warm ENSO generates a significant positive SWE anomaly in the southwest (55.2 mm), but has a weaker impact on the northwest SWE (-3.7 mm). The cold ENSO produces a strong positive SWE anomaly in the northwest (117.8 mm), but has a mild effect on the southwest SWE (-21.5 mm). Under the positive PNA pattern without oceanic forcing, the entire WUS has negative SWE anomalies (-80.2 mm in the northwest and -71.2 mm in the southwest), while under the negative PNA pattern, the WUS has positive SWE anomalies (73.1 mm in the northwest and 88.8 mm in the southwest). Table 1 also indicates that the positive SWE anomaly results from the stronger precipitation and colder temperature, whereas the negative SWE anomaly is caused by weaker precipitation and warmer temperature. The empirical orthagonal function (EOF) analysis further shows that the PNA patterns contribute to 39% of the total SWE variance, and the ENSO episodes account for only 18%, indicating that the atmospheric internal variability has a dominant impact on the SWE variations in the WUS.

Regions / Events	Northwest			Southwest		
	SWE(mm)	P(mm)	T(°C)	SWE(mm)	P(mm)	T(°C)
Warm ENSO	-21.5	-11.0	0.52	55.2	32.7	-0.14
Cold ENSO	117.8	44.7	-0.81	-3.7	-3.1	-0.28
Positive PNA	-80.2	-22.6	0.77	-71.2	-27.2	0.69
Negative PNA	73.1	20.5	-1.09	88.8	26.6	-0.56

Table 1. SWE, temperature, and precipitation anomalies averaged over the snow course stations, where the SWEs pass the 95% Student's *t* test (P is precipitation and T is temperature)

SIGNIFICANCE OF FINDINGS

Our study shows that the oceanic impact on WUS snow is likely overestimated, and that atmospheric internal variability also plays an important role in WUS snow volume. This study provides significant insight into forecasts of winter and spring snow mass in the WUS, where snow is the major water resource.

RELATED PUBLICATIONS

Jin, J., N.L. Miller, S. Sorooshian, and X. Gao, Relationship between atmospheric circulation and snowpack in the western United States. Hydrological Processes (in press), 2005. Berkeley Lab Report LBNL-55404.

ACKNOWLEDGMENTS

Support was provided by the California Energy Commission Climate Change Program.

Development of a Coupled Land Surface and Groundwater Model

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RESEARCH OBJECTIVES

Land-Surface Models (LSM), used for numerical weather simulation, climate projection, and as inputs to water management decisions, do not treat the LSM lower boundary in a fully process-based fashion. This lower boundary is often assumed to be zero flux, or the soil moisture content is set to a constant—an approach that while mass conservative, ignores processes that alter surface fluxes and water quantity and quality. Conversely, groundwater models (GWM) for saturated and unsaturated flow often have overly simplified upper-boundary conditions that ignore soil heating, runoff, snow, and root-zone uptake. The objectives of this study are to indicate a new approach and methodology for coupling a state-of-the-art CLM (Common Land Model) and a variably saturated GWM (ParFlow), and to replicate this study for CLM and the Berkeley Lab Earth Sciences Division GWM, TOUGH2.

APPROACH

The water-balance equations represent the link between the LSM and the GWM. The CLM and ParFlow models were coupled at the land surface and soil column by replacing the soil column/root zone soil moisture formulation in CLM with the ParFlow formulation. All processes within CLM, except for those that predict soil moisture, are preserved within the original CLM equations.

The coupled model, CLM.PF, communicates over the 10 soil layers in CLM, with the uppermost cell layer in ParFlow. Soil saturation is calculated from the hydraulic pressure solution over the entire domain, with the water content at the upper ten layers passed back to CLM, where soil surface temperatures, heat fluxes, and energy balances are calculated.

ACCOMPLISHMENTS

Simulations for both the coupled (CLM.PF) and uncoupled (CLM) models are compared to the Usad Watershed observations. The simulations of sensible heat flux and evapotranspiration for the coupled and uncoupled models agree closely. However, the runoff rates are more accurately simulated by the coupled model, with the uncoupled model tending to underestimate the observed flow rate. The differences in runoff result from the explicit simulation of the water table (WT) in the coupled model.

The three plots of soil saturation provide insight into the differences in model simulation and agreement with observations. Shallow simulations (20 cm) show that soil saturation for the coupled and uncoupled models are very similar, particularly during the summer months. This corresponds to the similarities in the simulated evapotranspiration between the two models. Deeper simulations of soil saturation (40 cm and greater) are quite different; with the coupled model agreeing well with observations (see Figure 1). CLM.PF stores water in the subsurface, and includes a memory effect on model behavior that extends beyond seasonal time cycles. This effect can be seen in the figure, where WT storage and soil moisture memory affect other modeled processes.

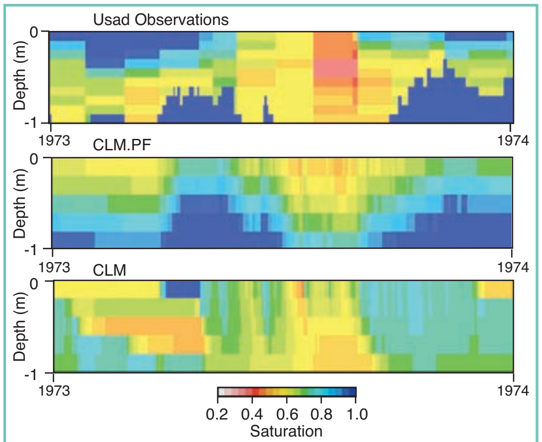

Figure 1. Plot of observed and simulated soil saturations for Valdai as a function of time and depth for 1973. Average soil moisture observations for the Usad catchment are plotted in the first panel, with CLM.PF model simulations in the middle and CLM simulations at the bottom. Note that only the first 1 m of model simulations are plotted to match the observations. Note also that the solid blue regions denote completely saturated conditions where the WT depth is less than one meter.

SIGNIFICANCE OF FINDINGS

CLM.PF behaves much differently from CLM and expands the capabilities of the groundwater model to include land surface processes. CLM.PF provides simulations of the subsurface, which, because of the explicit accounting for water up to and below the WT, have a memory of water stored in the deep subsurface. The simulations presented here show that this scheme balances mass across the land surface/groundwater boundary and provides new insights into coupled processes. The coupled model also has a different depiction of the root-zone soil moisture than the uncoupled model, leading to more realistic behavior that more closely matches observations at the Usad site. The coupled model demonstrates the need for better groundwater representation in land surface schemes. This study has been duplicated for CLM and TOUGH2 with similar results, and we expect to use this for new applications.

RELATED PUBLICATION

Maxwell, R.M., and N.L. Miller, Development of a coupled land surface and groundwater model. Journal of Hydrometeorology, 6 (3), 233–247, 2005. Berkeley Lab Report LBNL-55029.

ACKNOWLEDGMENTS

This work was conducted under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract No. W-7405-Eng-48, and Berkeley Lab under the DOE Fossil Energy Environmental Program, Contract No. DE-AC03-76F00098.

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

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[1]Oak Ridge National Laboratory, [2]Brookhaven National Laboratory, [3]Los Alamos National Laboratory, [4]Argonne National Laboratory
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RESEARCH OBJECTIVES

The DOE Water Cycle Pilot Study represents a successful multi-laboratory investigation to better understand water cycle variability—by evaluating DOE climate models, developing water isotopic data to constrain such climate models, and to test process descriptions and their sensitivity at multiple scales. The research objectives are to: (1) evaluate predictions of components of the water budget, using a set of nested models with different spatial resolutions, along with archived and new field data from the Walnut River Watershed (WRW); (2) evaluate multiscale water isotope modeling as a means of tracing sources and sinks within and external to the WRW and the Atmospheric and Radiation Measurements Program-Southern Great Plains (ARM SGP) site; (3) identify water-budget-model improvements and data needs over a range of scales. The DOE Water Cycle Pilot was funded for two years by DOE's Office of Basic Energy Research (BER), and resulted in several follow-on studies, including a paper by Sharif et al. (2005) on a 51-year simulation and derivation of scaling relationships for the Red-Arkansas River Basin.

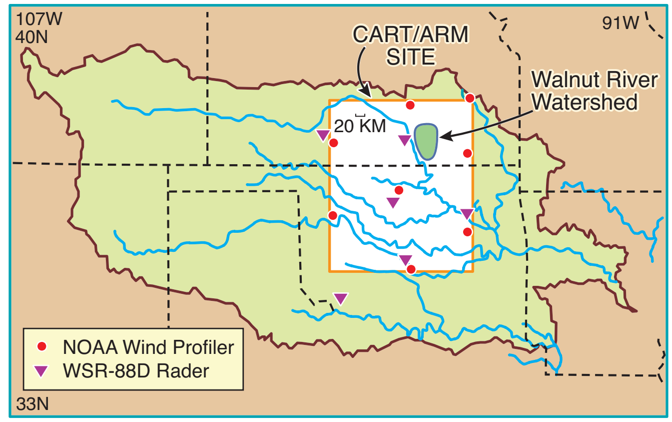

Figure 1. The ARM/CART Southern Great Plains Site within the Red-Arkansas River Basin

APPROACH

Water isotopic measurements of precipitation, surface water, soils, plants, and atmospheric water vapor were collected every three months and during the DOE Intensive Observing Period, April 1 to June 30, 2002. Land-surface modeling compared 1 km fluxes for different modes and for a 51-year simulation. Different wetting and drying conditions caused by different controls were investigated. Multi-scale atmospheric simulations using the MM5 and radar-based data have been analyzed and are discussed below (Miller et al., 2005).

ACCOMPLISHMENTS

It was shown that isotopic sampling of rivers and lakes provides a good long-term average of precipitation patterns and helps to validate water cycle simulations in regional climate models, such as MM5. Analysis of the simulated MM5 6-hour precipitation and radar-derived precipitation has indicated that MM5 slightly underestimates at a 4 km resolution and lags behind the radar-precipitation onset. MM5 exhibits strong capabilities in predicting precipitation occurrences, with somewhat less accuracy in predicting precipitation amounts.

The TOPLATS land surface model was evaluated for a number of scenarios, resolutions, and periods. Eleven simulations were performed with different modes, with several variations in the representations of spatial variability of precipitation, land use, topography, and soils—to assess the sensitivity of the model response. Model results suggest that in parts of the catchment, evapotranspiration switched between being atmospherically controlled to soil-moisture controlled.

SIGNIFICANCE OF FINDINGS

The DOE WaterCycle Pilot Study resulted in a number of findings that are highlighted in Miller et al. (2005b). One key finding is the MM5 analysis indicating that simulations at 12 km resolution are more accurate than at 4 km, because of the scale-dependent parameterizations. Another key finding is the TOPLATS simulations indicating that a low parameter semi-distributed simulation replicates a high-parameter, fully distributed simulation with fair to good accuracy.

RELATED PUBLICATIONS

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Sharif, H. O., W. T. Crow, N. L. Miller, and E. F. Wood, Multi-decadal high-resolution land surface modeling study in the Southern Great Plains. J. of Hydrometeorology (submitted), 2005.

ACKNOWLEDGMENTS

This work was supported by the Director, Office of Science, Office of Biological and Environmental Research, Climate Change Research Division, of the U.S. Department of Energy under Contract No. DE-AC03-76SF00098.

New Emission Scenarios and California Climate Impacts: An Analysis of Extreme Heat

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RESEARCH OBJECTIVES

Two global climate models, the low-sensitivity NCAR/DOE Parallel Climate Model and the medium-sensitivity UK Met Office HadCM3 model, were used to calculate climate change resulting from the B1 (lower) and A1fi (higher) emissions scenarios. These scenarios bracket a large part of the range of Intergovernmental Panel on Climate Control (IPCC) nonintervention emissions futures, with atmospheric concentrations of CO_2 reaching ~550 ppm (B1) and ~970 ppm (A1fi) by 2100. The objectives of this Extreme Heat Analysis component of the larger study (Hayhoe et al., 2004) is to quantify the change in likelihoods of extreme heat days for urban population centers, for the higher and lower emission scenarios of 2045–2054 and 2090–2099, compared to the reference period 1989–1998.

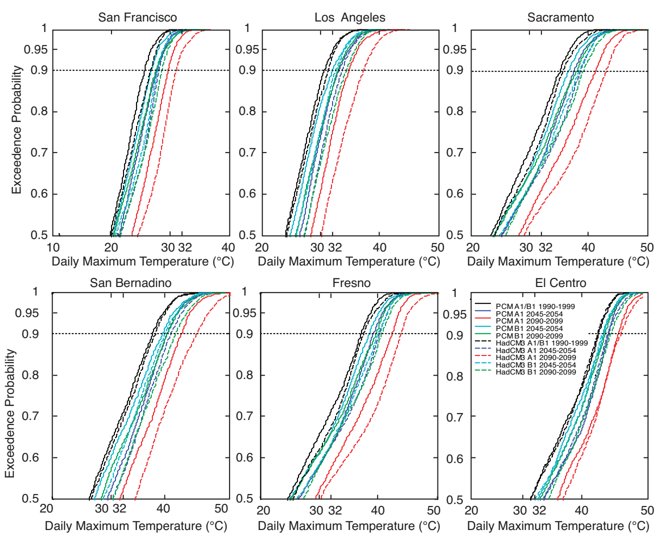

Figure 1. Temperature exceedance probabilities for PCM (dashed) and HadCM3 (solid) projections under emission scenarios A1fi (Red) and B1 (Green) for 2090–2099 for San Francisco, Los Angeles, Sacramento, San Bernadino, Fresno, and El Centro

APPROACH

Changes in local temperature extremes were evaluated based on calculated exceedance probability (EP) analyses, using the distribution of daily maximum temperatures downscaled to representative locations and ranked. Exceedance probabilities define a given temperature for which the probability exists that X% of days throughout the year will fall below that temperature. Conversely, there is a probability that (100-X)% days will lie above that threshold. For example, if the 35°C EP averages 95% for 2070–2099, an average of 95% or ~347 days per year lie below 35°C. Exceedance probabilities of daily time series have been used to indicate the likelihood of occurrence of temperature, precipitation, and runoff (Miller et al., 2003).

ACCOMPLISHMENTS

The maximum daily temperature (Tx) EP at San Francisco, Los Angeles, Sacramento, San Bernadino, Fresno, and El Centro for emission scenarios A1fi and B1, using PCM and HadCM3, are shown in Figure 1. The 2090–2099 50% and 95% Tx EPs for San Francisco increase by more than 7°C for the HadCM3 A1FI scenario, and 6°C for the PCM A1FI scenario. The 1990–1999 baseline 95% EP becomes 58% and 70% for HadCM3 and PCM A1FI, and 86% and 78% for B1, respectively. Such shifts indicate that San Francisco's historic 5% warmest days may occur as frequently as 30–42% of the year for A1FI and 14-22% for B1, by the end of this century.

Los Angeles has a more dramatic shift. In the 2090–2099 HadCM3 and PCM B1 projections under the A1fi emission scenario, the heat threshold is exceeded by 35% and 22%, respectively. (See Figure 1). The lengthening of future heat-wave seasons results primarily from earlier onset, with the season beginning 25–40 days earlier under B1, and twice that (50–80 days earlier) under the A1fi scenario. Under A1fi, 49–83 more heat-wave days are seen, which represents an increase of ~20–30 more days than under the B1 scenario.

SIGNIFICANCE OF FINDINGS

The significance of this extreme heat analysis is the well-established link between extreme heat and excess summer mortality. A simple temperature threshold approach without acclimatization suggests that heat mortality in Los Angeles may increase by 2–4 times under B1 and 6–10 times under A1fi by the 2090s. With acclimatization, these estimates are 15–20% lower. Individuals likely to be most affected include the elderly, children, economically disadvantaged, and already ill.

RELATED PUBLICATIONS

Hayhoe, K, D. Cayan, C.B. Field, P.C. Frumhoff, E.P. Maurer, N.L. Miller, S.C. Moser, S.H. Schneider and others, Emissions Pathways, Climate Change, and Impacts on California. Proc. Nat'l Acad. Sci., 101, 12422–12427, 2004. Berkeley Lab Report LBNL-56119.

Miller, N.L., K.E. Bashford, and E. Strem: Potential impacts of climate change on California hydrology. J. Amer. Water Resourc. Assoc, 39, 771–784. 2003. Berkeley Lab Report LBNL-51313.

ACKNOWLEDGMENTS

This work was supported by the California Energy Commission's Climate Change Program.

The California Water and Energy System: An Approach for Addressing Future Crises

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RESEARCH OBJECTIVES

The purpose of this fundamental-climate-science, applied-hydrology and economics project is to better understand how natural processes and human intervention interact to influence California's water supply, and the sensitivity of this system to potential disruptions.

Our research objectives are to: (1) quantify the climate drivers impacting mountain front recharge, snowmelt runoff, and net infiltration in the Sierra Nevada and Central Valley; (2) investigate the sensitivity of the water table to these inputs and to pumping withdrawals; (3) adapt existing geophysical logging and monitoring techniques for characterizing the depth distribution of groundwater contaminants; and (4) develop a regional resource management model to demonstrate economic tradeoffs between agricultural and environmental groundwater pumping, incorporating long-term aquifer degradation.

APPROACH

Our research team brings together hydroclimate science, water resources engineering, and economic analyses through drought-sensitivity simulations, groundwater-surface water response studies—at both Central Valley and Merced Basin scales—and studies of the economic impact associated with water supply limitations. Three integrated studies representing climate science, water resources, and economics are merged, resulting in a new type of multidisciplinary analysis. A schematic of this approach is given in Figure 1.

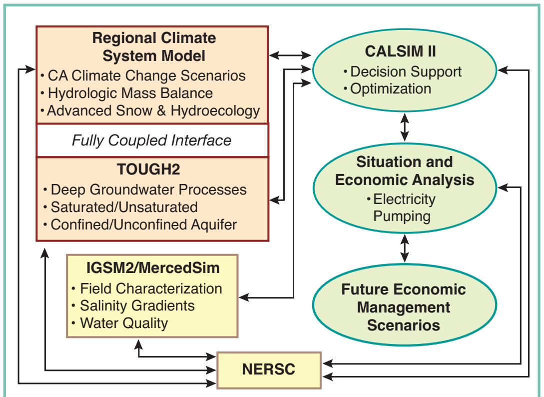

Figure 1. Flow chart of connections between project components: Scientific research to simulate projected California climate change impacts, as well as to understand the hydrologic mass balance and related snow and ecohydrologic processes (upper left box), is fully coupled to a dynamic groundwater model with saturated/unsaturated and confined/unconfined aquifers (middle left box). Comparison and improvements on the CDWR Integrated Ground Surface Model, modified for the Merced River Basin field research to characterize the subsurface water and salinity profiles (lower left box).

ACCOMPLISHMENTS

Our water-energy system project accomplishments have advanced around three interrelated components. The first component involved coupling climate, land surface, and groundwater models to simulate the water flux and balance. Research focused on the new coupling, testing, and simulations of the LBNL Regional Climate System Model with a state-of-the-art land-surface/shallow subsurface model (NCAR Community Land Model version 3: CLM3), an advanced groundwater-surface water coupling with CLM and the Berkeley Lab Earth Sciences Division (ESD) TOUGH2 code, and a 104-year atmospheric-land surface simulation with a 25-year drought simulation for the Merced River Basin Transect. The second component of our work includes salinity with depth characterization at four wetlands sites with difficult-to-access well casings, using an advanced ESD geophysical logging approach. This data has been prepared to calibrate our surface-groundwater code for the Merced Basin.

The third component includes the development of economic models for the value of water supply reliability and the value of groundwater-surface water storage. The water supply reliability model has been calibrated using regional water-source and land value data. A conceptual version of water storage model has been developed using data from the Merced Basin.

SIGNIFICANCE OF FINDINGS

The success of our water-energy system has resulted in a California Energy Commission (CEC) grant for significantly more comprehensive advances in our climate, water, and pricing models, as well as new analyses. This project has resulted in the synthesis of hydrological simulations and economic analysis, representing a new approach for guiding water management under climate change.

RELATED PUBLICATIONS

Brekke, L.N., N.L. Miller, K.E. Bashford, N.W.T. Quinn, and J.H. Dracup, 2004: Climate Change Impacts Uncertainty for the San Joaquin River Basin. J. Amer. Water Resources Assoc. 40, 149-164.

ACKNOWLEDGMENTS

This work was supported by Laboratory Directed Research and Development (LDRD) funding from Berkeley Lab, provided by the Director, Office of Science, of the U.S. Department of Energy under Contract No. DE-AC03-76SF00098. We thank the California Energy Commission and California Department of Water Resources (CDWR) for working with us on advancing this research and developing a new drought response scenario for California policy makers.

Analyzing the Impact of the Three Gorges Dam on Local Climate

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RESEARCH OBJECTIVES

The Three Gorges Dam (TGD), on the Yangtze River in China, represents the world's largest man-made reservoir, with a hydroelectric potential of 84.7 billion kilowatt hours and flood reduction in low-lying regions downstream. By 2009, the TGD is expected to fill the projected 39.3 billion m^3 storage capacity. The submerged 663 km length of the Yangtze River will have a 1,040 km^2 wet surface area, representing a significant land-use change in topography and evaporation, which in turn is expected to cause changes in regional weather and climate patterns. Previous studies suggest that the annual average near-surface air temperature in the vicinity of the TDG will increase by 0.3°C. However, the impact on local climate resulting from the change in surface area and weather patterns has not been systematically quantified and is not fully understood.

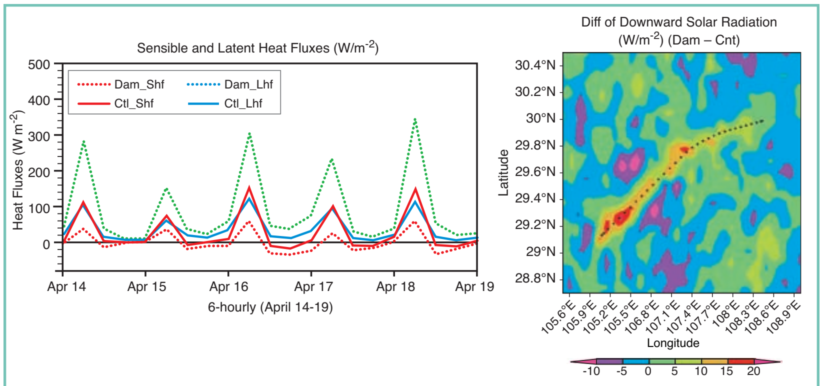

Figure 1. MM5 simulations for April 2–May 16, 1990, indicating (a) a 2 m air temperature, and (b) the difference in downward solar radiation with and without the presence of TGD, which showed a net increase of 10–25 W/m^2 along the Yangtze River Valley area.

The objectives of this sensitivity study are to determine the changes in surface characteristics within the TGD area, from one of steep, vegetated terrain to a large, flat saturated surface, with a potential evaporating rate. We investigate changes in local circulation and moisture patterns and seek to quantify the relative change in temperature, precipitation, and energy fluxes using a regional atmospheric model coupled to a land-surface model.

APPROACH

Simulations were conducted and results analyzed for the period April 2–May 16, 1990, using the nonhydrostatic version of the Penn State/National Center for Atmospheric Research (NCAR) Mesoscale Model Version 5 (MM5) coupled with the Community Land Model Version 2 (CLM2).

ACCOMPLISHMENTS

Initial analyses suggest that increased surface evaporation leads to a colder surface with decreased sensible heat flux (Figure 1a), which further cools the atmospheric column, producing stronger downdrafts of air mass and dissipation of clouds. The reduction in clouds in turn causes an increase in solar radiation (Figure 1b), countering the decrease in surface temperature. However, the increase in descending air mass appears to divert atmospheric moisture out of the region in the lower troposphere, which tends to reduce any precipitation enhancement resulting from the intensified surface evaporation.

SIGNIFICANCE OF FINDINGS

This preliminary examination of the mechanisms associated with local climate change in the TGD region suggests a more comprehensive study, using a fine-scale mesoscale (1 km resolution) simulation for periods up to several years, and a further analysis utilizing remote-sensed observation. The full manuscript to this initial study has been published in *Geophysical Review Letters* (Miller et al., 2005), and a second-phase, more comprehensive analysis is currently being completed by the authors of this study.

REFERENCES

Miller, N.L., J. Jin, and C.-F. Tsang, Local climate sensitivity of the Three Gorges Dam. Geophysical Review Letters 32, L16704, doi:10.1029/2005GRL02821, 2005. Berkeley Lab Report LBNL-58249.

ACKNOWLEDGMENTS

This work was supported by the Director, Office of Science, Office of Biological and Environmental Research, Climate Change Research Division, of the U.S. Department of Energy under Contract No. DE-AC03-76SF00098.

West Coast Regional Carbon Sequestration Partnership

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RESEARCH OBJECTIVES

The goal of the West Coast Regional Carbon Sequestration Partnership (WESTCARB) is to address several key issues that impact the development of practical, commercially ready sequestration technologies. WESTCARB is one of seven partnerships established by the DOE to evaluate carbon dioxide capture, transport, and sequestration (CCS) technologies best suited for different regions of the country. WESTCARB is evaluating both terrestrial and geologic sequestration options for the region comprising Arizona, California, Nevada, Oregon, Washington, Alaska, and British Columbia.

APPROACH

WESTCARB is carrying out five major tasks: (1) collecting data to characterize major CO_2 point sources, the transportation options, and the terrestrial and geologic sinks in the region; (2) addressing key issues affecting deployment of CCS technologies; (3) conducting public outreach and education work; (4) integrating and analyzing data to develop supply curves and cost-effective sequestration options; and (5) identifying appropriate terrestrial and geologic demonstration projects in the region. WESTCARB has assembled a diverse consortium of nearly 50 participants, including state natural resource, environmental protection, and other agencies; national labs and universities; private companies working on CO_2 capture, transportation, and storage technologies; nonprofit organizations; commercial users of CO_2, such as the oil and gas industry; policy/governance coordinating organizations; and others.

ACCOMPLISHMENTS

Data on 81 major point sources, which account for more than 75% of the CO_2 emissions in the region, have been compiled and organized into a geographic information system (GIS) database, which is maintained at the Utah Advanced Geographic Reference Center. The WESTCARB geologic sink GIS database contains data on the significant sedimentary basins in the region. In California, screening of 104 sedimentary basins excluded 77 on the basis of insufficient depth (<800 m), lack of seals, or lack of access. The estimate of the storage capacity of saline formations in the ten largest remaining basins ranged from 146 to 840 Gt CO_2, depending on assumptions about what fraction of the formations is used, what fraction of the pore volume is filled with separate-phase CO_2, and salinity. The amount of CO_2 that could be stored in oil reservoirs associated with EOR was found to be 3.4 Gt. If existing plants are retrofitted for capture, about 50 M tons of CO_2 per year could be sequestered for $35 per ton CO_2 avoided.

Terrestrial sequestration studies are using GIS databases to characterize the carbon baseline in the region and to develop supply curves for major classes of land use. Analysis of changes in carbon stocks in California for the decade of the 1990s revealed that forests and rangelands were responsible for a net removal of carbon dioxide from the atmosphere of 7.55 $MMTCO_2eq/yr$, and that agricultural lands were responsible for a net emission of 0.35 $MMTCO_2eq/yr$. In California, it was found that rangeland conversion yielded the greatest carbon benefits. For an afforestation project of 80 years duration, it was found that 5.6 GT of carbon could be stored at less than $50/MT C, involving an area of about 21 million acres.

Storage site permitting, monitoring, and injection regulations, as well as health, safety, and environmental (HSE) risks, are key issues affecting the deployment of geologic sequestration technologies. A screening-level risk assessment tool has been developed to help select sites with minimum HSE risk. The regulatory framework in each state has been defined as a first step in addressing regulatory issues. These issues are also being addressed through public outreach efforts.

SIGNIFICANCE OF FINDINGS

Though analyses are continuing in several WETCARB states, results to date show that significant sequestration opportunities are available in the region. In California, the Central Valley, alone, has capacity for several hundred years of CO_2 emissions from utilities. Because of its capacity, and the presence of oil and gas reservoirs, the Central Valley also is favored as a location for field pilot studies. Terrestrial sequestration opportunities have been identified in afforestation and forest fire mitigation. Though smaller in magnitude than the geologic opportunities, the terrestrial opportunities are much less expensive.

ACKNOWLEDGMENTS

This work was supported by the Assistant Secretary for Fossil Energy, Office of Coal and Power Systems, of the U. S. Department of Energy through the National Energy Technology Laboratory, under DOE Cooperative Agreement No. DE-FC26-03NT41984, and DOE Contract No. DE-AC03-76SF00098, and by the California Energy Commission through Work Authorization Contract #500-02-014, Work Authorization #MR-021, and Interagency Agreement 500-03-018.

Screening and Ranking Framework for Geologic CO_2 Storage

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RESEARCH OBJECTIVES

The injection of CO_2 into deep geologic formations for geologic CO_2 storage involves the risk that CO_2 will leak from the target formation to the near-surface environment. Once in the near-surface environment, CO_2 can cause detrimental health, safety, and environmental (HSE) effects. One consideration in the selection of geologic CO_2 storage sites is the minimization of potential HSE risks. The objective of this work is to develop a screening and ranking framework (SRF) to evaluate the relative risk that CO_2 will leak to the near-surface environment and cause HSE effects. The SRF is designed so that it can be applied to sites with limited data as appropriate for pilot studies. The expected users of the SRF are geoscientists or hydrologists with access to limited published information about the site in reference books or maps. In short, the framework is designed to answer the question, "From a choice of several potential sites, which site has the lowest HSE risk?"

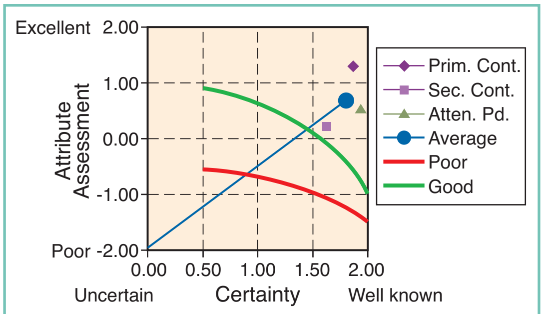

Figure 1. Summary graphic showing the attribute assessment (y-axis) and uncertainty (x-axis) of the three fundamental characteristics along with qualitative regions of "poor," "fair," and "good" HSE risk for the Rio Vista gas field

APPROACH

The approach stems from the realization that HSE risk is related to three fundamental characteristics of a geologic carbon storage site:

1. Potential of the target formation for long-term containment of CO_2
2. Potential for secondary containment, should the primary target site leak
3. Potential of the site to attenuate and/or disperse leaking CO_2, should the primary formation leak and secondary containment fail

The SRF tool is designed to provide a qualitative and independent assessment of each of these three characteristics, through a numerical evaluation of properties/values associated with various attributes of the three general characteristics. For example, three attributes of the potential for the target formation to contain CO_2 for long periods are (1) the nature of the primary seal, (2) the depth of the reservoir, and (3) the properties of the reservoir. The properties of the primary seal attribute are thickness, lithology, demonstrated sealing capacity, and lateral continuity. Similar properties for all of the other attributes are listed in the spreadsheet. The user simply assigns numerical values to these attributes, based on suggestions in the spreadsheet. In addition, the user must assign weights and uncertainties to the properties, which are carried along to the final display. The results are summarized and displayed graphically in the summary worksheet, one graphic from which is shown in Figure 1.

ACCOMPLISHMENTS

An HSE screening and ranking framework has been developed, based on the three fundamental characteristics of a CO_2 sequestration site. The system allows the user to arbitrarily weight and assign uncertainty to the properties associated with the attributes of the fundamental characteristics, to evaluate and rank two or more sites relative to each other. We emphasize that the SRF tool is intended to guide the selection of the most promising sites, for which more detailed risk assessment would be carried out. Testing and further development of the SR framework are under way.

SIGNIFICANCE OF FINDINGS

The SRF shows that comparative evaluations of prospective sites with limited characterization data can be accomplished, and that the ranking offers a way of screening sites based on potential for CO_2 leakage and seepage, as well as related HSE risk.

RELATED PUBLICATION

Oldenburg, C.M., HSE screening risk assessment (SRA) for geologic CO_2 sequestration. Fourth Annual Conference on Carbon Capture and Sequestration, Alexandria, Virginia, May 2–5, 2005. Berkeley Lab Report LBNL-57280.

ACKNOWLEDGMENTS

This work was supported in part by WESTCARB through the Assistant Secretary for Fossil Energy, Office of Coal and Power Systems, through the National Energy Technologies Laboratory (NETL), and Lawrence Berkeley National Laboratory, under Department of Energy Contract No. DE-AC03-76SF00098.

NEAR-SURFACE CO_2 LEAKAGE MIGRATION

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RESEARCH OBJECTIVES

The ultimate failure of geologic CO_2 storage is the seepage of injected CO_2 out of the ground surface into the atmosphere, with associated potential health, safety, and environmental (HSE) risks. To evaluate (1) potential HSE risks, (2) near-surface monitoring strategies for CO_2 storage verification, and (3) the effectiveness of geologic CO_2 storage even in leaky systems, we must understand the behavior of leaking CO_2 in the near-surface environment. The objective of this research is to study CO_2 migration in the near surface environment by numerical simulation and theoretical analyses. The near-surface environment relevant to our studies is approximately ± 10 m from the ground surface and includes porous media (e.g., sediments, fractured rock, and soils), surface water (e.g., lakes, rivers, estuaries, and shallow marine environments), and the lower part of the atmospheric surface layer. We define leakage as CO_2 migration in the subsurface away from the primary target formation, while seepage is CO_2 migration across an interface, such as the ground surface or the basement wall of a building.

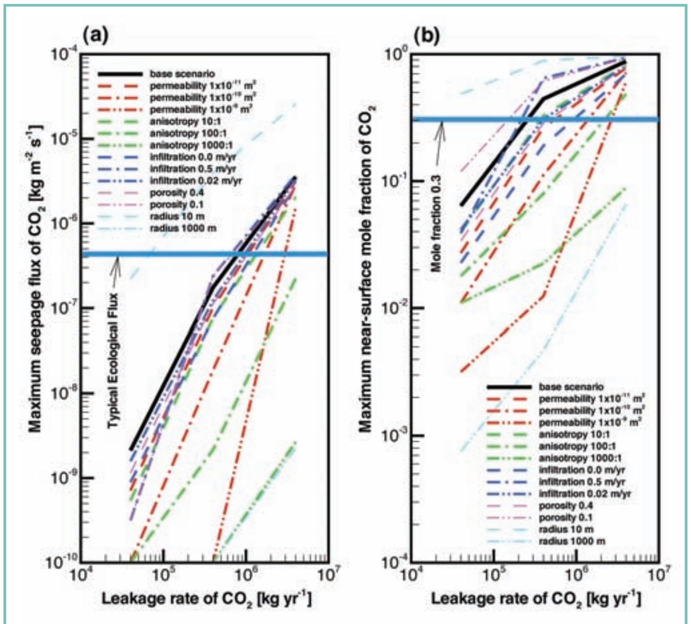

Figure 1. (a) Maximum seepage flux of CO_2 and (b) near-surface gas-phase mole fraction of CO_2 as a function of leakage rate at steady-state seepage conditions for three leakage fluxes and a variety of vadose zone properties.

APPROACH

We have developed and applied T2CA, a TOUGH2 module for simulating CO_2 and air in the near-surface environment. In addition, we have used solubility models and related theoretical analyses of ebullition potential of CO_2 in NaCl brines to evaluate the process of CO_2 entering surface water from below. Our approach is to model simple systems with variable properties to cover a range of natural conditions. The domain for the simulations is a radial 30 m thick vadose zone with a constant leakage flux specified at the bottom and a surface rainfall infiltration recharge of 10 cm/yr.

ACCOMPLISHMENTS

Shown in Figure 1 are the near-surface fluxes and concentrations for three different leakage fluxes and a variety of system properties. As shown in Figure 1, seepage flux and concentration are most sensitive to the strength of the leakage source. Note that concentrations can be quite large even for fluxes that are not much larger than a typical biological flux. From our theoretical studies of CO_2 entry into surface water, we found that ebullition and bubble flow will be the dominant form of transport of CO_2 leakage in shallow surface water.

SIGNIFICANCE OF FINDINGS

The finding that small fluxes can lead to relatively large CO_2 concentrations in the shallow subsurface points to the utility of monitoring the subsurface for anomalous CO_2 concentrations. As for surface water, ebullition appears to be the expected process, making seepage detection in surface water relatively simple because bubbles are easy to detect by visual and acoustic methods. Our results suggest that once CO_2 is in the near-surface environment, it will tend to seep to the atmosphere. If seepage fluxes are small, integrated measurement and modeling strategies will be needed for CO_2 storage verification, in order to discern weak leakage and seepage signals from natural background variability.

RELATED PUBLICATIONS

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Oldenburg, C.M., J.L. Lewicki, and R.P. Hepple, Near-surface monitoring strategies for geologic carbon dioxide storage verification, Berkeley Lab Report LBNL-54089, October 2003.

ACKNOWLEDGMENTS

This work was supported by the Office of Science, U.S. Department of Energy under Contract No. DE-AC03-76SF00098, and by a Cooperative Research and Development Agreement (CRADA) between BP Corporation North America, as part of the CO_2 Capture Project (CCP) of the Joint Industry Program (JIP), and the U.S. Department of Energy through the National Energy Technologies Laboratory (NETL).

Self-Enhancing and Self-Limiting Effects During CO_2 Leakage from Geologic Disposal Reservoirs

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RESEARCH OBJECTIVES

The amounts of CO_2 that would have to be stored in geologic reservoirs are very large, and it appears inevitable that such plumes would encounter imperfections in the caprock, causing leakage. This raises a concern over whether it may be possible for a CO_2 leak to be self-enhancing, in such a way as to give rise to runaway discharge at the land surface with potentially serious consequences. CO_2 has physical properties—including lower density, much lower viscosity, and higher compressibility than aqueous fluids—which suggest that such a possibility should be taken seriously. The purpose of this research is to explore the behavior of leaking CO_2, and to identify conditions, if any, in which CO_2 could be discharged at the land surface in an eruptive manner.

APPROACH

Using information from natural systems, including CO_2 degassing in volcanic areas, and hydrothermal and pneumatic eruptions, we attempt to identify hydrogeologic conditions that would facilitate CO_2 discharge. Numerical simulations using our general-purpose simulator TOUGH2 and a special fluid property module for water-CO_2 mixtures were performed to study the behavior of proposed leakage systems that may involve supercritical as well as gaseous and liquid CO_2.

ACCOMPLISHMENTS

A 1 m thick vertical fault was prepared with initial conditions typical for continental crust (land surface conditions of 15°C temperature and 1 bar pressure; geothermal gradient of 30°C/km and hydrostatic pressures). Carbon dioxide was then introduced at a constant overpressure of approximately 9.5 bar relative to hydrostatic at a depth of 710 m. The CO_2 flows upward and outward from the injection point, displacing most of the water. Substantial cooling effects are observed as the CO_2 rises, caused by decompression and boiling of liquid CO_2 into gas. The interplay between multiphase flow and heat-transfer effects causes nonmonotonic discharge behavior at the land surface (see Figure 1). The strong feedback between fluid flow and heat transfer tends to limit CO_2 fluxes, gives rise to quasi-periodic variations in flow rates, and makes it difficult to envision scenarios in which leakage of CO_2 as a free phase could develop a self-enhancing runaway discharge at the land surface.

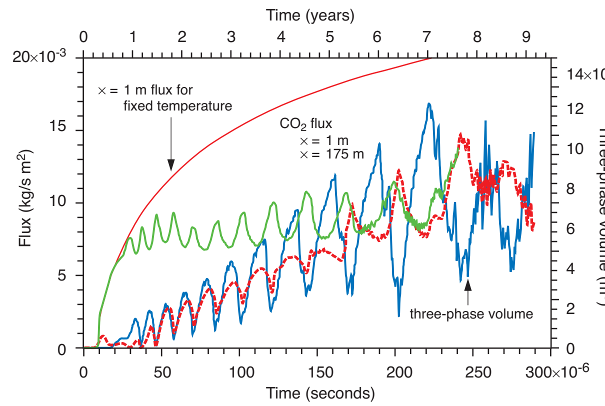

Figure 1. CO_2 discharge behavior from a fault zone. The curves labeled "1 m" and "175 m" show simulated leakage fluxes at the land surface at 1 m and 175 m lateral offset, respectively, from the injection point along the fault strike. Flux predictions obtained for a simulation in which temperatures are held constant at initial values are also shown for comparison. The blue curve shows total fault zone volume in three-phase conditions (aqueous–liquid CO_2–gaseous CO_2).

SIGNIFICANCE OF FINDINGS

Leakage of CO_2 along a fault or fracture zone is accompanied by strong cooling effects. These effects limit CO_2 discharge rates and give rise to nonmonotonic leakage behavior.

RELATED PUBLICATION

Pruess, K., Numerical studies of fluid leakage from a geologic disposal reservoir for CO_2 show self-limiting feedback between fluid flow and heat transfer. Geophys. Res. Lett., 32 (14), L14404, doi:10.1029/2005GL023250, 2005. Berkeley Lab Report LBNL-57362.

ACKNOWLEDGMENTS

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

Spatially Distributed CO_2, Sensible Heat, and Latent Heat Fluxes over the Southern Great Plains

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RESEARCH OBJECTIVES

We have developed a method to estimate regional-scale ecosystem CO_2 and energy exchanges at the Atmospheric Radiation Measurement Southern Great Plains (ARM-SGP) facility. This work addresses U.S. national goals of estimating regional CO_2 sources and sinks, and provides inputs to forward and inverse models.

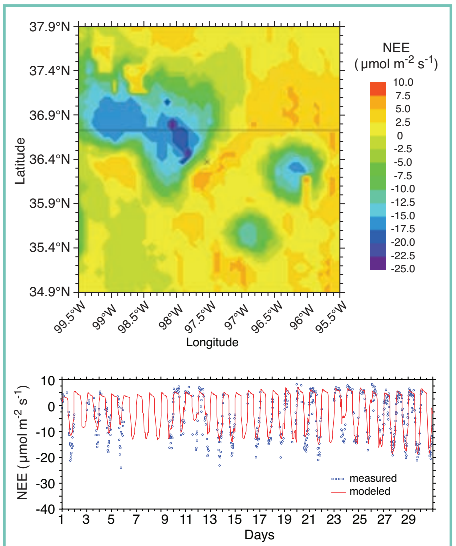
APPROACH

Our method incorporates meteorological data from over 120 Oklahoma and Kansas Mesonet sites into a distributed land surface model (ISOLSM [Cooley et al., 2005; Riley, 2005; Riley et al., 2002], which is based on LSM1.0) of fluxes between ecosystems and the atmosphere. In addition to CO_2 and energy exchanges, ISOLSM predicts fluxes and pools of ^{18}O in CO_2 and H_2O and ^{13}C in CO_2. The meteorological datasets, compiled by ARM, contain fields for precipitation, radiation, wind speed, air temperature, and atmospheric pressure. Our interpolation provides meteorological input for ISOLSM at user-specified resolution across the ARM domain.

We modified the land surface (vegetation) types in ISOLSM to correspond to the dominant land covers in the domain. Soil hydraulic characteristics are determined from the USGS STATSGO 1 km resolution soil map. We have tested ISOLSM in the dominant crop (winter wheat) in the SGP region [Riley et al., 2003] and calibrated to the dominant vegetation types with measurements made by portable 4 m systems comprised of a sonic anemometer and an open-path infrared gas analyzer (http://www.arm.gov/instruments/carbon.stm). Our preliminary calibration was accomplished by manipulating the maximum carboxylation rate and soil-organic-matter content associated with each vegetation type. Future work will improve on this approach by statistically minimizing errors in net ecosystem exchange (NEE) with these and other parameters.

ACCOMPLISHMENTS

Our results show that the interpolated meteorological fields are in good agreement with independent measurements in the area's dominant vegetation types. The bottom panel shows predicted and measured net CO_2 fluxes in a wheat field. Excellent agreement was also obtained for two other portable eddy flux sites (in pasture and sorghum fields).



Top panel: Midday NEE at noon May 15, 2004, in the ARM-SGP domain. Bottom panel: Predicted and measured net CO_2 fluxes in a wheat field during May 2004.

SIGNIFICANCE OF FINDINGS

Typical midday NEE variations across the ARM-SGP domain can be large (up to 25 μmol m^{-2} s^{-1} (top panel), implying that estimating regional NEE requires accurate characterization of spatial heterogeneity in vegetation characteristics and meteorological forcing. Currently, the region is typically modeled as homogeneous cropland. Our approach allows us to quantify uncertainty in regional flux estimates associated with uncertainties in vegetation type, soil types, and spatial and temporal scaling of surface characterization and meteorological forcing. This work will benefit both "bottom-up" and "top-down" approaches to quantifying regional-scale surface CO_2 and energy exchanges.

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Multi-Decadal High-Resolution Hydrologic Modeling of The Arkansas-Red River Basin

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RESEARCH OBJECTIVES

This follow-on study of the DOE Water Cycle Pilot (Miller et al. 2005) evaluates the contrast between fine spatial scales at which heterogeneity is significant (1 km and finer) and coarser scales at which climate simulations are generated. The objectives of this study are to identify physiographic and climatic controls on the spatial variability of soil moisture; to develop new subgrid parameterizations for soil moisture during wet and dry conditions; to examine the spatial scaling properties of soil moisture; and to perform a statistical analysis of the teleconnections between climatic variables and land surface states and processes, such as soil moisture and evapotranspiration.

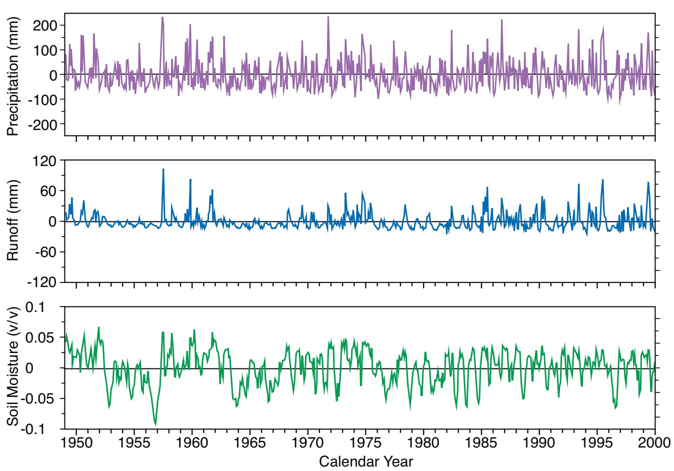

Figure 1. Time series of monthly anomalies of precipitation, runoff, and soil water storage. Notice that while runoff amplifies positive anomalies in precipitation, soil water storage amplifies negative anomalies.

APPROACH

We generated a 51-year simulation of water and energy fluxes over the Arkansas-Red River Basin, using the fully distributed land surface model, TOPLATS, at fine temporal (hourly) and spatial (1 sq. km) resolutions, to bridge the gap between traditional hydrologic modeling and regional land-surface modeling. We focused on the accuracy of streamflow simulations at the sub-basin scale, with physically based descriptions of heat and water exchange at the land-atmosphere interface, because sub-basin scale biases may grow nonlinearly over time, leading to larger basin-scale biases.

ACCOMPLISHMENTS

The surface runoff did not show a distinct shift of the east-west gradient during the summer months as observed for precipitation. The variability of interannual basin-averaged precipitation varied strongly and decreased during the simulation period. Results indicate that precipitation variability amplified in the runoff, but decreased with time. Both basin-averaged precipitation and surface runoff increased during the simulation period, on average, at different rates, suggesting that evapotranspiration increased. This conclusion is supported by analysis of evapotranspiration at the sub-basin scale and observed discharge. Results agree with mounting evidence of an accelerating hydrologic cycle over the conterminous United States. Monthly precipitation and runoff have also increased over the simulation period, except during May and July. It was also found that runoff amplifies positive precipitation anomalies, while soil water storage amplifies negative anomalies.

SIGNIFICANCE OF FINDINGS

The study enhances understanding of the correlation between mean-monthly, seasonal, and annual variations in surface energy fluxes, soil moisture, and stream flow and large-scale atmospheric patterns. The results of this analysis will help clarify the sources of long-term hydrologic variability at regional scales.

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A Noniterative Model for CO_2-H_2O Mutual Solubilities in Chloride Brines

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RESEARCH OBJECTIVES

The objective of this study was to develop a numerically efficient model to compute the mutual solubilities of CO_2 and H_2O in chloride brines, for applications to CO_2 geologic sequestration studies. One specific goal was to avoid degrading the performance of numerical fluid-flow simulations when using such a model.

APPROACH

We previously developed a numerically efficient thermodynamic model for phase partitioning without salt effects. This model was shown to provide an excellent match to experimental data in the range 12–100°C and up to 600 bar. Here, the model is extended to NaCl and $CaCl_2$ solutions by including an activity coefficient for aqueous CO_2, and taking the activity of water as its mole fraction on the basis of a fully ionized salt. Several published activity coefficient formulations were evaluated, two of them based on a Pitzer formulation and providing best results (Figure 1).

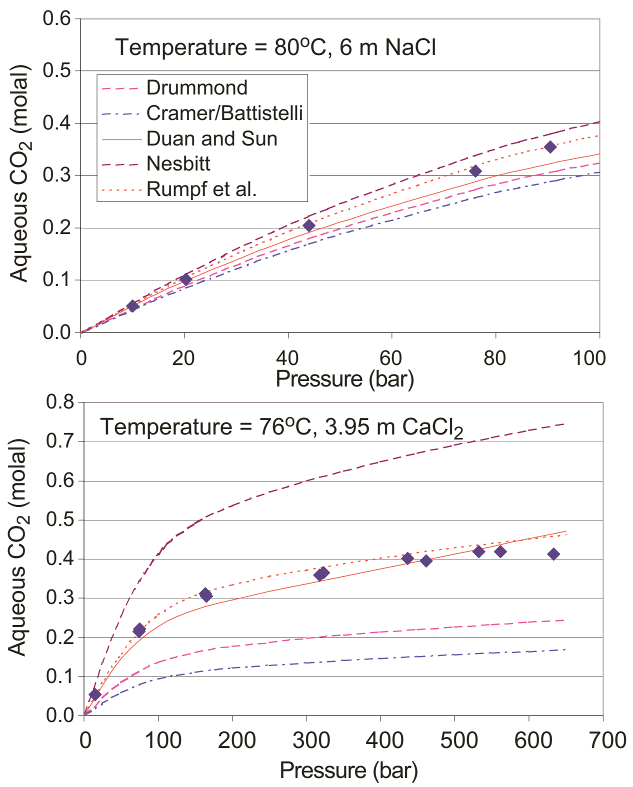

Figure 1. Measured (symbols) versus predicted (lines) CO_2 solubilities using five different activity coefficient models

ACCOMPLISHMENTS

For solutions up to 6 molal NaCl and 4 molal $CaCl_2$ (Figure 1), the best activity coefficient formulations yield calculated CO_2 solubilities within less than 7% (root-mean-square error) of experimental data. Thus, the new model allows computing mutual solubilities in a noniterative manner and with an accuracy typically within experimental uncertainty.

SIGNIFICANCE OF FINDINGS

Previously published models involve complex correlations requiring an iterative solution and/or do not cover temperatures below ~100°C at high pressures. The approach followed here is noniterative, thus numerically efficient, and reproduces experimental solubilities with sufficient accuracy for the study of geologic CO_2 disposal.

RELATED PUBLICATIONS

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Carbon Cycling in the Southern Great Plains: The ARM/LBNL Carbon Project

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RESEARCH OBJECTIVES

The DOE Atmospheric and Radiation Measurement (ARM)/Berkeley Lab Carbon Project is making a coordinated suite of carbon concentration, isotope, and flux measurements to support a range of scaling and integration exercises, including those proposed for the North American Carbon Program:

- Quantifying regional atmospheric CO_2 sources and sinks
- Developing land-surface models and testing carbon exchange parameters
- Predicting the effect of land use and climate on carbon and energy fluxes
- Testing innovative methods for inferring carbon fluxes

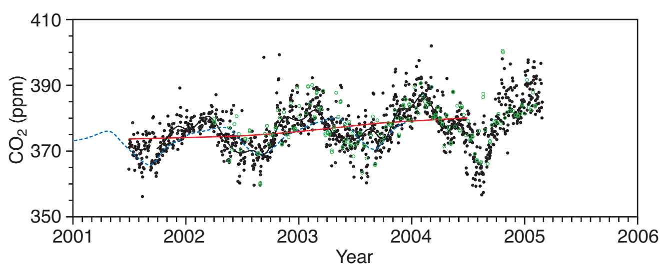

Figure 1. Precise atmospheric CO_2 concentrations (black circles) measured at 60 m, during well-mixed, afternoon conditions (14:00–17:00 CST daily). The running average (black line) shows the seasonal cycle amplitude at ~15 ppm, with a minimum at the peak N Hemisphere growing season, rather than peak local growing season in late spring. The average annual trend in ARM data (red line) matches the NOAA network trend for the SGP latitude band (dashed line). The NOAA flasks were collected ~14:30 CST weekly.

APPROACH

We are working in the ARM Southern Great Plains test bed, a 300 × 300 km area of Oklahoma and Kansas. Most of our carbon measurements are collected at the 60 m tower of the ARM Central Facility, including precise CO_2 concentration profiles, carbon eddy covariance fluxes, National Oceanic and Atmospheric Administration (NOAA) flasks in the mixed layer and free troposphere (by aircraft), and diurnal profiles of ^{13}C and ^{18}O in CO_2. The precise CO_2 measurements and NOAA flasks tie the ARM site to the global atmospheric network. This year, we have added continuous CO measurements and are in the process of adding continuous airborne CO_2 and $^{14}CO_2$ flask sampling to assist with source attribution.

ACCOMPLISHMENTS

By comparing airborne and tower data, we have found that the 60 m tower is tall enough to sample well-mixed boundary-layer air during the afternoon, when convective mixing is active. As a result, our data can be used to estimate regional CO_2 levels. Figure 1 shows daily CO_2 concentrations measured in the afternoon during well-mixed conditions. The annual increase over three years was more than 2 ppm y^{-1}. This trend nearly matches the global background trend (2.3 ppm y^{-1}) reported by NOAA at Mauna Loa.

Using multiple eddy flux towers, we find large heterogeneity in surface fluxes among replicate wheat fields and even larger variability between different cover types. These findings reinforce the need for model parameters that accurately represent heterogeneity in land use, to replace the typical application of a single parameter set for all crop types. We have begun testing distributed ecosystem model predictions against the eddy flux measurements, and plan to compare the distributed model results with atmospheric inversion results for estimating mesoscale carbon fluxes.

SIGNIFICANCE OF FINDINGS

As shown in Figure 1, global atmospheric CO_2 concentrations are rising rapidly. The rate of increase is the difference between anthropogenic emissions and uptake by land and oceans. The ability to predict or manage future CO_2 concentrations, and thus climate itself, depends on our ability to understand and predict terrestrial carbon exchanges. Our research at ARM addresses this need by quantifying subcontinental-scale ecosystem-atmosphere fluxes, and predicting the effects of land use and climate on atmospheric CO_2 concentrations.

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RELATED WEB SITE

ARM Carbon Web Site: http://esd.lbl.gov/ARMCarbon/

ACKNOWLEDGMENTS

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

Soil Organic Matter and Root Turnover: The Enriched Background Isotope Study

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RESEARCH OBJECTIVES

In the summer of 1999 there was a large atmospheric release of $^{14}CO_2$ near the Oak Ridge Reservation (ORR), Tennessee, presumably from a local incinerator. The rapid photosynthetic uptake of the $^{14}CO_2$ created a pulse label for studying carbon (C) cycling through the ORR forests. As part of a team from four DOE labs and UC Irvine, we are utilizing this whole-ecosystem isotopic label to study, and improve modeling of, processes in terrestrial carbon cycling. At Berkeley Lab, we are investigating (1) soil organic matter (SOM) dynamics, (2) the longevity of fine roots, and (3) leaf versus root inputs to SOM.

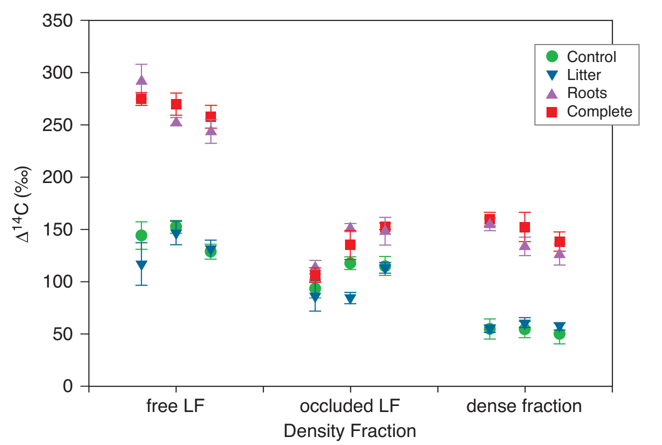

Figure 1. The radiocarbon content of SOM fractions from 0–15 cm depth at the Ultisol EBIS sites. The treatments are named for the source of elevated ^{14}C to the soil: roots, leaf litter, enriched leaves and roots (complete) or no enriched plant inputs (control). The three repeated symbols for each treatment and fraction are for the three years of sampling, 2001–2003.

APPROACH

The ORR team used a reciprocal transplant of enriched and near-background leaf litter to create four treatments, depending on type of plant ^{14}C inputs to soil: roots, leaf litter, both, or neither (no enrichment). We used a simple density fractionation method to separate SOM into interaggregate particulate organic matter (free light fraction), particulate organic matter occluded within aggregates (occluded light fraction), and organic matter complexed with minerals to form a dense fraction. We determined fine-root longevity by tracking the radiocarbon label in live and dead root populations. For fungal dynamics, ectomycorrhizae were hand-picked from freshly harvested roots. For microbial biomass, chloroform fumigation-extracts of soils were freeze-dried and combusted for graphitization. Radiocarbon content was measured at Lawrence Livermore National Laboratory by accelerator mass spectrometry. As a guide to interpreting the results, the more ^{14}C-depleted a sample, the slower its rate of input or turnover in the ecosystem.

ACCOMPLISHMENTS AND SIGNIFICANCE

The $\Delta^{14}C$ values of the SOM fractions reveal two important aspects of carbon cycling in these forest soils. First, considering only the control treatment, the mineral-associated (dense fraction) carbon is the most depleted in ^{14}C, showing that this fraction has the slowest turnover time, while the free light fraction is the fastest cycling. The depleted signature (and thus slow turnover time) of the occluded light fraction was unexpected, because it is chemically similar to the free light fraction. These results mean that the dominant mechanisms of carbon stabilization were interaction with minerals and physical protection by occlusion, rather than intrinsic recalcitrance of the organic matter.

Second, only the soils receiving elevated ^{14}C from roots (roots and complete treatments) become enriched, and in fact there is no significant difference between control and litter soils, showing that only root inputs are contributing to SOM. The importance of root inputs relative to leaf litter was also seen in the results for ectomycorrhizal fungi and total microbial biomass. These results directly contradict the predominant assumption that litterfall is the main source of soil carbon, and its corollary that carbon inputs to soil can be approximated by litterfall rates.

The Enriched Background Isotope Study (EBIS) data are used to improve models of soil C cycling . For example, in the root study, new roots grew from a mixture of recent photosynthate and 10–20% stored reserves from the previous year. These findings are helping us parameterize a root model and estimate fine-root turnover based on trends in atmospheric $^{14}CO_2$.

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The Importance of Belowground Plant Allocation for Terrestrial Carbon Sequestration and Climate Feedbacks

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RESEARCH OBJECTIVES

Soil organic matter (SOM) plays a central role in the carbon (C) cycle, by sequestering atmospheric carbon and by forming a feedback to climate change. The long turnover time of SOM compared to most plant tissues means that soils are a more efficient storage pool for C (i.e., more sequestration per unit net primary productivity [NPP]), with less interannual variability or disturbance-driven losses. We are conducting research to fill critical gaps in understanding of belowground carbon cycling in temperate forests, by quantifying:

- The lifetime of fine roots and its effect on belowground NPP
- Decomposition of root versus needles/leaves
- Total residence time of belowground C, including SOM
- Resource constraints on plant allocation

APPROACH

When plants allocate C belowground, the C cascades through several reservoirs—live roots, dead roots, microbial biomass, and humic organic matter—each with their own residence time and respiratory losses (Figure 1). A longer residence time results in more storage per unit C input. To predict C sequestration or the potential for ecosystem feedbacks to climate change, we need to understand the turnover times of C in each soil carbon pool, the pathways of C movement among pools, and the potential feedbacks to productivity.

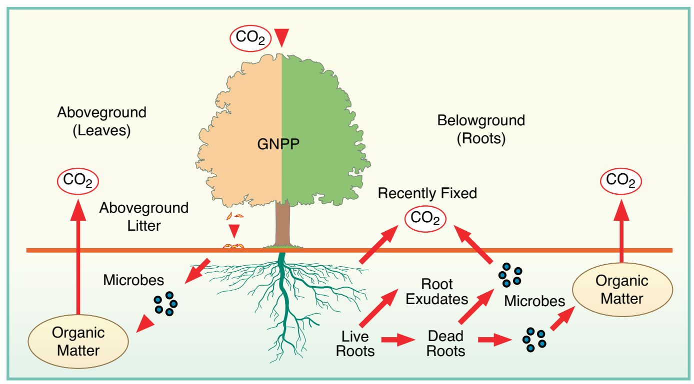
Accordingly, we have conducted field isotope-based experiments, including (1) natural abundance ^{14}C, to determine fine-root lifetimes; (2) litterbags and *in situ* incubations of ^{13}C-labeled litter, to estimate litter decay rates; and (3) ^{13}C-labeled litter, to track root and needle decay into soil-respired CO_2, microbial biomass, and soil organic fractions. The accomplishments represent work in ponderosa pine, mixed conifer-deciduous hardwood, and Norway spruce forests.

ACCOMPLISHMENTS

We find that fine roots live 2–5 years, longer than the historical assumption of annual turnover. The main implication of longer root life spans is that belowground NPP currently may be overestimated. We have begun modeling to produce better estimates of root turnover and NPP allocation. For decomposition, our experiments provide multiple lines of evidence that roots decay more slowly than needles or leaves, and there are differences in the microbial communities mediating decomposition of the tissues. For SOM, we have documented the importance of depth and mineralogy in long-term carbon storage. We have published eight peer-reviewed articles, presented at a dozen venues, and supported two post docs, one Ph.D. student, and more than 10 undergraduates.

SIGNIFICANCE OF FINDINGS

Our results to date imply that the same amount of primary productivity leads to more C storage if it is allocated to fine roots rather than to leaves or needles in these temperate forests. Translating these results to a sequestration strategy or analysis of feedbacks poses challenges that we are addressing in the second phase of our research. It appears from our early results that plant allocation patterns influence the plant's ability to acquire and use belowground and aboveground resources, which may in turn feed back to shape productivity and long-term C sequestration.



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Earth Sciences Division Staff 2004–2005

A Special Note: Looking Forward to A Big Event—The year 2007 will be the Earth Sciences Division's 30th anniversary. We are currently planning to celebrate scientific breakthroughs and achievements, as well as take a look back at the people and events that made ESD what it has been through the years.

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Front Cover

Photo Montage of equipment and personnel in the field, working on the Frio Brine Project: CO_2 injection system. Tanks with hoses connecting to heat exchanger and pump (left), sampling vessels for U-Tube apparatus (top right), tanks at Frio Brine Project (bottom right)

Back Cover

Photos in column: U-Tube apparatus; crew with downhole packer assembly and U-Tube; evaporator and nitrogen tank used with U-Tube to collect samples; seismic testing truck

Page 1 **Division Director's Perspective**

Aerial View of Lawrence Berkeley National Laboratory, on the hill overlooking the campus of the University of California, Berkeley

Page 9 **Resource Departments**

Barry Freifeld (left) and Rob Trautz (right), lifting an x-ray diffraction device to image cores

Page 11 **Hydrogeology**

Rohit Salve in Alcove 8, Yucca Mountain, NV

Page 13 **Geophysics**

Preparation of an injection test at the Frio Brine CO_2 Sequestration Pilot in Texas
Photography by Barry Freifeld

Page 15 **Geochemistry**

Tom Owen in the Center for Isotope Geochemistry

Page 19 **Ecology**

Terry Hazen (left) and Gary Andersen, microbiologists with Berkeley Lab, are shown here with the 16s phylochip they developed that can analyze a sample for the unique DNA signatures of all known species of bacteria.

Page 21 **Research Programs**

Oil drilling program to deploy an x-ray diffraction apparatus
Photography by Barry Freifeld

Page 23 **Fundamental and Exploratory Research**

Monitoring CO_2 and He emissions at Mammoth Mountain

Page 41 **Nuclear Waste**

Yucca Mountain cross section
Illustration by Diana Swantek

Page 65 **Energy Resources**

Alaska rig

Page 85 **Environmental Remediation**

Boris Faybishenko collecting sediment samples at Hanford, 100-H site, for biogeochemical analyses

Page 121 **Climate Change and Carbon Management**

Markus Kleber (in pit), Alejandro (Alex) Morales (left), and Margaret Torn (right) describing a soil profile before collecting soil for a global change project, Hopland, CA

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