LBL--27900

DE91 004108

EARTH SCIENCES DIVISION ANNUAL REPORT 1989

Lawrence Berkeley Laboratory
University of California
Berkeley, California 94720

June 1990

Prepared for the U.S Department of Energy under Contract No. DE-AC03-76SF00098

MASTER

DISTRIBUTION OF THIS DOCUMENT IS UNLIMITED

ACKNOWLEDGMENTS

This work was supported through U.S. Department of Energy Contract No. DE-AC03-76SF00098 by (1) the DOE Director, Office of Energy Research, (i) Office of Basic Energy Sciences and (ii) Office of Health and Environmental Research; (2) the DOE Director, Office of Civilian Radioactive Waste Management, (i) Office of Systems Integration and Regulation and (ii) Office of Facilities Siting and Development; (3) the DOE Assistant Secretary for Conservation and Renewable Energy, Office of Renewable Technologies; (4) the DOE Assistant Secretary for Fossil Energy, Office of Oil, Gas, Shale and Special Technologies; (5) U.S. Government Offices in (i) Agency for International Development, (ii) Bureau of Reclamation, (iii) Environmental Protection Agency, (iv) Geological Survey, and (v) National Science Foundation through various Universities; (6) the State of California, (i) Department of Health Services, (ii) State Lands Commission, and (iii) University of California; (7) the Gas Research Institute; and (8) the Swedish Nuclear Power Inspectorate.

CONTENTS

INTRODUCTION 1

RESERVOIR ENGINEERING AND HYDROGEOLOGY 3

An Analytic Solution Relating Wellbore and Formation Velocities, with Application to the Tracer-Dilution Problem
P. Bidaux and C.F. Tsang 5

Some Considerations on Resource Evaluation of The Geysers
G.S. Bodvarsson, S.W. Gaulke, and M. Ripperda 7

Fracture Flow Models of the Fracture Zone at the Migration Investigation Site
A. Davey, K. Karasaki, J.C.S. Long, M. Landsfeld, and S.J. Martel 10

Unsaturated-Zone Thermal-Energy Storage: Modeling the 1989 Module Experiment
C. Doughty, A. Nir, and C.F. Tsang 14

The Semianalytical Similarity Solution for Two-Phase Fluid and Heat Flow: A Tool for High-Level Nuclear Waste Studies
C. Doughty and K. Pruess 16

Numerical Simulation of Steam Injection for the Removal of Organic Liquids from the Subsurface
R.W. Falta, K. Pruess, I. Javandel, and P.A. Witherspoon 19

Numerical Modeling Studies on Cerro Prieto
S.E. Halfman-Dooley, M.J. Lippmann, and G.S. Bodvarsson 23

Hydrologic Characterization of Faults and Other Potentially Conductive Geologic Features in the Unsaturated Zone
I. Javandel and C. Shan 27

Application of the PTST Solution to Field Data
K. Karasaki 32

Fractal Study and Simulation of Fracture Roughness and Apertures
S. Kumar and G.S. Bodvarsson 35

Permeability of a Parallel-Walled Fracture with Cylindrical Asperities
S. Kumar, R.W. Zimmerman, and G.S. Bodvarsson 37

The Hydrogeologic-Geochemical Model of Cerro Prieto Revisited
M.J. Lippmann, A.H. Truesdell, S.E. Halfman-Dooley, and A. Mañón M. 40

An Analytical Expression for the Permeability of Random Two-Dimensional Poisson Fracture Networks
J.C.S. Long and K. Hestir 45

Preliminary Calculations of Inflow to the D-Holes at the Stripa Mine
J.C.S. Long, K. Karasaki, A. Davey, J.E. Peterson Jr., M. Landsfeld, J.M. Kemeny, and S.J. Martel 48

An Interdisciplinary Methodology for Modeling Fracture Systems, with Application to the US/BK Site, Grimsel Laboratory, Switzerland
S.J. Martel and J.E. Peterson Jr. 52

First-Order Kinetics-Controlled Multiple-Species Reactive Transport of Dissolved Organic Compounds in Groundwater: A Numerical Model

W.W. McNab, Jr., and T.N. Narasimhan 56

On the Potential Importance of Transient Air Flow in Advective Radon Entry into Buildings

T.N. Narasimhan, Y.W. Tsang, and H.-Y. Holman 60

Disposal of High-Level Wastes at Yucca Mountain, Nevada: A Hierarchy of Hydrological Issues Relating to the Vadose Zone

T.N. Narasimhan and J.S.Y. Wang 62

Development and Verification of a Numerical Technique for Coupled Hydromechanical Phenomena in Rocks

J. Noorishad and C.F. Tsang 65

Aqueous Foams for Control of Gas Migration and Water Coning in Aquifer Gas Storage

P. Persoff, C.J. Radke, K. Pruess, S.M. Benson, Y.S. Wu, and P.A. Witherspoon 70

Flow to Wells in Fractured Rock with Fractal Structure

J. Polek, K. Karasaki, J.C.S. Long, and J. Barker 74

Numerical Modeling of Gas Migration at a Proposed Repository for Low- and Intermediate-Level Nuclear Wastes at Oberbauenstock, Switzerland

K. Pruess 77

On Two-Phase Relative Permeability and Capillary Pressure of Rough-Walled Rock Fractures

K. Pruess and Y.W. Tsang 79

An Exploitation Model and Performance Predictions for the Ahuachapan Geothermal Field, El Salvador

M. Ripperda, G.S. Bodvarsson, M.J. Lippmann, and C. Goranson 82

A Simplified Analytical Solution for Dissolution and Transport of Nonaqueous Phase Liquids in Groundwater

C. Shan, I. Javandel, and P.A. Witherspoon 86

A Broad View of Model Validation

C.F. Tsang 89

Validation of a Method for Analyzing Borehole-Fluid-Conductivity Logs to Determine Fracture-Inflow Parameters

C.F. Tsang, P. Hufschmied, and F.V. Hale 95

A Permeability, Porosity, and Capillary-Radius Relationship for Rocks and Soils

J.S.Y. Wang 98

Sensitivity Analysis of Partially Saturated Flow through Welded-Nonwelded Tuff Units Using a Path-Integration Technique

J.S.Y. Wang and T.N. Narasimhan 101

Scaling Law for Absorption of Water into Porous Blocks of Various Shapes and Sizes

R.W. Zimmerman, G.S. Bodvarsson, and E.M. Kwicklis 104

GEOLOGY AND GEOCHEMISTRY 107

Behavior of Isotopic Ratios during Reactive Transport in Saturated Geologic Media

D.J. DePaolo 109

Paleoclimatic Implications of Oceanic Strontium Isotopic Variations over the Past 2.5 Million Years

D.J. DePaolo and R.C. Capo 111

The Hydrothermal Alteration and Carbonation of Oceanic Crust: Implications for Global Cycles of CO₂ and the Oxygen Isotopes

B.M. Smith and H. Staudigel 114

¹⁴C Transport in a Partially Saturated Fractured Porous Medium

W.B. Light, P.L. Chambre, W.W.-L. Lee, and T.H. Pigford 117

Analytic Solution of Pseudocolloid Migration in Fractured Rock

Y. Hwang, T.H. Pigford, W.W.-L. Lee, and P.L. Chambre 119

Preliminary Derivation of a Gas-Flow Source Term from a Nuclear Waste Container

E.D. Zwahlen, T.H. Pigford, P.L. Chambre, and W.W.-L. Lee 120

Simulation of Reactive Chemical Transport in a Varying Thermal Field with Reaction-Flow Coupling

C.L. Carnahan 123

Nonsteady-State Simulation of Coupled Transport Processes in Geological Materials

C.L. Carnahan and J.S. Jacobsen 125

Development of UTHCC—A Computer Program for Simulating Reactive Chemical Transport through Unsaturated Media

J.S. Jacobsen, C.L. Carnahan, and K. Pruess 128

Hydrothermal Mineralogy and Alteration Temperatures in the Shady Rest Drill Hole, Long Valley Caldera

S. Flexser 130

Solubility and Speciation Studies for the Yucca Mountain Project

H. Nitsche, A. Müller, R.C. Gatti, T. Prussin, R.S. Deinhammer, and S.C. Carpenter 134

Synthesis and Spectroscopic Studies of Uranium Carbonate

D.L. Perry 136

Thermodynamics of High-Temperature Brines

K.S. Pitzer, R.T. Pabalan, and L.M. Connaughton 138

Selection and Characterization of a Radon Experimental Site

H.A. Wollenberg, S. Flexser, R.G. Sextro, and A.R. Smith 140

GEOPHYSICS AND GEOMECHANICS 147

One-Dimensional Least-Squares Inversion of Surface-to-Borehole and Cross-Hole Electromagnetic (EM) Data

M. Deszcz-Pan, K.H. Lee, and H.F. Morrison 149

Evaluating the Performance of Cross-Hole Diffusion Tomography

K.T. Nihei and Q. Zhou 150

Cross-Hole Tomographic Imaging for Fracture Characterization

E.L. Majer, J.E. Peterson Jr., L.R. Myer, K. Karasaki, T.M. Daley, and J.C.S. Long 155

Seismic Imaging for Fracture Characterization at Yucca Mountain, Nevada

E.L. Majer, J.E. Peterson Jr., T.V. McEvilly, and M.A. Tura 158

Anisotropic Inversion of VSP Travel-Time Data, with an Example from The Geysers

I. Pšenčík, J. Jech, V. Cervený, D. Gajewski, T.M. Daley, T.V. McEvilly, and E.L. Majer 162

Modeling Elastic Waves in Fractured Rock with the Kirchhoff Method

K.T. Nihei, L.R. Johnson, and N.G.W. Cook 166

Compaction of Porous Rock under an Indenter <i>R. Suarez-Rivera, N.G.W. Cook, G. Cooper, and Z. Zheng</i>	169
The Effects of Tortuosity on Flow through a Natural Fracture <i>A.M. Cook, L.R. Myer, N.G.W. Cook, and F.M. Doyle</i>	172
The Effects of a Clay Coating on Fluid Flow through Simulated Rock Fractures <i>J.J. Carter, L.R. Myer, and N.G.W. Cook</i>	175

APPENDIXES 181

Appendix A: Abstracts of Journal Articles	181
Appendix B: Other Publications	188

INTRODUCTION

Scientists and engineers of the Earth Sciences Division, following the mission of a multipurpose National Laboratory, conduct research on a wide variety of topics relevant to the nation's energy development programs. This report summarizes the activities for 1989. The Earth Sciences Division has developed unique expertise in several research areas. This expertise is due in part to the special resources and facilities available to researchers at the Lawrence Berkeley Laboratory and in part to the Laboratory's commitment to technical and scientific excellence. In addition to the permanent Laboratory staff, University faculty members, postdoctoral fellows, students, and visiting scientists participate in many investigations. Each year, several Ph.D. and Masters theses are founded in research within the Division. Interlaboratory cooperation within the U.S. Department of Energy system and collaboration with other research institutions provide access to unmatched intellectual and technological resources for the study of complex problems.

Much of the Division's research deals with the physical and chemical properties and processes in the earth's crust, from the partially saturated, low-temperature near-surface environment to the high-temperature environments characteristic of regions where magmatic-hydrothermal processes are active. Strengths in laboratory and field instrumentation, numerical modeling, and in situ measurement allow study of the transport of mass and heat through geologic media—studies that now include the appropriate chemical reactions and the hydraulic-mechanical complexities of fractured rock systems. Related and parallel laboratory and field investigations address the effects of temperature, pressure, stresses, pore fluids, and fractures on the elastic and electrical properties of rock masses. These studies are concerned with rock behavior in the brittle and ductile crustal regimes, and they drive the development of improved geomechanical and geophysical tools and techniques for mapping and characterizing heterogeneity in the subsurface. Recent initiatives in special areas of research have been generated in response to needs perceived by Congress, by DOE, by industry, or by the scientific community at large. Of particular note are three major new Division efforts addressing problems in the discovery and recovery of petroleum, the application of isotope geochemistry to the study of geodynamic processes and earth history, and the development of borehole methods for high-resolution imaging of the subsurface using seismic and electromagnetic waves. In 1989 a major DOE-wide effort was launched in the areas of Environmental Restoration and Waste Management. Many of the methods previously developed for and applied to deeper regions of the earth will in the coming years be turned toward process definition and characterization of the very shallow subsurface, where man-induced contaminants now intrude and where remedial action is required.

This Annual Report presents summaries of selected representative research activities grouped according to the principal disciplines of the Earth Sciences Division: Reservoir Engineering and Hydrogeology, Geology and Geochemistry, and Geophysics and Geomechanics. We are proud to be able to bring you this report, which we hope will convey not only a description of the Division's scientific activities but also a sense of the enthusiasm and excitement present today in the Earth Sciences.

RESERVOIR ENGINEERING AND HYDROGEOLOGY

The scientists and engineers in the Reservoir Engineering and Hydrogeology group are primarily concerned with several different approaches to the fundamental problem of the movement of mass and energy through rocks. For a number of years, we have been striving to understand geothermal systems and to unravel the complex physics that controls such systems. This has required the perfection of mathematical models and their application to rather large and complicated field projects. Several articles in this section present the results of recent developments and serve to illustrate the level of sophistication that has been attained in geothermal reservoir modeling.

Several years ago we began to investigate the phenomenon of flow in fractured rocks, and this has now become a major effort. The importance of fractures in fluid flow arose in connection with our work on geothermal systems and has become a central theme in our investigations of problems related to the isolation of radioactive and toxic wastes. One of these problems is to be able to characterize the fracture system of a rock mass; several articles discuss the difficulties in the evaluation of field data and the use of well tests. Another problem is to develop models that are appropriate to use in evaluating the factors that control fluid movement in fractures; different approaches are being pursued in this area, and they address a vast range of spatial scales, from small (cored) sections of individual rough-walled fractures to three-dimensional fracture networks in the field. Single- and multiphase flow as well as chemical transport in fractures are being studied.

High-level radioactive wastes generate substantial amounts of heat, and once the waste is placed underground the dissipation of this thermal energy and its effects on the rock mass must be understood. Our previous work on geothermal systems has provided us with an excellent background for confronting this problem; the results of several investigations are included here. Another problem of great practical importance concerns the migration of chemical species in the unsaturated zone and in groundwater systems. Our studies in this area involve the development and field application of quantitative techniques for monitoring and predicting the behavior of organic as well as inorganic contaminants in the subsurface.

Recently there has been considerable interest in utilizing the unusual properties of foam to improve the efficiency of oil recovery and underground gas storage. Results of our laboratory experiments and theoretical attempts to understand foam flow in porous media are reported.

Our research program is rounded out by a number of topical studies. These relate to the design and interpretation of hydrologic tests and to the improvement of mathematical-modeling capabilities.

An Analytic Solution Relating Wellbore and Formation Velocities, with Application to the Tracer-Dilution Problem

P. Bidaux* and C.F. Tsang

The natural groundwater flow velocity in an aquifer is ignored in most problems concerning water supply because its value is considered as too small to have any effect. However, the importance of the regional flow velocity has been noticed in certain cases where one needs to predict aquifer vulnerability to contaminants, plan an aquifer cleanup operation (Javandel and Tsang, 1986), or estimate the longevity of a geothermal doublet (Aubertin et al., 1987). Attempts have been made to measure formation velocity using the point-dilution technique in a single well at rest (Aubertin et al., 1987). In that case, the Darcy velocity in the formation is related to the apparent velocity at the wellbore by a convergence factor that reflects the deformation of streamlines near the wellbore.

In the work summarized here (Bidaux and Tsang, 1989), we studied the influence of a damage zone around the borehole on the convergence factor and on the measurements of formation velocity, and we studied the combined pattern of regional flow and production (or injection) at the well.

Calculations were made for two cases: natural regional flow with and without pumping (or injecting) in the wellbore. For natural flow without pumping, the ratio between formation velocity and wellbore velocity is a constant that depends on the skin factor and on the thickness of the damaged zone. When pumping (or injecting), two different flow patterns can be distinguished, depending on the flow rate. If the flow rate is above a critical value, which is a function of the formation velocity, the wellbore radius, and the skin factor, the flow at the wellbore is purely convergent for pumping and purely divergent for injecting. However, if the flow rate is below the critical value for the case of injection, the flow leaving the well and entering the formation is a combination of injected fluid and fluid from the formation upstream. Thus, if tracer is injected into the borehole at a subcritical flow rate, the concentration of tracer fluid entering the formation can be calculated and will be lower than the tracer concentration in the injected fluid. For the case of pumping, only part of the flow from the formation upstream is produced; the rest re-enters the formation downstream. The formation velocity can still be calculated by an analytic relationship involving upstream and downstream flow rates, wellbore radius, and skin factor.

Our study (Bidaux and Tsang, 1989) suggests an alternative method of measuring the regional flow velocity. It also suggests that a dilution factor should in some cases be taken into account when injecting a tracer at low flow

rate in a borehole during tracer-transport testing. These two applications of our study are briefly described below.

The alternative method of measuring regional flow velocity involves the injection of water with tracer. When water is injected at a flow rate less than the critical value of the pumping rate, Q_{crit} , the water entering the formation downstream is a mixture of injected water and water from the formation upstream (Fig. 1). Here Q_{crit} is defined as $4\pi e R_w V_\infty / (1 + s\alpha)$, where $\alpha = (1 - R_w^2/R_d^2)/2 \ln(R_d/R_w)$ and where e is the aquifer thickness, R_w is the well or drift radius, V_∞ is the Darcy velocity of the unperturbed regional flow, s is the skin factor, and R_d is the outer radius of a conventional skin. If we let the injected water have a concentration C_0 , let the water in the formation upstream have a concentration C_f in some element, and introduce the dimensionless concentration

Figure 1. Injection of a tracer in an aquifer with a regional flow. (a) Subcritical injection rate. (b) Supercritical injection rate. [XBL 902-552]

*Permanent address, CNRS-URA 1359, Laboratoire d'Hydrogéologie, Montpellier, France.

$$c = \frac{C - C_f}{C_0 - C_f},$$

then our semianalytic calculations give the dimensionless concentration c as a function of the dimensionless injected flow rate $q = Q/Q_{crit}$:

$$c(q) = \frac{q\pi}{q \arccos(-q) + 2\sqrt{1-q^2}}$$

for $0 \leq q \leq 1$. As there is no flow from the formation to the borehole for an injection at a flow rate over the critical value, we have $c(q) = 1$ for $q > 1$. The variations of c as a function of q are plotted in Fig. 2.

Thus, by measuring the steady-state concentration C in the borehole, corresponding to various values Q of injected flow rate of deionized water ($C = C_0$), one gets an experimental curve $C = C(Q)$. When the critical flow rate is reached, C equals C_0 . It should be easy to measure the critical flow rate in this way because the sensitivity of C as a function of Q increases sharply when Q approaches its critical value, as shown in Fig. 2. Note that, contrary to the procedure based on tracer-dilution method in the well without pumping (at rest), we measure only the steady-state concentrations for various injected flow rates and not the change in concentration with time.

Our study also points out the need to consider the regional flow rate (or flow field imposed by pumping from nearby wells) when performing tracer tests in an aquifer. If water is injected into the borehole at a subcritical flow rate Q_{crit} , formation water will still flow into the borehole and dilute the tracer before it enters the formation. If the skin factor, the α coefficient, and the regional flow velocity have been measured or estimated, one can calculate the critical value Q_{crit} of the injection flow rate and use the theoretical curve given in Fig. 2 to determine the real concentration of the water entering the formation. For that reason, tracer tests in boreholes should be carried out carefully and the injection flow rate controlled; otherwise there is no way to know the tracer concentration in the water entering the formation.

Indeed, what we need to know for this particular problem is Q_{crit} , and not necessarily the formation velocity. Thus a direct measure of Q_{crit} may be enough. Estimates of

Figure 2. Effective concentration obtained in a borehole by the injection of a tracer as a function of the injection flow rate. [XBL 902-553]

s and α are not specifically required if we just want to know how much a tracer will be diluted when it is injected into the wellbore. However, if tracer tests are planned in several wells with different characteristics in the same aquifer, it may be worth determining the regional velocity rather than measuring directly the critical flow rate for all the wells.

REFERENCES

- Aubertin, G., Benderitter, Y., Cordier, E., Doillon, F., Fabris, H., Gable, R., Gaillard, B., Ledoux, E., and DeMarsily, G., 1987. Experimental measurement of the natural flow velocity of the Dogger geothermal aquifer in the Paris basin. *Bull. Soc. Geol. Fr.*, v. 8, t. III, no. 5, p. 991-1000.
- Javandel, I., and Tsang, C.F., 1986. Capture-zone type curves: A tool for aquifer cleanup. *Groundwater*, v. 24, no. 5, p. 616-625 (LBL-19843).
- Bidaux, P., and Tsang, C.F., 1989. A semi-analytic study of the regional flow patterns around a well or an underground drift with complex skin effects. Submitted to *Water Resour. Res.* (LBL-28072).

Some Considerations on Resource Evaluation of The Geysers

G.S. Bodvarsson, S.W. Gaulke, and M. Ripperda

The Earth Sciences Division of Lawrence Berkeley Laboratory (LBL) is conducting research studies on The Geysers geothermal field for the California State Lands Commission (SLC). SLC receives royalties for steam produced from State-owned leases at The Geysers, and the funds are used for the California Teachers Retirement Fund.

The LBL project on The Geysers started in 1985 with the development of a comprehensive computerized data base; the following year various geological and reservoir engineering studies were conducted using the data base. During the last two years numerical modeling studies were carried out with the purpose of understanding the reservoir response to production and injection.

This article summarizes the various aspects of resource assessment of The Geysers discussed in Bodvarsson et al. (1989). The available data are briefly described and some results of data analysis presented. The limitations of the data base for numerical modeling are then discussed, and poorly known reservoir parameters are identified. Different modeling approaches are evaluated in terms of The Geysers data, and information regarding appropriate initial and boundary conditions are summarized. Finally, two-dimensional fractured/porous-medium models of The Geysers and some simulation results are described.

AVAILABLE DATA

Over 500 wells have been drilled at The Geysers, providing large amounts of data for this resource. These data include lithologic logs, directional surveys, steam-entry locations, static and flowing temperature and pressure surveys, production and injection histories, pressure decline, pressure transient tests, and geochemical data. In terms of the overall resource evaluation the most important data are the production and injection histories and the pressure-decline data. Figure 1 shows pressure contours based on the limited open-file data for 1988.

Most of the current proprietary data are for wells located in recently drilled areas, such as Northwest and Southeast Geysers, hence the pressure drawdown in these areas is not well defined. The original pressure at The Geysers was close to 35 bars (500 psi). By 1988 the pressure had declined to less than 14 bars (200 psi) over a large portion of the field. In the last few years the pressure decline has accelerated considerably due to recent development in the Southeast Geysers, causing large decreases in flow rates of producing wells. The field is currently producing about 1400–1500 MW_e, which is significantly below the total installed capacity of about 2000 MW_e.

From lithologic logs, the graywacke has been identified as the main producing reservoir rock, with typically 2

Figure 1. Pressure contours based upon open file data for 1988. [XBL 902-554]

to 8 major steam entries per productive well. Most of the wells are directionally drilled because of the rugged topography in the area, but overall the deviated wells do not have more steam entries, or higher production rates, than the near-vertical wells. This suggests that the permeability at The Geysers is not limited to major near-vertical faults and that lateral permeability is significant; this is also indicated by the pressure-decline data. Many of the major steam entries are associated with intervals containing a significant fraction of shale or micrograywacke, suggesting high contact permeability between the shale layers and the main graywacke.

Pressure-transient data (primarily pressure-buildup data) indicate that there is a high fracture kH product at The Geysers in the range 10–100 D-m (30,000–300,000 md-ft). Few open-file data are available on matrix porosities or permeabilities, but the average matrix porosity is believed to be within the range 3–5%. Analysis of flow-rate-decline data yielded values for the so-called recharge factor between 1 and 10 (Ripperda et al., 1989). The recharge factor R is defined as

$$R = C \frac{k_m}{D^2}$$

where k_m is the matrix permeability, D is the average fracture spacing, and C is a constant. Steam-entry data suggest average fracture spacing on the order of 100 m (300 ft),

yielding matrix permeabilities in the range 1–10 μd . This range of values for the matrix permeability is consistent with the measurements from other geothermal fields.

POORLY KNOWN PARAMETERS

There are several parameters that are poorly known at The Geysers and greatly affect resource evaluations using analytical or numerical models. These parameters include the initial distribution and amount of liquid water, reservoir thickness, matrix permeability, and data on the characteristics of the fracture network.

It is well known that most of the fluid reserves at The Geysers must be in liquid form, because of the large volume of steam that has already been produced. The amount of liquid and its spatial distribution is not known at present. It is commonly believed that the liquid is primarily stored in the "tight" matrix blocks, and not concentrated in a deep "water table." Pruess and Narasimhan (1982) showed that the matrix would have to possess low permeability (μd) for the matrix water to boil to steam on its way to the fractures. Analysis of noncondensable gases indicate that most of the steam originated as liquid water in the reservoir (D'Amore et al., 1982).

In vapor-dominated systems the liquid saturation in the fractures must be small (vaporstatic pressure gradient), but the liquid saturation in the matrix could be anywhere between zero and unity. This makes the determination of reservoir fluid reserves difficult.

The reservoir thickness is generally not well known for most geothermal reservoirs, and The Geysers reservoir is no exception. Estimates for the average reservoir thickness at The Geysers vary from 2 to about 6 km (1.2–4 miles). The depth to the top of the reservoir ranges from less than 330 m (1000 ft) in the Thermal area to over 1500 m (5000 ft) in the Northwest Geysers. Wells have been drilled to depths exceeding 3500 m (12,000 ft) without encountering the reservoir bottom.

Open-file data on matrix permeability is scarce, but this parameter is very important, as it, along with average fracture spacing, controls the amount of steam flow recharging the fractures. The characteristics of the fracture system are not well known. However, the connectivity of the fracture system seems to be good on the basis of pressure-decline data. Other important unknown parameters include the relative-permeability functions for the fracture networks and the matrix blocks.

CONSIDERATIONS FOR MODELING THE GEYSERS

Fractured versus Porous Media

The Geysers reservoir is characterized by high fracture permeabilities providing pathways for steam flow and low-permeability matrix blocks providing the liquid

reserves. The relatively high steam mobility can be represented by a porous-medium model, but the time- and pressure-dependent steam recharge from the matrix blocks and the associated in situ boiling cannot adequately be represented. It seems that the best approach is to use discrete (and approximate) modeling for the major faults known to be predominant steam conduits or barriers to steam flow and to represent the less predominant fractures (or faults) using double-porosity concepts. Fracture spacing and porosity may be spatially variable, as indicated by drilling results, geological features, and other data.

Model Dimensionality

In most cases one must use a three-dimensional model to simulate adequately the natural state of the reservoir and its behavior under exploitation. However, it is often beneficial to start with a two-dimensional fractured/porous-medium model and investigate its applicability. In the case of The Geysers a two-dimensional model can reasonably well assess lateral steam migration and yield good first estimates for spatial variations in fracture and matrix permeabilities. This is because vertical permeabilities at The Geysers are high and vertical pressure gradients therefore small and near vaporstatic. A two-dimensional model is less useful for investigating effects of water injection because of the strong vertical pressure and temperature gradients that develop with the associated vertical mass and heat flows.

Initial Conditions

All reservoir models require data on the appropriate initial conditions before exploitation. Over most of The Geysers the initial pressure was about 35 bars (msl) (500 psi msl) and was vaporstatic with depth. The corresponding temperature was about 240°C (460°F). In some areas of The Geysers much hotter reservoir conditions have been found with temperatures exceeding 300°C (600°F); an example is the deep reservoir in Northwest Geysers (Drenick, 1986). It is often beneficial to perform natural-state model studies to obtain the proper initial conditions, as well as to obtain coarse estimates of the permeability distribution. This involves balancing the natural mass and heat inflow into the system with mass and heat losses through surface manifestations and through conduction. As there are little spatial variations in pressures and temperatures at The Geysers (except for the deeper hotter zones), natural-state modeling should consider the large observed gradients in noncondensable gases and isotopes. These data may yield estimates for the initial in situ liquid saturations (reserves), which is much needed information.

TWO-DIMENSIONAL DOUBLE-POROSITY MODELS OF THE GEYSERS

As a part of our work for SLIC, LBL has developed several double-porosity models of The Geysers, using the

Multiple Interacting Continuum method (MINC; Pruess, 1983a) and the numerical simulator MULKOM (Pruess, 1983b). Here we will briefly describe the approach used and the assumptions employed in developing these models.

Reservoir Boundaries

The boundaries of the reservoir were inferred from the locations of dry wells (DW) and from the available heat-flow data. All boundaries were assumed to be no-flow boundaries both in terms of mass and heat flow.

Reservoir Thickness

Over most of The Geysers, the reservoir was assumed to be 3 km (~2 miles) thick. A thinner reservoir was assumed in some areas on the basis of geological information. The depth to the reservoir varied according to first-reported steam entries.

Initial Conditions

Near-uniform initial conditions of about 35 bars (500 psi) and 240°C (460°F) were used. A gravity equilibration was done to account for the varying elevation of the grid blocks and to ensure stable initial conditions. Different initial liquid saturations were assumed for the matrix blocks as will be described below; the initial liquid saturation in the fractures was assumed to be 2%.

Fracture Network Parameters

It is assumed that three orthogonal fracture sets are present in the reservoir, with an average fracture spacing of 100 m (330 ft) based on steam-entry data. As mentioned earlier, the fracture spacing and matrix permeability jointly affect the flow of steam from the matrix blocks to the fractures, so that if the proper fracture spacing is not used in some parts of the reservoir the matrix permeability, adjusted to match the pressure-decline data, should offset this error. A fracture porosity of 1% was assumed, but that parameter does not affect the results significantly. A matrix porosity of 5% was assumed, and the initial estimate for the matrix permeability was 3 μ d based on our estimates for the recharge factor from flow-rate-decline data. The initial estimate of the fracture kH product distribution was based upon Fetkovich analysis of flow-rate declines. Linear relative-permeability fractions were used for both the fractures and the matrix blocks.

Approach

The main unknown reservoir parameters at The Geysers are the initial liquid saturation, the matrix permeability, and the relative-permeability. Three different models were developed, the first two with initial liquid sa-

turations of 50% and 25%, respectively, and the third one with a constant average matrix permeability and variable initial liquid saturation. Thus matrix permeability and fracture kH product were the adjustable parameters for the first two models and initial liquid saturation and fracture kH product for the third. All three models used 250 gridblocks and were developed and calibrated against the pressure-decline data.

History Matching and Results

All three models could be calibrated to match the pressure-decline data, and their respective matches were similar in quality. Figure 2 shows the observed and calculated pressure-decline data for an area at The Geysers for Model 1. The match is reasonably good and representative of the history matches for all of the other areas. The results of the history matching yielded fracture permeability thickness products in the range 10–75 D-m (30,000–225,000 md-ft). Matrix permeabilities for Models 1 and 2 were in the range 1–3 μ d. For Model 3 an average matrix permeability of 1.8 μ d was used, and the initial liquid saturation was used as an adjustable parameter along with the fracture transmissivities. This yielded initial liquid saturation values ranging from about 5% to over 60% for the different areas of The Geysers.

The three models were used to predict the future behavior of the different areas of The Geysers. The performance predictions for the three models were surprisingly similar, given the drastically different assumptions made. Moreover, the results indicate that injection has significantly helped in halting the pressure decline, suggesting that increased injection would greatly enhance the long-term generating capacity of the resource.

Figure 2. Observed and calculated pressures for Area 1 for Model 1. [XBL 902-555]

CONCLUSIONS

1. Large amounts of open-file data are available for The Geysers resource, but an assessment of the future generating capability of the field is difficult because crucial parameters, such as the initial liquid saturation, the matrix permeability, and the characteristics of the fracture system, are poorly known.
2. A fractured/porous-medium model must be employed to evaluate The Geysers, because of the strong fracture-matrix interaction and low matrix permeabilities. Two-dimensional models are appropriate for initial studies, but three-dimensional models are required for reliable evaluations.
3. Several two-dimensional fractured/porous-medium models have been developed for the entire Geysers field. These models are based upon different assumptions regarding initial liquid saturations and matrix permeabilities. All three models match the observed pressure decline equally well, and the predicted reservoir performance is remarkably similar for all models. The results of the history matching yielded fracture transmissivities in the range 10–75 D-m (30,000–225,000 md-ft) and matrix permeabilities in the range 1–3 μ d.

REFERENCES

- Bodvarsson, G.S., Gaulke, S., Ripperda, M., 1989. Some considerations on resource evaluation of The Geysers. Presented at the Geothermal Resources Council 1989 Annual Meeting, Santa Rosa, California, October 1–4, 1989 (LBL-27598).
- D'Amore, F., Celati, R., and Calore, C., 1982. Fluid geochemistry applications in reservoir engineering (vapor-dominated systems). *In* Proceedings, Eighth Workshop on Geothermal Reservoir Engineering, Stanford, California, December 14–16, p. 295–308.
- Drenick, A., 1986. Pressure-temperature-spinner surveys in wells at The Geysers. *In* Proceedings, Eleventh Workshop on Geothermal Reservoir Engineering, Stanford, California, January 21–23, 1986, p. 197–206.
- Pruess, K., 1983a. GMINC — A mesh generator for flow simulations in fractured reservoirs. Lawrence Berkeley Laboratory Report LBL-15227, 64 p.
- Pruess, K., 1983b. Development of the general purpose simulator MULKOM. *In* Earth Sciences Division Annual Report 1982. Lawrence Berkeley Laboratory Report LBL-15500, p. 133–134.
- Pruess, K., and Narasimhan, T.N., 1982. On fluid reserves and the production of superheated steam from fractured, vapor-dominated geothermal reservoirs. *J. Geophys. Res.*, v. 87, no. B11, p. 9329–9339.

Fracture Flow Models of the Fracture Zone at the Migration Investigation Site

A. Davey, K. Karasaki, J.C.S. Long, M. Landsfeld, and S.J. Martel

The disposal of nuclear waste is the subject of research internationally, and many countries are considering storage in underground facilities. The need to accurately predict the long-term effects of storing waste underground has led to greater effort in developing and validating models of flow and transport in fractured rock. The Swiss National Cooperative for the Storage of Radioactive Waste (NAGRA) has hosted a variety of experiments over the past few years at its underground Grimsel Rock Laboratory directed toward improving understanding of fracture flow. Lawrence Berkeley Laboratory (LBL) has worked with NAGRA for several years to help develop site-characterization techniques at the Grimsel laboratory.

The Migration Investigation (MI) Experiment at Grimsel Rock Laboratory, Switzerland, was designed by NAGRA as an investigation of transport phenomena in fractures. The field experiments at the MI site were

designed to provide realistic information on migration and retention of radionuclides through a fractured rock matrix; to validate models for flow and transport; and to apply, evaluate, and improve current experimental and modeling methods. A fairly simple fracture zone was chosen, with wells placed so that groundwater transport could be measured over a few meters within the zone.

LBL has been investigating the use of a new inverse model for flow and advective transport through the fractures, which we have applied to data from the MI Experiment. A statistical inversion technique called simulated annealing is used to search for an equivalent-discontinuum model that simulates the observed behavior of the system (Long et al., 1982; Davey et al., 1989). Two cases using field data collected at the Migration Investigation site by NAGRA were studied (Frick et al., 1988; preliminary version, NAGRA Technical Report 87-14 by Keusen et al.,

1989; Vomvoris, personal communication, 1989). For the first case we used annealing to match the steady-state head distribution resulting from drawdown to the drift intersecting the MI fracture zone. For the second we used a transient well test that was conducted by Solexperts at the MI site between January 12, 1989 and February 16, 1989 (Solexperts, 1989). This was a long-term constant-rate pumping test with eight observation wells located at different points in the same fracture.

A cross-validation technique was applied to see how well our model predicts the distribution of head in the system. We can calculate an estimated prediction error for head if we leave out some of the data we have when we build our models and use the resulting model to predict the data we left out. For example, our estimate of the prediction error for the steady-state head value at a new well is based on how successfully we can predict the steady-state value at that well by using the measurements at all the other wells.

THE SIMULATED ANNEALING ALGORITHM

We briefly describe how to use annealing to find an equivalent fracture-network model. The fracture-network model is "annealed" by continually modifying the base model, or "template," such that the modified systems behave more and more like the observed system (Tarantola, 1987). To do this, we set up a template of allowed conducting elements. Then we look at different configurations of these elements by turning some of them off, i.e., making them nonconducting. For each configuration we can compute the behavior of a well test that was also conducted in the field (Karasaki, 1987). The "energy" of the configuration is then defined as a function of the difference between the observed and the simulated responses. The problem of finding the appropriate model now becomes one of finding configurations that have low values of the energy function.

The algorithm starts from some arbitrarily selected configuration and computes the energy, which is proportional to the difference between observed and measured values. Then an alternative configuration is selected and the energy for this configuration computed. If the alternative energy is lower than the energy for the current configuration, the alternative matches the observed data better, and the algorithm will decide to move to the alternative configuration. A move to an alternative with a higher energy function will be taken randomly, with a probability that depends on the increase in energy and on a weighting parameter called the temperature. The temperature, T , is decreased as the number of iterations increases to make it more and more unlikely that an unfavorable change will be accepted. At first, a high value of T allows the algorithm to jump out of local minima and continue searching for a better region of the function. Later, lowering the temperature tends to confine the search for a minima, so that the algorithm can converge. The final configuration is then said

to be a solution to the inverse problem of finding a system that conforms to the geologic data and matches the observed hydraulic behavior. A more complete description of the simulated annealing algorithm may be found in Kirkpatrick et al., 1983.

THE MI FIELD STUDIES

Steady-State Case

The MI zone is a narrow fracture zone that strikes northeast and is intersected by two tunnels and eight boreholes (Keusen et al., 1989). Figure 1 shows the MI zone in the geological setting of the southern part of the Grimsel Rock Laboratory. The anisotropic fracture structure of the NE-striking fracture zones at Grimsel indicates that the MI zone would be hydrologically anisotropic. The average hydraulic conductivity along the zone probably is greater than that across it. Marked differences in the structure of the zone observed in intersecting tunnels and the presence of fault-filling materials indicate that the hydrologic properties may vary along the fracture zone.

We have modeled the MI zone as a two-dimensional system. The template for the MI site was based on the geology of the MI zone. The grid has a coarse border that surrounds a fine mesh in the vicinity of the eight wells and the drift. The region with the fine mesh is where we expect

Figure 1. Geologic setting of the southern part of the Grimsel Rock Laboratory. [XBL 898-7693]

annealing to be able to resolve the finest details in the pattern of conductance. The conductance was chosen to be the same for each element. We used the annealing algorithm to develop channel models for the steady state and the transient case.

In the steady-flow case, the heads at the various wells were measured in response to drawdown to the drift that intersects the fracture. The heads measured at the end of the recovery period were used for the steady-state case. For the transient case we used a transient well test that was conducted by Solexperts at the MI site between January 12 and February 16, 1989. This was a long-term constant-rate pumping test with eight observation wells located at different points in the same fracture (Fig. 2).

A crude estimate of the model outer-boundary condition was obtained using the method of images. The medium is assumed to be homogeneous, and the water table is assumed to be flat and constant in the model. The boundary condition along the perimeter of the modeled area is relatively constant except for the left and right sides, where the effects of the nearby drifts are felt.

The annealing algorithm was used five times to find configurations that matched the observed data. The five solutions have similar geometries: one of the solutions is shown in Fig. 3. We can see that the annealed models show a lack of connection between wells 7, 11 and wells 4, 6, 9. Annealing has also revealed a lack of connection between well 11 and the boundary. This is happening because well 11 had a very low head, close to zero. As the drift boundary is zero head and the outer boundaries are held at a head of 100 m, steady-state annealing encourages a connection to the drift. All the solutions give well-test results that are within the measurement error of the observations.

Figure 2. Constant-flow withdrawal test followed by a buildup test. [XBL 8910-3872]

Figure 3. One of five solutions with similar geometries. [XBL 902-454]

An estimate of prediction error for steady-state response is calculated using a statistical method called cross-validation (Stone, 1974). At the MI site, we have eight wells and a drift. We use the steady-state observed pressure response, H_{obs}^i , at each well, i , under conditions of steady flow to the drift. We calculate the prediction error associated with using our annealing model to predict the steady-state head response at an arbitrary nearby point.

We used cross-validation to estimate a prediction error for predictions made using one solution and for predictions made by generating five solutions and using the median value as the predictor. The one-solution estimated prediction error was 4.3 m, and that for the median of five solutions was 3.3 m. The prediction error for well 11 was very large and tends to have a big effect on the average prediction error.

The large average prediction error reflects the abrupt change in permeability of the zone somewhere between wells 11 and 7 and wells 4, 6, and 9. If we attempt to predict the steady-state head response in this region, we may be far off the mark. However, predictions made in other areas of the zone are probably much more accurate.

Transient Case

The annealing solution for the transient case and the well-test results for the solution are given in Figs. 4 and 5. The transient data were derived from a pumping test in well 9. Annealing these data required constructing an energy function that differences head measurements taken at different times and locations. A larger region has been modeled in order to avoid problems with "seeing" the boundaries.

Figure 4. The annealed configuration for the transient case at iteration number 15510. [XBL 8910-3876]

Figure 4 shows that the annealing procedure attempted to disconnect the wells from the boundary. There are only three connections left to the outer boundary from wells 4, 9, 6, 8, 10, and 5. This may be indicating a low-permeability zone surrounding the high-permeability zone. Or the boundary conditions, which are based on data collected several years ago, may be too high. The minimum energy mesh also shows that most of the vertical elements between wells 9 and 5 were deleted. This has the effect of removing much of the storage capacity between the wells

Figure 5. Simulated well-test response on the annealed configuration. [XBL 8910-3877]

while maintaining a strong hydrological connection. This is necessary to minimize the energy, since well 5 is such a great distance from the pumping well but behaves similarly to wells 4 and 6, which are much closer. We can see that the low head at well 11 has been taken care of by isolating this well from the rest of the network, a solution quite different from the steady-state response.

Another interesting feature of this network is that annealing was unable to match the response of well 7. Even though well 7 is physically close to the pumping well, 9, it is hydraulically isolated. Annealing is not able to find a tortuous enough path to account for this. This can be handled through mesh refinement in the vicinity of well 7. The tortuosity might be due to the fact that the real flow system is three dimensional and analysis is restricted to two dimensions. However, we would have to construct an unrealistically fine mesh to account for the much lower permeability surrounding well 7. Another approach is to allow mesh elements to have different properties. A variable-aperture pipe model is currently being tested for the transient pressure response at the MI site.

CONCLUSION

The application of these techniques to fracture hydrology represent a new approach to finding equivalent models. The models are not equivalent porous-media models. Nor do they require knowledge of all details of the fracture network. The models are simplifications of the discontinuous pattern of the conductors. They are designed to capture the first-order behavior of the system, which both equivalent-continuum and discrete-fracture models have failed to do. The results of the analysis of the MI data are preliminary but offer encouragement for the utility of this new approach. It is clear, however, that annealing is able to identify much about the connectivity in the vicinity of the wells.

REFERENCES

- Davey, A., Karasaki, K., Long, J., Landsfeld, M., Mensch, A., and Martel, S., 1989. Analysis of the hydraulic data of the MI experiment. Lawrence Berkeley Laboratory Report LBL-27864 (NDC-15).
- Frick, U., Baertschi, P., and Hoehn, E., 1988. Migration investigations. NAGRA Special Bulletin, p. 23-34.
- Keusen, H.R., Ganguin, J., Schuler, P., and Buletti, M., 1989. NAGRA Technical Report 87-14, 120 p.
- Karasaki, K., 1987. A new advection-dispersion code for calculating transport in fracture networks. Lawrence Berkeley Laboratory Report LBL-22090.
- Kirkpatrick, S., Gelatt, D.C., and Vecchi, M.P., 1983. Optimization by simulated annealing. *Science*, v. 220, p. 661-680.
- Long, J.C.S., 1983. Investigation of equivalent porous medium permeability in networks of discontinuous

fractures (Ph.D. Thesis). University of California at Berkeley. Lawrence Berkeley Laboratory Report LBL-16259.

Long, J.C.S., Remer, J.S., Wilson, C.R., and Witherspoon, P.A., 1982. Porous media equivalents for networks of discontinuous fractures. *Water Resour. Res.*, v. 18, no. 3, p. 645-658 (LBL-12874).

Solexperts, 1989. 566 NAGRA Migration Long Term Constant Q Test in BOMI 87.009, Test Analysis and Description., 2/20/1989. Solexperts.

Stone, M., 1974. Cross-validatory choice and assessment of statistical predictions. *J. R. Stat. Soc., Series B*, (2), p. 111-147.

Tarantola, A., 1987. *Inverse Problem Theory*. Elsevier, New York.

Unsaturated-Zone Thermal-Energy Storage: Modeling the 1989 Module Experiment

C. Doughty, A. Nir, and C. F. Tsang*

Seasonal heat storage is an important element in the utilization of alternative energy sources with low-temperature heat supplies, as it addresses the common problem of out-of-phase energy supply and demand. Unsaturated-zone soils have been identified as the most suitable medium for this purpose in warm climatic zones, where the use of groundwater aquifers is generally not feasible (Nir et al., 1986). Since 1981, detailed theoretical development of such a storage system has been underway, in a cooperative effort between Lawrence Berkeley Laboratory (LBL) and Ben-Gurion University of the Negev (BGU) (Doughty et al., 1983; Nir et al., 1986). In the proposed storage system heat transfer to the soil is performed through a heat exchanger constructed of a 3-cm-diameter polybutylene pipe, wound into a 1-m-diameter, 12-m-long helical configuration and inserted into a 16-m-deep well. The top of the heat exchanger is 4 m below the ground surface. The well is then refilled with the original soil, with the option to add a phase-change material in the future to increase the heat-storage capacity of the system.

In 1987 a three-year Binational Science Foundation project began, aimed at validating this heat-storage concept by means of a field experiment. The project is called the module experiment; it is being conducted at the Beer-Sheva campus of BGU. During the first 2 years of the project, site evaluation, including assessment of local geology and meteorology, and engineering design work for the heat exchanger and well construction were carried out. In 1988 a scaled-down storage system was constructed, consisting of a 6-m-long heat exchanger emplaced in a 10-m-deep well. Moisture sensors and thermocouples were positioned near the heat exchanger before the well was refilled with soil. No phase-change material was included, because none was found to be practical for the planned temperatures of opera-

tion (initial soil temperature 20°C, energy supply temperature 65-75°C).

From February to November 1989 a storage cycle consisting of 8 months of charge followed by 1 month of discharge was conducted.

Throughout the three-year project LBL has conducted mathematical modeling studies to complement the field work, primarily using the computer code PT (Bodvarsson, 1982). Although PT is designed to calculate coupled fluid and heat flows in a fully saturated medium, for the present work fluid flow is restricted to the heat exchanger and heat flow in the soil is purely by conduction, with constant thermal properties representative of a soil-water-air mixture.

In 1987 previously developed numerical models of unsaturated-zone thermal-energy storage were applied to the specific conditions of the module experiment. Additionally, local soil-temperature profiles were analyzed to determine soil thermal properties and surface-temperature time dependence (Nir et al., 1988).

In 1988 two of the basic assumptions made for the mathematical model of the module experiment were examined. First, the model assumes that the heat transfer in the soil is purely by conduction, with constant thermal properties. In a partially saturated soil, however, convective heat transfer and phase-change effects may also be important. A simplified version of the problem, with a one-dimensional radial geometry, was examined using the computer code TOUGH (Pruess, 1987), which includes both convection and phase change. Results showed that for the regime of temperature (20-75°C) and moisture content (>50% liquid saturation) under consideration, conduction appears to be the dominant heat-transfer mechanism. Second, the helical heat exchanger is modeled as a cylindrical conduit, enabling use of an axisymmetric model. This assumption was tested by a detailed comparison of the modeled heat transfer from one turn of the helix compared with that for the equivalent length of cylindrical conduit.

*Also at Institute of Desert Research, Ben-Gurion University of the Negev, Israel.

The cylindrical-conduit approximation was seen to be justified. The results also demonstrated the feasibility of using larger spacing between turns of the helix, yielding a decrease in cost and weight of the heat exchanger.

In 1989 the module experiment was modeled. A uniform temperature of 21.5°C was assumed for the soil initial condition. Heat-exchanger inlet temperature and flow rate were time-averaged and specified as boundary conditions for the numerical model (Fig. 1). The experiment was interrupted several times by electrical breakdowns, providing unintentional tests of short-term responses of the storage system. Ground-surface temperature provided another boundary condition for the models; it was assumed to vary sinusoidally, with a mean temperature of 22.7°C, an amplitude of variation of 10.2°C, a 1-year period of variation, and a maximum temperature on July 10. These parameters were determined from the 1987 analysis of soil-temperature profiles, which also provided an estimate for soil diffusivity of $8.6 \times 10^{-7} \text{ m}^2/\text{s}$.

Figure 2 shows the calculated temperature distribution in the soil surrounding the heat exchanger at the end of the charge period; observed temperatures from the field experiments at various thermistor locations are also shown. Figure 3 shows the calculated and observed values of the heat-exchanger outlet temperature as a function of time. Note that the inlet location for the charge period becomes the outlet location for the discharge period, and vice versa. Also shown are calculated and observed temperatures from observation well A at a depth of 4 m (see Fig. 2 for location).

Generally, the calculated temperatures agree with the observed ones. Both the short-term and long-term changes in temperature are properly calculated, but there is a systematic 1–2°C underprediction of the absolute value of the temperature at sensor locations within the heat exchanger. Sensitivity studies using a range of values for soil thermal properties are underway. Although the in situ value of soil

Figure 2. Calculated temperature distribution around the heat exchanger at the end of the charge period of the module experiment. Observed temperatures for various thermistor locations, shown as black dots, are also shown (temperatures are in °C). [XBL 901-6703]

diffusivity was estimated from the 1987 temperature-profile studies described above, the actual value within the heat exchanger may differ because of variations in temperature, moisture content, or soil density resulting from the excavation and refilling procedure. Further studies considering effects such as unexpected heat flow from the upper 4 m of the center pipe of the heat exchanger are also being investigated.

Figure 1. Heat-exchanger inlet temperature and flow rate for the module experiment (gray lines) and the time-averaged values input to the numerical model (heavy black lines). [XBL 901-6702]

Figure 3. Calculated and observed values of heat-exchanger outlet temperature as a function of time during the module experiment. The 4-m-depth temperature in observation well A is also shown. [XBL 901-6704]

REFERENCES

- Bodvarsson, G.S., 1982. Mathematical modeling of the behavior of geothermal systems under exploitation (Ph.D thesis). University of California at Berkeley. Lawrence Berkeley Laboratory Report LBL-13937.
- Doughty, C., Nir, A., Tsang, C.-F., and Bodvarsson, G.S., 1983. Heat storage in unsaturated soils: Initial theoretical analysis of storage design and operational methods. *In* Proceedings, International Conference on Subsurface Heat Storage in Theory and Practice, June 6-8, Stockholm, p. 518-523 (LBL-14957).
- Nir, A., Doughty, C., and Tsang, C.-F., 1986. Seasonal heat storage in unsaturated soils: Example of design study. *In* Proceedings, 21st Intersociety Energy Conversion Engineering Conference, August 25-29, San Diego, California, p. 669-675 (LBL-21026).
- Nir, A., Doughty, C., and Tsang, C.-F., 1988. Unsaturated-zone thermal energy storage: Model development and field validation. *In* Earth Sciences Division Annual Report 1987. Lawrence Berkeley Laboratory Report LBL-24200.
- Pruess, K., 1987. TOUGH user's guide. Lawrence Berkeley Laboratory Report LBL-20700.

The Semianalytical Similarity Solution for Two-Phase Fluid and Heat Flow: A Tool for High-Level Nuclear Waste Studies

C. Doughty and K. Pruess

The Yucca Mountain Project is investigating the feasibility of constructing a geologic repository for heat-generating high-level nuclear wastes at Yucca Mountain, Nevada, in a partially saturated, highly fractured volcanic formation. We have developed a semianalytical similarity solution to an idealized version of the problem of fluid and heat flow near the waste packages; this solution is capable of addressing a wide range of problems relevant to repository design (Doughty and Pruess, 1989). Certain simplifications necessary for the similarity solution preclude its use for rigorous predictions of repository behavior, but other important applications exist. Although the similarity solution treats a geometrically simplified problem, all the complex physical mechanisms for coupled two-phase fluid and heat flow are taken into account in a rigorous way. Thus the similarity solution may be used to study the impact of various flow and heat-transport parameters on physical conditions near the waste canisters. Furthermore, the ability to rigorously solve a class of highly nonlinear two-phase fluid and heat-flow problems has important applications in the verification of complex numerical simulations, such as the TOUGH code (Pruess, 1987).

THERMAL AND HYDROLOGIC CONDITIONS NEAR WASTE PACKAGES

The ambient temperature in the formation around the repository is well below the saturation temperature, hence water is primarily in the liquid phase and the initial heat transfer in the host rock is mainly conductive. As temperatures around the repository increase to the saturation temperature (approximately 94°C at the elevation of Yucca Mountain), evaporation increases and vapor partial pressure becomes appreciable. Heat-pipe effects may contri-

bute to or even dominate heat transfer in this regime. In the heat-pipe region, heat transfer is primarily convective. Near the canister, liquid water vaporizes, causing pressurization of the gas phase and gas-phase flow away from the canister. The water vapor condenses in cooler regions away from the canister, depositing its latent heat of vaporization there. This sets up a saturation profile, with liquid saturation increasing away from the canister. The saturation gradient drives the backflow of the liquid phase toward the canister through capillary forces. The liquid then vaporizes again and repeats the cycle. This convective heat transfer is much more efficient than conduction, so it occurs under nearly isothermal conditions. With time the heat pipe moves away from the waste canister, leaving a gas-phase zone in which heat transfer is again conduction-dominated.

THE SIMILARITY-SOLUTION APPROACH

In the similarity solution, the region surrounding the waste packages is modeled as an infinite homogeneous medium with uniform initial conditions and thermohydrologic properties; the waste canisters are modeled as an infinitely long linear heat source of constant (time-independent) strength. Gravity effects are neglected, so that the system has a one-dimensional radial symmetry. With these simplifications, the coupled partial differential equations governing fluid and heat flow for radial geometry can be transformed into simpler ordinary differential equations through the use of a similarity variable, $\eta = r/\sqrt{t}$. The resulting equations are nonlinear, so a numerical integration from $\eta = 0$ to $\eta = \infty$ is required to solve them. Because some of the boundary conditions are specified at the $\eta = 0$ limit of integration and the remainder at the $\eta = \infty$

limit, an iterative integration scheme is used, which is known as the shooting method (Press et al., 1986).

NEW FEATURES

Initially we considered a one-component two-phase fluid (water, present as liquid or vapor) saturating the formation surrounding the repository (Doughty and Pruess, 1989). This led to a set of four coupled first-order differential equations to describe heat and fluid flow (two equations for mass conservation and flow and two for energy conservation and flow). Subsequently, the approach was extended to a two-component two-phase fluid (water and air, both of which may be present in the liquid or gas phase). This increases the number of equations to six: two for mass conservation and flow for each component and two for energy conservation and flow. Although there is a notable increase in computations required when solving six equations instead of four, there is no real conceptual difference between the similarity solutions with and without air. In practice, the coupling between the various equations becomes more complicated when air is included, requiring more careful use of the similarity solution. The inclusion of air has some interesting effects on conditions around the repository (see below).

Our earlier work was limited to relative permeability curves that have a residual liquid saturation of zero ($S_{lr} = 0$; Doughty and Pruess, 1989). With this constraint, there is no two-phase region in which liquid is immobile, making solution of the coupled differential equations straightforward. Recently we have achieved an extension to the more realistic case of finite residual liquid saturation. The similarity-solution algorithm has been encoded in a computer program "SIM4A," which is being released for general use. Internal and external documentation of the program is available (Doughty, 1990).

ILLUSTRATIVE RESULTS

Figure 1 shows an example of a similarity solution with a residual liquid saturation of $S_{lr} = 30\%$ and realistic boundary conditions including air (see Table 1 for additional specifications). The horizontal axis is $z = \ln(\eta) = \ln(r/\sqrt{t})$, so that these profiles may be viewed as spatial profiles for a given time, with radial distance increasing from left to right, or as a time sequence for a given point in space, with time increasing from right to left. Figure 1a shows temperature, pressure, liquid-saturation, and air-mass-fraction profiles. Figure 1b shows heat-flow and water-flow profiles; at this scale air flow is too small to see. The large linear temperature gradient in the single-phase gas zone ($z < -12$) indicates that heat transfer is conduction-dominated there. The more gradual temperature decline for $-12 < z < -8$ indicates that convective heat transfer, the heat-pipe process, accounts for much of the heat transfer in this region, while for $z > 8$ conduction again dominates. Figure 1b shows that the only region where mass flows are large is in the heat-pipe region,

Figure 1. (a) Profiles of temperature, pressure, saturation, and air-mass-fraction. (b) Profiles of heat flow (Q_g), water flow (Q_w), liquid-phase flow (Q_l), and gas-phase flow (Q_r) for the problem described in Table 1. Note that $Q_w = Q_l + Q_g$. [Part a, XBL 902-455; part b, XBL 902-456]

where a countercurrent flow of liquid and gas is seen. The sharp air-mass-fraction profile that coincides with the outer edge of the heat pipe illustrates how the heat pipe effectively purges the near-canister region of air.

Temperature, pressure, and saturation profiles for the same problem without air are shown in Fig. 2. In this problem, single-phase liquid conditions prevail at $\eta = \infty$; all other boundary conditions and material properties are given in Table 1. The extent of the heat pipe is much greater in this case.

Figure 3 shows a comparison of the similarity solution with results of the numerical simulator TOUGH (Pruess, 1987). A description of the material properties and boundary conditions used for this case may be found in Doughty (1990).

Figure 2. Temperature, pressure, and saturation profiles for a problem without air. [XEL 902-457]

Figure 3. A comparison of the similarity solution (solid lines) with results of the numerical simulator TOUGH (closed circles). [XBL 902-458]

Table 1. Boundary conditions and material properties used for the similarity-solution results shown in Fig. 1.

Boundary Conditions	
$z = \ln(\eta) = -\infty$	$Q_{wo} = 0$ $Q_{ae} = 0$
$z = \ln(\eta) = +\infty$	$Q_{eo} = 500 \text{ W/m}$ $P_0 = 101,325 \text{ Pa}$ $T_0 = 26^\circ\text{C}$ $S_{l0} = 0.8$
Material Properties	
Permeability	10^{-15} m^2
Porosity	0.40
Characteristic Curves [†]	
k_{rl}	$\sqrt{S_l^*} [1 - (1 - (S_l^*)^{1/\lambda})^\lambda]^2$
k_{rg}	$1 - k_{rl}$
P_c	$-P_0 [(S_l^*)^{-1/\lambda} - 1]^{1-\lambda}$
S_l^*	$(S_l - S_{lr}) / (S_{ls} - S_{lr})$
S_{lr}	0.3
S_{ls}	1.0
λ	0.45
P_0	13.93 bars

[†]van Genuchten, 1980.

REFERENCES

- Doughty, C., and Pruess, K., 1989. A similarity solution for two-phase fluid and heat flow near high-level nuclear waste packages emplaced in porous media. Int. J. Heat Mass Transfer, in press (LBL-26057).
- Doughty, C., 1990. SIM4A users guide. Lawrence Berkeley Laboratory Report LBL-28384.
- Press, W.H., Flannery, B.P., Teukolsky, S.A., and Vetterling, W.T., 1986. Numerical Recipes: The Art of Scientific Computing. Cambridge University Press, New Rochelle, New York, Ch. 16.
- Pruess, K., 1987. TOUGH user's guide. U.S. Nuclear Regulatory Commission Report NUREG/CR-4645; Lawrence Berkeley Laboratory Report LBL-20700.
- van Genuchten, M.Th., 1988. A closed-form equation for predicting the hydraulic conductivity of unsaturated soils. Soil Sci. Soc. Am. J., v. 44, p. 892-898.

Numerical Simulation of Steam Injection for the Removal of Organic Liquids from the Subsurface

R.W. Falta, K. Pruess, I. Javandel, and P.A. Witherspoon

Subsurface contamination by nonaqueous-phase liquids (NAPLs), such as organic solvents and hydrocarbon fuels, is a serious problem in the United States and other industrialized countries. The complete removal of these chemicals by conventional technologies is difficult, time-consuming, and expensive. Recently, the sweeping of contaminated areas with steam has been examined as an alternative remediation method. Several laboratory-scale experiments (Hunt et al., 1988; Basel and Udell, 1989; Udell, personal communication, 1989) and a field experiment (Udell and Stewart, 1989) have demonstrated that steam treatment may be an effective cleanup method. A schematic illustration of a possible steam-injection remediation system is shown in Fig. 1. To gain a better quantitative understanding of the steam-injection process, and to aid in the design of future experiments and remedial efforts, we have developed a numerical simulator that can model all of the complex fluid- and heat-flow processes arising in a steam-sweep operation. This article presents a brief description of the simulator along with some numerical results obtained using the simulator. Full details of the numerical formulation along with several examples of the code's application may be found in Falta (1990).

NUMERICAL FORMULATION

The numerical simulator, which will be referred to as STMVOC, has been developed for the purpose of modeling true three-phase flow in systems undergoing rapid changes

Figure 1. Diagram of a possible steam-injection remediation system. [XBL 903-712]

in temperature. The simulator is based on a general integral-finite-difference multiphase formulation known as MULKOM (Pruess, 1983, 1988). Several versions of MULKOM have been developed for solving various multiphase flow problems. The features and capabilities of these different versions have been summarized by Pruess (1988).

In the present formulation, the multiphase system is assumed to be composed of three mass components: air (or some other noncondensable gas), water, and a slightly miscible organic chemical. These three components may be present in different proportions in any of the three phases, gas, water, and NAPL. The components and phases present in the STMVOC simulator are listed in Table 1. Each phase flows in response to pressure and gravitational forces according to the multiphase extension of Darcy's law, including effects of relative permeability and capillary pressure between the phases.

Transport of the three mass components occurs by advection in all three phases and by multicomponent diffusion in the gas phase. It is assumed that the three phases are in local chemical and thermal equilibrium and that no chemical reactions are taking place other than interphase mass transfer. Mechanisms of interphase mass transfer for the organic chemical component include evaporation and boiling of the NAPL, dissolution of the NAPL into the liquid-water phase, condensation of the organic chemical from the gas phase into the NAPL, and equilibrium phase partitioning of the organic chemical between the gas, water, and solid phases. Interphase mass transfer of the water component includes the effects of evaporation and boiling of the water phase, dissolution of water in the NAPL (not usually important), and condensation of water vapor from the gas phase. The interphase mass transfer of the air component consists of equilibrium phase partitioning of the air between the gas, liquid-water, and NAPL phases.

Heat transfer occurs due to conduction, multiphase convection, and gaseous diffusion. The heat-transfer effects of phase transitions between the NAPL, water, and

Table 1. Components and phases.

Components	Phases
Air	Gas
Water	Aqueous
Organic chemical	NAPL
Heat	

gas phases are fully accounted for by considering the transport of both latent and sensible heat. The overall porous-media thermal conductivity is calculated as a function of water and NAPL saturation and depends on the chemical characteristics of the NAPL.

Secondary water and NAPL phase parameters such as saturated vapor pressure and viscosity are calculated as a function of temperature, whereas parameters such as specific enthalpy and water density are computed as functions of both temperature and pressure. The density of the NAPL phase is assumed to be a function of temperature only. The gas-phase properties, such as specific enthalpy, viscosity, density, and component molecular diffusivities, are considered to be functions of temperature, pressure, and gas-phase composition. The solubility of the organic chemical in water may be specified as a function of temperature and the gas-water Henry's constant for the organic chemical is calculated as a function of temperature. The gas-water and gas-NAPL Henry's constant for air is assumed to be constant, as is the water solubility in the NAPL phase.

By virtue of the fact that the integral-finite-difference method (Narasimhan and Witherspoon, 1976) is used for spacial discretization, the present formulation makes no reference to a global coordinate system other than the direction of the gravitational acceleration vector, and no particular dimensionality is required. The STMVOC simulator may be used for one-, two-, or three-dimensional anisotropic, heterogeneous porous or fractured systems having complex geometries. The porous-media porosity may be specified to be a function of pore pressure and temperature, but no stress calculations are made. The simulator has been verified by comparisons with analytical solutions for one-dimensional two-phase flow (Buckley and Leverett, 1942) and with a semianalytical solution for a two-phase heat pipe with a noncondensable gas (Udell and Fitch, 1985).

VALIDATION WITH A ONE-DIMENSIONAL LABORATORY EXPERIMENT

The results of a series of laboratory-scale column experiments were recently reported by Hunt et al. (1988). The experiments were designed to evaluate the mobilization and transport of a NAPL during water- and steam-flooding. These experiments were conducted in a sand-packed glass column with a length of 91 cm and diameter of 5.1 cm. The sand in the column had a porosity of 0.385 and a permeability of about $1.6 \times 10^{-11} \text{ m}^2$ and was initially water saturated. The column was fully instrumented with pressure transducers and thermocouples providing detailed pressure and temperature measurements during the experiments. A diagram of the experimental geometry is shown in Fig. 2. Further details of the experimental apparatus and methodology are given by Hunt et al. (1988).

Figure 2. Experimental geometry used by Hunt et al. (1988). [XBL 903-713]

Three experiments were performed, each using a different NAPL: trichloroethylene (TCE), a mixture of benzene and toluene, and gasoline. In each experiment, 18 ml of the NAPL was injected into the column centerline 27.0 cm from the inlet. This was followed by cold-water injection at a Darcy velocity of 15 m/d for several pore volumes. The flow rate was then lowered to about 1.5 m/d prior to steam injection. During the TCE experiment, cold water was injected at a rate of 15 m/d for 9.5 pore volumes, and at a rate of 1.5 m/d for 3 pore volumes. Following the cold-water injection, steam with a quality of about 0.5 (a specific enthalpy of about 1560 kJ/kg) was injected at a rate of 0.127 kg/h until some time after steam breakthrough at the outlet. The water mass flow rate used during the steam injection is equivalent to that used during the 1.5 m/d waterflood.

For the purpose of validating the STMVOC simulator, the TCE experiment was modeled. The one-dimensional mesh consisted of 50 elements with a uniform mesh spacing of 1.82 cm. During the course of the simulation, several boundary conditions were required to model the different experimental conditions (i.e., NAPL injection, water injection, steam injection). The three-phase capillary pressure curves were calculated by using functions given by Parker et al. (1987). The values of the empirical constants used in the calculation of the capillary pressures are those suggested by Parker et al. (1987) for use in sandy systems. The three-phase NAPL relative permeability was computed by Stone's first method (Stone, 1970) with the normalization of Aziz and Settari (1979). The water- and gas-phase relative permeabilities were taken to be the respective scaled saturations cubed (see, for example, Stewart and Udell, 1988). The residual TCE phase saturation (below which separate-phase TCE flow cannot occur) was assumed to be 0.05. Most of the TCE thermophysical constants required by the STMVOC code are given by Reid et al. (1987).

Figure 3 shows the simulated TCE phase saturation after the waterflood and the temperature profile and TCE phase saturation during the steamflood. In the simulation, the TCE becomes distributed over a large portion of the column at a saturation of slightly more than 0.05 during the high-flow-rate waterflood. At this point, the separate-

Figure 3. Calculated NAPL saturation after waterflood, and calculated temperature profile and NAPL saturation during steamflood. [XBL 903-714]

phase TCE is nearly immobile and the transport of TCE in the column is dominated by dissolution of the upstream edge of the TCE and advection in the flowing water phase. When steam is injected into the column and the steam-condensation front reaches the zone containing the TCE, the TCE is very effectively mobilized. As the steam front propagates through the column, the TCE (which has a normal boiling point of 87°C) forms a sharp NAPL bank just ahead of the steam-condensation front. In the narrow zone occupied by the TCE, transport of the TCE occurs primarily due to advection in the gas-phase and separate-phase TCE flow. As the trailing edge of the TCE boils and evaporates, it is carried ahead by the gas phase to a cooler part of the column, where it condenses. Due to the rapid drop in temperature ahead of the steam-condensation front, and the strong dependence of TCE vapor pressure on temperature, the region in which TCE boiling, evaporation, and condensation occur tends to be very small. This results in an increase in the TCE phase saturation in this area to a value greater than the residual saturation. As a result of this increased TCE saturation and the decreased TCE liquid viscosity at the higher temperatures, separate-phase TCE flow is facilitated.

Stewart and Udell (1988) present a theoretical evaluation of the mechanisms of NAPL displacement by steam injection and conclude that the maximum possible NAPL saturation ahead of the steam-condensation front is determined mainly by the ratio of NAPL and water viscosities. The maximum NAPL saturation shown in Fig. 3 of about 0.3 is in approximate agreement with their theoretical results.

Figure 4 shows a comparison of the experimental data with the numerical simulation results for the pressure gradient between the first two pressure transducers. As explained by Hunt et al. (1988), the pressure-gradient data re-

Figure 4. Comparison of numerical solution with the experimental data of Hunt et al. (1988) for the pressure gradient between the first two pressure transducers. [XBL 903-715]

flect three distinct multiphase-flow conditions. The early part of the curve, from about 12.5 to about 12.65 displaced pore volumes is indicative of single-phase liquid-water flow between the pressure ports. The center part of the curve, from about 12.65 to about 13.0 displaced pore volumes, reflects multiphase flow between the pressure ports. The large rise in the pressure gradient from about 12.65 to about 12.7 displaced pore volumes occurs as the steam front passes the first pressure transducer and is a result of the rapid change in capillary pressure at this location.

From about 12.7 to about 12.9 displaced pore volumes, the pressure gradient continues to increase as a high-velocity steam zone develops between the pressure ports. At about 12.9 displaced pore volumes, the steam front passes by the second pressure transducer, and the capillary pressure gradient between the transducers diminishes. In the final part of the curve, from about 13.0 to 13.5 displaced pore volumes, the pressure gradient becomes nearly constant at a value of about 25 kPa/m and is representative of single-phase high-velocity steam flow between the transducers. The calculated pressure gradient shown in Fig. 4 reflects the different flow conditions discussed above and approximately matches the experimental data.

Figure 5 shows the measured and calculated cumulative volume of TCE removed from the column during the experiment. Prior to steam injection at 12.5 displaced pore volumes, TCE was removed from the column by dissolution and advection in the water phase only. Hunt et al. (1988) report that the concentration of TCE in water leaving the column was at the TCE solubility limit. After about one pore volume of fluid was displaced by the steam injection, and just before steam breakthrough at the outlet, separate-phase TCE was produced. The numerically calculated result is in good quantitative agreement with the experimental data. The experimentally measured and numerically calculated locations of the steam-condensation front are compared in Fig. 6. Again, the numerical simulation closely matches the experimental data.

Figure 5. Comparison of numerical solution with the experimental data of Hunt et al. (1988) for the cumulative volume of TCE removed from the column. [XBL 90-716]

SUMMARY

A numerical simulator has been developed for modeling three-phase flow in nonisothermal systems. The code has been successfully verified with analytical solutions for multiphase flow and heat transfer. The simulator has been validated in part by the simulation of a laboratory-column steamflood experiment involving TCE. In addition to the validation effort summarized here, we have been able to successfully simulate a series of two-dimensional steamflood experiments performed by Basel and Udell (1989) and by Udell (personal communication, 1989). These two-dimensional experiments included the effects of gravity, variable initial water saturation, and heterogeneity. The two-dimensional simulation results are presented in Falta (1990).

With validation of the code nearly complete, our future efforts in this area will largely be directed toward the simulation of field-scale experiments and the effective design of remedial systems.

Figure 6. Comparison of numerical solution with the experimental data of Hunt et al. (1988) for the location of the steam-condensation front in the column. [XBL 903-717]

REFERENCES

- Aziz, K., and Settari, A., 1979. Petroleum Reservoir Simulation. Applied Science Publishers, London.
- Basel, M.D., and Udell, K.S., 1989. Two dimensional study of steam injection into porous media. Presented at the 1989 ASME Winter Annual Meeting, Multiphase Transport in Porous Media, San Francisco, California.
- Buckley, S.E., and Leverett, M.C., 1942. Mechanism of fluid displacement in sands. AIME Trans., v. 146, p. 107-116.
- Falta, R.W., 1990. Multiphase transport of organic chemical contaminants in the subsurface (Ph.D. thesis). University of California at Berkeley.
- Hunt, J.R., Sitar, N., and Udell, K.S., 1988. Nonaqueous phase liquid transport and cleanup, 2. Experimental studies. Water Resour. Res., v. 24, no. 8, p. 1259-1269.
- Narasimhan, T.N., and Witherspoon, P.A., 1976. An integrated finite difference method for analyzing fluid flow in porous media. Water Resour. Res., v. 12, no. 1, p. 57-64.
- Parker, J.C., Lenhard, R.J., and Koppusamy, T., 1987. A parametric model for constitutive properties governing multiphase flow in porous media. Water Resour. Res., v. 23, no. 4, p. 618-624.
- Pruess, K., 1983. Development of the general purpose simulator MULTOM. Earth Sciences Division Annual Report 1982. Lawrence Berkeley Laboratory Report LBL-15500.
- Pruess, K., 1988. SHAFT, MULTOM, TOUGH: A set of numerical simulators for multiphase fluid and heat flow. Lawrence Berkeley Laboratory Report LBL-24430.
- Reid, R.C., Prausnitz, J.M., and Poling, B.E., 1987. The Properties of Gases and Liquids. McGraw-Hill, New York.
- Stewart, L.D., and Udell, K.S., 1988. Mechanism of residual oil displacement by steam injection. SPE Res. Eng., November, p. 1233-1242.
- Stone, H.L., 1970. Probability model for estimating three-phase relative permeability. J. Pet. Technol., v. 22, no. 1, p. 214-218.
- Udell, K.S., and Fitch, J.S., 1985. Heat and mass transfer in capillary porous media considering evaporation, condensation and non-condensable gas effects. Heat Transfer in Porous Media and Particulate Flows, ASME HTD Vol. 46.
- Udell, K.S., and Stewart, L.D., 1989. Field study of *in situ* steam injection and vacuum extraction for recovery of volatile organic solvents. University of California, UCB-SEHRL Report No. 89-2.

Numerical Modeling Studies on Cerro Prieto

S.E. Halfman-Dooley, M.J. Lippmann, and G.S. Bodvarsson

More than 150 deep wells have been drilled in the Cerro Prieto geothermal field, Mexico (Fig. 1). About 85 wells are now supplying steam to three power plants in the field (total installed electrical generating capacity: 620 MWe). Three major reservoirs (or reservoir zones) have been identified at Cerro Prieto: (1) the α reservoir, the shallowest one, between about 1000 and 1500 m depth, restricted to the western part of the field (i.e., area west of the railroad tracks); (2) the β reservoir, extending over the entire field, between about 1500 and 3000 m depth; and (3) the γ reservoir, found below 3000 m depth only in the eastern and southeastern parts of the field.

A three-dimensional numerical model of Cerro Prieto was constructed on the basis of the hydrogeologic model developed by Halfman et al. (1984, 1986b). According to that model, under pre-exploitation conditions, the hot fluids originate at great depths in the eastern portion of the system, recharging the reservoirs in the field (Fig. 2) through the SE-dipping normal fault H.

METHODOLOGY

The three-dimensional, multiphase simulator MULKOM (Pruess, 1988) was used to compute the heat and mass flow in the system. First, a natural steady-state model of Cerro Prieto was developed. It was calibrated by varying the rock properties and boundary conditions of the model until reasonable matches between calculated and observed temperatures and pressures (Rivera et al., 1982; M. A. Ayuso, personal communication, 1988) were obtained. After that, the 1973–1987 exploitation of the field

Figure 1. Plan view of the computational mesh used in this study. [XBL 849-9022C]

Figure 2. Schematic west-east cross section of the Cerro Prieto field, showing geothermal fluid flow and cold groundwater (GW) recharge prior to exploitation (top) and during exploitation (bottom) (from Lippmann et al. 1989). [XBL 891-7427A]

was simulated. The results of the model were compared with the observed reservoir pressure and enthalpy changes (Bermejo et al., 1979; M. A. Ayuso, personal communication, 1988).

Computational Mesh

The three-dimensional computational mesh incorporates the most important geologic features that control the flow of fluids and heat in Cerro Prieto. These are the lithology (permeable sandy layers and less permeable shales; Fig. 3) and the normal faults H and L (Halfman et al., 1984; Figs. 1 and 2). The horizontal dimensions of the mesh are 9000 m (NW-SE) by 8600 m (NE-SW); the vertical extent is from 800 to 4000 m in depth.

In the first simulation runs, the rock properties assigned to the various mesh zones were similar to the ones used by Lippmann and Bodvarsson (1983), but these were adjusted as the modeling work progressed, in order to match the observed and computed temperatures and pressures. The results of the model giving the best matches indicate that the permeability of the sandy materials varies

Figure 3. Southwest-northeast cross section through the grid elements just north of the fault H. Hatched zones represent layers of lower permeability. [XBL 861-10527]

between 1 and 100 md and that of the shale layers between 0.005 and 1 md. The horizontal permeability of the three reservoirs (α , β , and γ) is 100 md; the vertical value is between 1 and 10 md. These permeabilities agree reasonably well with the results of well tests and with values used in earlier simulations of the field (Lippmann and Bodvarsson, 1983; Ayuso, personal communication, 1988). A constant rock density of 2650 kg/m³ was used for all materials. Thermal conductivities ranged from 2.35 to 3.00 W/m°C, depending on rock type (these values are somewhat high, especially for shaly materials, but the effect on the results is minimal). Constant-temperature and constant-pressure boundary elements are located along all sides of the computational mesh (i.e., surrounding the internal elements), except in some areas along the bottom.

RESULTS

Natural-State Model

The natural-state model provides quantification of the fluid (and heat) movement and the distribution of temperatures, pressures, and steam saturations in the system before commercial fluid production started in March 1973. The validity of the model is supported by comparison with the geothermal fluid-flow pattern inferred by the hydrogeologic study of Halfman et al. (1984) and the reasonable match obtained with best known initial temperatures and pressures at Cerro Prieto (Bermejo et al., 1979; F.J. Bermejo, personal communication, 1982; M.A. Ayuso, personal communication, 1988.)

The observed and calculated temperatures for the α and β reservoirs match fairly well (Halfman-Dooley et al., 1989). For example, Fig. 4 shows close correspondence between the observed and calculated temperature distributions for the α reservoir (1300 m depth). Both figures show an elongation of the isotherms in a NE-SW direction. At this level, the hotter part of the field corresponds to the α reservoir. To the east of the railroad tracks (see Fig. 1), the calculated isotherms at 1300 m depth extend farther east than the observed ones. Future simulations will rectify this situation. For the α reservoir, the observed pressures increase toward the center of the mesh, ranging from 122.3 to about 126 bars. The calculated pressures differ by only a few bars and show a similar trend. The three-dimensional numerical model for the natural state shows a

Figure 4. (Left) Observed temperature distribution (in °C) at 1300 m depth, based on data from M.A. Ayuso (personal communication, 1988). (Right) Calculated temperature distribution (in °C) at 1300 m depth. [Left, XBL 901-55; right, XBL 901-56]

fluid-circulation pattern that corresponds to that in the hydrogeologic model of Halfman et al. (1984). Figure 2 is a schematic diagram of the model, with arrows indicating the direction of geothermal fluid flow.

Exploitation Model

In the second phase of this numerical modeling study, fluid production at Cerro Prieto was simulated between 1973 and 1987; the study by Halfman et al. (1986a) considered production only up to 1979. Actual production data from individual wells was simulated by assigning appropriate fluid sinks to various mesh elements. The α reservoir was the first to be exploited; and its exploitation continues today. Production from the β reservoir started in 1978. The bulk of the fluid is now being produced from this deeper reservoir. In the model, the β reservoir has been subdivided into four sections. A given area is assigned to one of these sections, depending on whether it is east or west of the railroad tracks or in the upthrown or downthrown block of fault H (Fig. 1).

The material properties and boundary conditions used for the exploitation model were identical to those of the natural-state model. The hot-water recharge (80 kg/s of 350°C water) into the deepest, easternmost mesh element of fault H was assumed to be constant and unaffected by reservoir drawdown. The constant-pressure and constant-temperature boundaries were considered to be adequate for simulating the early exploitation history. These boundary conditions will be modified to allow computation of the post-1987 behavior of Cerro Prieto.

Response of the α reservoir

In response to production-induced drawdown, the model indicated a rearrangement in the direction of fluid movement, similar to what is shown in Fig. 2. Figure 5

Figure 5. Observed (well M-38 and data of Bermejo et al., 1979) and calculated pressure histories for the α reservoir. [XBL 901-57]

shows the observed and calculated pressures in the α reservoir at 1200 m depth. The solid curve represents the pressures given by Bermejo et al. (1979), and the crosses represent reported well M-38 pressures. The solid curve shows for the 1973–1979 period a pressure drawdown of about 22 bars (from about 110 to 88 bars). On the other hand, well M-38 shows between 1973 and 1977 an initial drawdown of about 6 bars (from 97 to 91 bars), followed by pressure recovery. These results reflect the effects of changes in fluid production rates and an increasing influx of colder groundwaters.

In the α reservoir the observed enthalpy histories vary from well to well, but in most wells enthalpies rarely exceed 400 kcal/kg (about 1675 kJ/kg). Some wells show fairly constant enthalpy values; other wells show a decrease. Finally, for a number of wells, higher enthalpies were observed in the mid-1970s, which then decreased and soon afterwards leveled off. We chose well M-26 out of this last group and considered it to represent the enthalpy behavior of the α reservoir (Fig. 6).

Figure 6 also shows the calculated enthalpy history for the main portion of the α reservoir between fault L and the sandy gap. Cold-water recharge through fault L and from the west is reflected by a decrease in enthalpy starting about 1976, both in the observed M-26 enthalpies and in the calculated enthalpies. The model shows a similar trend. It agrees fairly well with the observed changes except around the 1975–1976 period, when higher enthalpies were observed associated with localized reservoir boiling (Grant et al., 1984; Truesdell et al., 1989; Lippmann et al., 1989).

Response of the β reservoir

The results from one of the four sections of the β reservoir, the eastern upthrown block, are given here. The other cases are described in Halfman-Dookey et al. (1989). Figure 7 shows the 1973–1987 observed and calculated

Figure 6. Observed (well M-26) and calculated enthalpy histories for the α reservoir. [XBL 901-58]

Figure 7. Observed (wells M-150 and M-133) and calculated pressure histories for the eastern upthrown block of the β reservoir. [XBL 901-59]

pressures for the eastern upthrown block of the β reservoir at 2100 m depth. Between 1979 and 1982 the observed representative pressures for the area near well M-150 (data from wells M-150 and M-133) show a slight decrease from 188 to 180 bars. Then they steeply decline to about 155 bars in 1986 (Fig. 7). This rapid and sudden decrease in pressure reflects the coming on line of power plant CPHI, as production greatly increased from about 105 kg/s in 1985 to 840 kg/s in 1986. The calculated and observed pressures match extremely well. The calculated pressures in the vicinity of M-150 show a pressure decline from 196 bars in 1973 to 178 bars in 1985, followed by a sharp decrease to 149 bars in 1986 (Fig. 7). In the eastern upthrown block of the β reservoir, two slightly different trends are seen in the enthalpy histories of observed wells. In the main portion of this part of the producing field (north of fault H, up to wells such as M-120 and M-150, Fig. 1), a trend toward increasing enthalpies is observed: up to 600 kcal/kg (about 2510 kJ/kg; e.g., well M-120, Fig. 8). The data indicate reservoir boiling due to stepped-up fluid production and the lack of significant fluid recharge into this portion of the reservoir.

Farther away from fault H, near the northern edge of the field (near well M-133, Fig. 1), increasing enthalpies are also observed, but in this area the enthalpies are lower; they do not exceed 450 kcal/kg (about 1880 kJ/kg; e.g., well M-133, Fig. 9). The location of the northern boundary of the field is inferred by the sudden and sharp deepening of the 300°C isotherm, from about 2000 m in well M-133 to below 3800 m in M-172 (Halfman et al., 1986b), indicating that the hot fluids probably do not migrate north much beyond well M-133. The observed enthalpies indicate that reservoir boiling has occurred at least during 1986 and 1987. The lower observed enthalpies in this region, as compared to the zone nearer to the fault, indicate that there is cold-water recharge in this northern fringe area of the geothermal system.

Figure 8. Observed (well M-120) and calculated enthalpy histories for the eastern upthrown block of the β reservoir near fault H. [XBL 901-125]

For the portion of the eastern upthrown block of the β reservoir nearest to fault H, the calculated increases in enthalpy are slightly delayed with respect to the observed ones (Fig. 8). This delay can be explained by mesh discretization effects. The calculated enthalpies for this area tend to be constant between 1979 and 1985 (around 385 kcal/kg; about 1610 kJ/kg) and then start to increase in 1986 (Fig. 8). This trend reflects the boiling in the model starting in 1986.

In the region farther away from the fault (e.g., near well M-133), the calculated and observed enthalpies (well M-133) match closely (Fig. 9). The enthalpies between 1978 and 1985 are constant (around 380 kcal/kg; about 1590 kJ/kg) and then rise to 460 kcal/kg (about 1925 kJ/kg) by 1988; the model shows reservoir boiling beginning in 1986.

Figure 9. Observed (well M-133) and calculated enthalpy histories for the eastern upthrown block of the β reservoir farther to the north of fault H (near M-133). [XBL 901-126]

CONCLUSIONS

Although the computational mesh needs to be refined, it reproduces the basic geologic features of this complex high-temperature system. For pre-exploitation (natural state) conditions the model gives fluid-flow patterns consistent with those of the hydrogeologic model of Halfman et al. (1984, 1986b). There is relatively good correspondence between the calculated and observed temperature and pressure distributions throughout the field. The 1973–1987 exploitation period has been simulated using the geometry and parameters of the natural-state model. Fluid production was modeled by incorporating time-dependent sinks in different mesh elements. There is a general good match between the observed and computed reservoir pressures and enthalpies. We tentatively conclude that the reservoir management plan for the Cerro Prieto system needs to be re-evaluated to reduce pressure drawdown that results in reservoir boiling and significant encroachment of colder groundwaters into the system. This issue is being discussed with the Comisión Federal de Electricidad, operator of the field.

REFERENCES

- Bermejo M., F.J., Navarro O., F.X., Castillo B., F., Esquer, C.A., and Cortéz A., C., 1979. Pressure variations at the Cerro Prieto reservoir during production. *In* Proceedings, Second Symposium on the Cerro Prieto Geothermal Field, Mexicali, Mexico, Oct. 17–19, 1979, p. 473–493.
- Grant, M.A., Truesdell, A.H., and Manón, A., 1984. Production induced boiling and cold water entry in the Cerro Prieto geothermal reservoir indicated by chemical and physical measurements. *Geothermics*, v. 13, p. 117–140.
- Halfman, S.E., Lippmann, M.J., Zelwer, R., and Howard, J.H., 1984. A geologic interpretation of the geothermal fluid movement in Cerro Prieto field, Baja California, Mexico. *Assoc. Pet. Geol. Bull.*, v. 68, p. 18–30 (LBL-15201).
- Halfman, S.E., Lippmann, M.J., Bodvarsson, G.S., 1986a. Quantitative model of the Cerro Prieto field. *In* Proceedings, 11th Workshop on Geothermal Reservoir Engineering, Stanford, California, January 21–23, 1986, p. 127–134 (LBL-20523).
- Halfman, S.E., Manón, A., and Lippmann, M.J., 1986b. Update of the hydrogeologic model of the Cerro Prieto field based on recent well log data. *Geoth. Resour. Counc. Trans.*, v. 10, p. 369–375 (LBL-21499).
- Halfman-Dooley, S.E., Lippmann, M.J., and Bodvarsson, G.S., 1989. Progress report on LBL's numerical modeling studies on Cerro Prieto. *In* Proceedings, Final Symposium—Agreement US/DOE and CFE Mexico in the Field of Geothermal Energy, San Diego, CA, April 4–5, 1989, p. 247–267 (LBL-27159).
- Lippmann, M.J., and Bodvarsson, G.S., 1983. Numerical studies of the heat and mass transport in the Cerro Prieto geothermal field, Mexico. *Water Resour. Res.*, v. 19, no. 3, p. 753–767 (LBL-15509).
- Lippmann, M.J., Truesdell, A.H., Manón M., A., and Halfman, S.E., 1989. The hydrogeologic-geochemical model of Cerro Prieto revisited. Presented at the 14th Workshop on Geothermal Reservoir Engineering, Stanford, California, January 24–26, 1989 (LBL-26819).
- Pruess, K., 1988. SHAFT, MULKOM, TOUGH: A set of numerical simulators for multiphase fluid and heat flow. *Geotermia, Rev. Mex. de Geoenergía*, v. 4, no. 1, p. 185–202 (LBL-24430).
- Rivera, R., Bermejo, F., Castillo, F. Pérez, H., and Abraján, A., 1982. Actualización en la distribución de temperaturas en el campo geotérmico de Cerro Prieto II y III. *In* Proceedings, Fourth Symposium on the Cerro Prieto Geothermal Field, Comisión Federal de Electricidad, Guadalajara, Mexico, August 10–12, 1982, p. 281–301.
- Truesdell, A.H., Terrazas, B., Hernández, L., Janik, C., Quijano, L., and Tovar, R., 1989. The response of the Cerro Prieto reservoir to exploitation as indicated by fluid geochemistry. *In* Proceedings, Final Symposium—Agreement US/DOE and CFE Mexico in the Field of Geothermal Energy, San Diego, CA, April 4–5, 1989, p. 123–132.

Hydrologic Characterization of Faults and Other Potentially Conductive Geologic Features in the Unsaturated Zone

I. Javandel and C. Shan

The capability of characterizing near-vertical faults and other potentially highly conductive geologic features in the vicinity of a high-level-waste repository is of great importance in underground waste-isolation site-characterization projects. The existence of such features near a repository

may provide a short travel-time flow path from the disturbed zone to the accessible environment.

Measurements of air-pressure changes at depth due to atmospheric-pressure fluctuations have been used before to estimate the permeability of geologic strata (Weeks,

1978). In those studies the assumption was made that no open borehole, fractures, or other geologic structures exist that would provide preferred flow paths for air movement. When a conductive fault cuts through layers of geologic materials with lower permeability, points located in the fault zone will experience pressure variations sooner and more strongly than points in the rock mass located at the same elevation. It is desirable to obtain a solution that allows the calculation of pressure response due to the atmospheric-pressure variations in a multilayer geologic system with a cross-cutting highly conductive fault. As a first step, we have developed a series of analytical solutions to calculate the propagation of atmospheric-pressure changes in a single-layer system that is intersected by a vertical fault or other planar conductive features. Comparison of pneumatic pressure variations between the fault zone and the surrounding rock mass could provide a means for estimating the permeability of the fault zone. This article summarizes two of these new analytical solutions.

MATHEMATICAL MODELS

Let us consider a single horizontal geologic layer that is cut by a vertical fault zone with a thickness of $2b'$, as shown in Fig. 1. We would like to derive solutions to calculate air-pressure changes due to atmospheric-pressure fluctuations as a function of time and position within the system. The medium is extensive both horizontally and vertically such that mathematically it could be assumed to be infinite in both directions. Since the mid-plane of the fault zone is a symmetry plane, only half of the system will be considered in the analysis. A Cartesian coordinate system is selected such that its origin is at the intersection of the ground surface, with the contact plane between the fault and the rock mass. The x' axis is horizontal and perpendicular to the rock/fault-zone interface, and the z' axis is oriented vertically downwards.

The partial differential equations governing the isothermal flow of air in the unsaturated porous media may be written as (Weeks, 1978)

Figure 1. Schematic cross section of the fault zone and surrounding rocks. [XBL 902-459]

$$\frac{\partial^2 \phi'^2}{\partial x'^2} + \frac{\partial^2 \phi'^2}{\partial z'^2} = \frac{\mu_a n_a}{k' \bar{p}} \cdot \frac{\partial \phi'^2}{\partial t'} \quad (1)$$

where $\phi' = (p/\rho_a g) - z' =$ pneumatic head, L; $\bar{p}$ = mean pressure of the system, M/L.T²; μ_a = viscosity of air, M/L.T; n_a = interconnected air-filled porosity at the prevailing moisture content; k' = air permeability of the medium at the prevailing moisture content, L²; and t' = time, T. The following assumptions are inherent in the development of Eq. (1):

1. The medium is homogeneous and isotropic with a constant moisture content.
2. The air permeability of the medium is large enough that the Klinkenberg (1941) effect is negligible.
3. The absolute pressure is small enough that the ideal gas laws apply.
4. The change in pressure with depth has a negligible effect on air density.

In our study, similar to that of Weeks (1978), we have assumed that pneumatic head varies only slightly from its mean value. Under this condition, Eq. (1) may be approximated to the following form, which is linear with respect to ϕ' .

$$\frac{\partial^2 \phi'}{\partial x'^2} + \frac{\partial^2 \phi'}{\partial z'^2} = \frac{1}{\alpha'} \cdot \frac{\partial \phi'}{\partial t'} \quad (2)$$

where $\alpha' = k' \bar{p} / \mu_a n_a$ is pneumatic diffusivity.

Furthermore, flow in the fault zone is assumed to be one-dimensional in the vertical direction, whereas the flux crossing the fault-rock interface is treated as a sink term in the governing equation for the fault zone. The validity and impact of the above assumptions on the results have been studied and reported elsewhere (Shan, 1990; Javandel and Shan, 1990). On the basis of the above assumptions, the mathematical model for the system under consideration may be written as follows. In a dimensionless form, the partial differential equations for the rock mass and the fault zone are

$$\frac{\partial^2 \phi_r}{\partial x^2} + \frac{\partial^2 \phi_r}{\partial z^2} = \frac{1}{\alpha} \cdot \frac{\partial \phi_r}{\partial t} \quad (3)$$

$$\frac{\partial^2 \phi_f}{\partial z^2} + k \left[\frac{\partial \phi_r}{\partial x} \right]_{x=0} = \frac{\partial \phi_f}{\partial t} \quad (4)$$

where the subscripts r and f refer to the rock mass and the fault zone, respectively. Dimensionless terms applied in the formulations are defined as

$$x = \frac{x'}{b'}, \quad z = \frac{z'}{b'}, \quad k = \frac{k'_r}{k'_f}, \quad \phi = \frac{\phi' - \phi'_0}{\phi'_b - \phi'_0}, \quad t = \frac{\alpha'_f t'}{b'^2}, \quad \alpha = \frac{\alpha'_r}{\alpha'_f} \quad (5)$$

where ϕ'_0 and ϕ'_b refer to the initial and upper boundary values of the pneumatic head.

As noted above, two types of boundary conditions have been considered for the variation of atmospheric pressure at the ground surface. Type one refers to a step function and type two to sinusoidal pressure variations. Except for the boundary conditions at the ground surface, the rest of boundary and initial conditions for both cases are the same, and may be written as

$$\phi_r(x, z, 0) = \phi_f(z, 0) = 0, \quad (6)$$

$$\phi_r(\infty, z, t) = \text{finite}, \quad (7)$$

$$\phi_r(x, \infty, t) = \phi_f(\infty, t) = 0, \quad (8)$$

$$\phi_r(0, z, t) = \phi_f(z, t). \quad (9)$$

The type-one boundary condition at the ground surface in nondimensional form translates to

$$\phi_r(x, 0, t) = \phi_f(0, t) = 1. \quad (10)$$

To simplify derivations of the type-two boundary condition, one may introduce a new definition for dimensionless pneumatic head:

$$\phi = \frac{\phi' - \phi'_0}{\phi'_a}, \quad (11)$$

where ϕ'_a is the amplitude of pressure-head variation, $p_a/\rho_a g$. The type-two boundary condition may now be written as

$$\phi_r(x, 0, t) = \phi_f(0, t) = \sin(\omega t). \quad (12)$$

SOLUTIONS

Case 1: Step-function atmospheric-pressure variation

The solution for case 1 may be presented as

$$\begin{aligned} \phi_r(x, z, t) = & \operatorname{erfc}\left[\frac{z}{2\sqrt{\alpha t}}\right] + \operatorname{erfc}\left[\frac{x}{2\sqrt{\alpha t}}\right] \\ & - \operatorname{erfc}\left[\frac{z}{2\sqrt{\alpha t}}\right] \operatorname{erfc}\left[\frac{x}{2\sqrt{\alpha t}}\right] \\ & + \frac{2(1-\alpha)}{\pi} \int_0^{\infty} [f_1(x, \rho, t) + f_2(x, \rho, t)] \sin(\rho z) d\rho, \quad (13) \end{aligned}$$

where

$$f_1(x, \rho, t) = \frac{\rho}{B_1(B_1 - B_2)} \exp\left[\frac{x}{\sqrt{\alpha}} B_1 + B_1^2 t - \alpha \rho^2 t\right] \times \operatorname{erfc}\left[B_1 \sqrt{t} + \frac{x}{2\sqrt{\alpha t}}\right] \quad (14)$$

$$f_2(x, \rho, t) = \frac{-\rho}{B_2(B_1 - B_2)} \exp\left[\frac{x}{\sqrt{\alpha}} B_2 + B_2^2 t - \alpha \rho^2 t\right] \times \operatorname{erfc}\left[B_2 \sqrt{t} + \frac{x}{2\sqrt{\alpha t}}\right], \quad (15)$$

in which B_1 and B_2 are defined as

$$B_1, B_2 = \frac{1}{2} \left[\frac{k}{\sqrt{\alpha}} \pm \sqrt{\Delta} \right] \quad (\Delta > 0), \quad (16)$$

$$B_1, B_2 = \frac{1}{2} \left[\frac{k}{\sqrt{\alpha}} \pm i \sqrt{-\Delta} \right] \quad (\Delta < 0), \quad (17)$$

with the determinant Δ defined by

$$\Delta = \frac{k^2}{\alpha} + 4(\alpha - 1)\rho^2. \quad (18)$$

The expression for the pneumatic head in the fault zone may be readily obtained from Eq. (13) by setting $x = 0$.

Case 2: Sinusoidal atmospheric-pressure variation

The procedure for solving the mathematical model with sinusoidal atmospheric-pressure variation is very similar to the one described above, and the expression for pneumatic head in the rock mass becomes

$$\begin{aligned} \phi_r(x, z, t) = & e^{-z \sqrt{\frac{\omega}{2\alpha}}} \sin\left[\omega t - z \sqrt{\frac{\omega}{2\alpha}}\right] + \frac{2\alpha\omega}{\pi} \int_0^{\infty} \frac{ue^{-\alpha u^2 t} \sin(uz)}{\omega^2 + \alpha^2 u^4} du \\ & + \omega \int_0^t \operatorname{erfc}\left[\frac{x}{2\sqrt{\alpha t}}\right] \left[1 - \operatorname{erfc}\left[\frac{z}{2\sqrt{\alpha t}}\right]\right] \cos[\omega(t-\tau)] d\tau \\ & + \frac{2(1-\alpha)\omega}{\pi} \int_0^{\infty} \sin(\rho z) d\rho \\ & \times \int_0^t [f_1(x, \rho, \tau) + f_2(x, \rho, \tau)] \cos[\omega(t-\tau)] d\tau. \quad (19) \end{aligned}$$

RESULTS AND DISCUSSION

Figures 2 through 5 present some of the results obtained for case 1, i.e., step-function atmospheric-pressure variation. Figure 2 shows variation of dimensionless pneumatic head versus dimensionless depth within the fault zone for three values of dimensionless time and for a fixed ratio of rock to fault-zone permeability $k = 0.02$. Figure 3 presents the variation of dimensionless pneumatic head with dimensionless distance from the fault-rock interface at a dimensionless depth of 20 and three values of dimensionless time. Corresponding values of pneumatic head in the absence of the fault are also shown. Figure 4 shows the change in pneumatic head with distance away from the rock/fault-zone contact for different levels of permeability ratio at the dimensionless depth of $z = 20$. To examine the effect of permeability contrast between the fault zone and the surrounding rocks, we have intentionally kept $\bar{p}/\mu_a n_a$ the same in the two regions.

As is apparent in Fig. 4, at a given time, the gradient of pressure variation in the direction perpendicular to the fault increases with the permeability contrast (i.e., decreasing k). The gradient, however, decreases with time, as shown in Fig. 3. Figure 5 presents time variation of pneumatic head within the fault zone and at points away from the fault at the depth corresponding to $z = 20$ and permeability ratio $k = 0.01$.

Figures 6 and 7 present results obtained from evaluation of the solution for case 2 (sinusoidal atmospheric-pressure variation). Figure 6 shows time variation of pneumatic head in the fault zone at three different depths for a permeability ratio $k = 0.02$. Figure 7A illustrates time variation of pneumatic head within the fault zone and at other points away from the fault at the same depth, for $z = 20$ and $k = 0.01$. Figure 7B shows results for the same set of parameters except for the permeability ratio of 0.005. Note

Figure 2. Variation of dimensionless pneumatic head versus dimensionless depth within the fault zone for three values of dimensionless time. [XBL 902-460]

Figure 3. Variation of dimensionless pneumatic head versus dimensionless distance from the fault zone at $z = 20$, for three values of dimensionless time. [XBL 902-461]

that when the permeability of the rock adjacent to the fault zone is significantly less than that of the fault zone, points located away from the fault will experience a smaller amplitude of pressure changes. The farther the points from the fault, the smaller the amplitudes. Furthermore, there is also a phase lag in the observed pressure changes. The farther the point from the fault, the larger the lag in the observed pressure changes. Such phenomena seem to magnify when the permeability contrast increases (i.e., k decreases).

Examination of Figs. 4, 5 and 7 reveals that when the contrast between permeability of the fault zone and surrounding rock is significant, the spatial pressure variation in the vicinity of the fault zone could be large enough to

Figure 4. Effect of permeability contrast on dimensionless pneumatic head. [XBL 902-462]

Figure 5. Dimensionless pneumatic head versus dimensionless time within the fault zone and three points within the rock mass at the same depth for $z = 20$ and $k = \alpha = 0.01$. [XBL 902-463]

lend itself to measurement by conventional instruments. Therefore, air-pressure data from isolated intervals in horizontal or inclined boreholes drilled through a fault zone may be analyzed to obtain the permeability ratio between the fault zone and surrounding rocks.

Figure 6. Dimensionless head versus dimensionless time in the fault zone at three dimensionless depths. [XBL 902-464]

Figure 7. Time variation of pneumatic head within the fault zone and two other points away from the fault at the same depth for $z = 20$ and (A) $k = \alpha = 0.01$, (B) $k = \alpha = 0.005$. [Part A, XBL 902-465; part B, XBL 902-466]

REFERENCES

- Javandel, I., and Shan, C., 1990. Hydrologic characterization of faults and other potentially conductive geologic features in the unsaturated zone. *In* Proceedings of the International High Level Radioactive Waste Management Meeting, April 8–12, 1990, Las Vegas, Nevada, p. 1185–1191.
- Klinkenberg, L.J., 1941. The Permeability of Porous Media to Liquids and Gases. American Petroleum Institute Drilling and Production Practice.
- Shan, C. 1990. Characterization of leaky faults (Ph.D. thesis). University of California at Berkeley.
- Weeks, E.P., 1978. Field determination of vertical permeability to air in the unsaturated zone. U.S. Geological Survey Professional Paper 1051.

Application of the PTST Solution to Field Data

K. Karasaki

Karasaki (1989) proposed a technique for analyzing the recovery data obtained from a prematurely terminated slug test (PTST). The purpose of the technique is to obtain a more-reliable estimate of the average system permeability and confirm the existence of a local heterogeneity near the well and, in some cases, to estimate the properties of the heterogeneity. This article summarizes the application of the PTST analysis technique to the field data furnished by the Nationale Genossenschaft für die Lagerung radioaktiver Abfälle (NAGRA) through the NAGRA/DOE Cooperative project. NAGRA has drilled some thirteen deep boreholes in northern Switzerland as part of the investigation of the feasibility of geologic isolation of nuclear wastes. The Leuggern borehole is drilled to a depth of 1688.9 m, penetrating the crystalline basement rock at a depth of 222 m. Since the completion of the borehole in early 1985, numerous hydraulic tests have been conducted. Readers interested in the details of the geology and the hydraulic testing are referred to the reports by NAGRA. Most of the tests conducted are slug tests and their variations such as pulse-injection/withdrawal tests and drill-stem tests (DST). The DST data from a couple of intervals are examined by using the PTST analysis method and compared with the results of conventional analyses presented in the literature.

PTST SOLUTION

Slug tests were originally developed for estimating flow parameters of shallow aquifers, which are often well approximated as homogeneous porous media. They have also been widely used to estimate the flow parameters of heterogeneous systems, such as fractured rocks. The attractiveness of slug tests is that they are inexpensive and easy to perform, and require a relatively short time to complete. On the other hand, analyses of slug-test results suffer a problem of nonuniqueness, more than other type of well tests, especially when skin is present (Karasaki et al., 1988).

Cooper et al. (1967) presented a solution for the change in water level for a finite-radius well subjected to a slug test in a homogeneous medium. Their solution assumes that there is no skin around the well. However, in fractured rocks there may exist regions around the well whose properties are different from those of the overall medium. These skin effects can be caused not only by drilling but by the inherent nature of the fracture system as well. Because the fracture permeability can be considered as a cubic function of the fracture aperture, the fracture permeability is expected to be distributed over a very wide range. Therefore, the particular fractures intersected by a well may cause skin-like effects. Several workers have investigated the effects of skin on observed fluid levels in

slug tests (Ramey and Agarwal, 1972; Ramey et al., 1975; Faust and Mercer, 1984; Moench and Hsieh, 1985; Sageev, 1986; and Karasaki, 1989).

Karasaki (1989) states that a more accurate estimate of the formation permeability can be obtained using a PTST than completing a slug test all the way to the end. Using a PTST method the transmissivity can be estimated by

$$K = \frac{(h_0 - h_i)C_w h_{wD}(10)}{2\pi b t_i (h_{10} - h_i)} \quad (1)$$

where the subscript t denotes the shut-in time, h_0 is the initial head, and h_{10} is the head value at $t/(t - t_i) = 10$. A value of unity for $h_{wD}(10)$ can be used in most cases. Otherwise the equation presented in Karasaki (1989) has to be used:

$$h_{wD}(t_D) = \int_0^\tau L_\lambda^{-1} \left\{ \frac{-\sqrt{p} K_1(\sqrt{p})}{p K_0(\sqrt{p}) + \omega_1 \sqrt{p} K_1(\sqrt{p})} \right\} \cdot L_{t_D - \lambda}^{-1} \left\{ \frac{K_0(\sqrt{p})}{\sqrt{p} K_1(\sqrt{p})} \right\} d\lambda + \int_\tau^{t_D} L_\lambda^{-1} \left\{ \frac{-\sqrt{p} K_1(\sqrt{p})}{p K_0(\sqrt{p}) + \omega_2 \sqrt{p} K_1(\sqrt{p})} \right\} \cdot L_{t_D - \lambda}^{-1} \left\{ \frac{K_0(\sqrt{p})}{\sqrt{p} K_1(\sqrt{p})} \right\} d\lambda, \quad (2)$$

where p is the Laplace space variable and L^{-1} denotes Laplace inversion. The subscript denotes the corresponding real-space variable.

APPLICATION OF THE PTST SOLUTION

In addition to pulse-injection/withdrawal tests and slug-injection/withdrawal tests, NAGRA conducted DSTs in several intervals. Although they were not terminated at the 50% fluid level as suggested in Karasaki (1989), a similar analysis method can be applied to these data. To demonstrate the application of the PTST method, DST data are chosen from a depth interval of 281.7 m for analysis and the results compared to those by Belanger et al. (1987). In this test the interval was shut in as early as 5% recovery. The numerical simulations by Belanger et al. (1987) yield reasonably good matches with the pulse-injection/withdrawal data and the flow-period data. However, they do not match the shut-in-period data very well. A much larger permeability has to be assumed in order to match the fast-recovery data. However, a permeability of 6×10^{-9} m/s was chosen for this interval. This is because

the goal of Belanger et al. (1987) was to find a single permeability that best matches all the data from an interval assumed to be a homogeneous medium, although the numerical simulator GTFM itself is capable of modeling a heterogeneous medium.

A skin would explain the discrepancy discussed above; i.e., a low-permeability model matches the pulse-injection/withdrawal data and the flow data during the DST, whereas a higher permeability explains the fast recovery after shut-in in DST. Because pulse tests and slug tests (DST flow period) are greatly affected by a low-permeability skin (Moench and Hsieh, 1986; Karasaki, 1988), the permeability value obtained by matching those data is probably a closer reflection of the permeability of the skin rather than the medium. The PTST technique calls for the recovery data to be plotted against Horner time (Fig. 1). As can be seen from the figure, the data approach a straight line from below. In theory, buildup data should approach from above, as seen in the next case. The reason why the buildup data approach from below may be that the zone was either repressurized when the valve was shut or the shut-in process was not instantaneous. Nonetheless, analysis can be attempted. The initial head h_i is 2722 kPa; the head at the start of the test, h_0 , is 1696 kPa; and the head at shut-in time, 3800 sec, is 1760 kPa. The radius of the delivery pipe is 0.05 m, and the interval length is 25 m. From Fig. 2, h_{10} is found to be 2703 kPa. Therefore, from Eq. (1) we obtain

$$K = \frac{(1696 - 1760) \text{ kPa} \cdot \pi (0.05)^2 \text{ m}^2 \cdot 1}{2\pi \cdot 25 \text{ m} \cdot 3800 \text{ sec} \cdot (2703 - 2722) \text{ kPa}}$$

$$= 4.4 \times 10^{-8} \text{ m/s}.$$

This value is about one order of magnitude larger than the previously reported value (Belanger et al., 1987). The next step is to estimate the formation specific storage and the skin parameters, i.e., the skin permeability and the radius.

Figure 1. Horner plot of the buildup data from 281.7 m. [XBL 902-556]

Figure 2. Flow-period match with curves of Ramey et al. (1975). [XBL 902-557]

However, when the storativity of the skin is equal to or smaller than that of the formation, which is often the case, it is virtually impossible to estimate these parameters separately from slug tests (Moench and Hsieh, 1986). Only the product ωe^{-2s} can be estimated. In theory this could be accomplished by employing the analysis of Ramey et al. (1972) alone, where the flow period data is used for type-curve matching. However, this is very difficult in many cases because the type curves for intermediate and large values of ωe^{-2s} are very similar to each other. In the present case, a unique match would be even more difficult because the slug test was shut in at a very early stage of the test (95% level). However, from the PTST analysis we already have the estimate of the formation permeability. Therefore, a match point can be calculated from

$$t' = \frac{2\pi T_i}{C_w} \quad (3)$$

In the present case, $T = 1.1 \times 10^{-6}$ and $C_w = 7.9 \times 10^{-3}$. Therefore, time t , which corresponds to dimensionless time t' (equal to, say, unity) is 1100 sec. Thus from Fig. 2, ωe^{-2s} is found to be 10^{-55} . In open-well tests ω generally ranges from 10^{-3} to 10^{-6} . Therefore, a skin coefficient, s , of about 60 is suggested. It is worth recalling here that in most practical cases the curves of Cooper et al. (1967) and those of Ramey et al. (1975) are identical if the curve labeled ω in the former work is relabeled as ωe^{-2s} . Therefore, exceptionally small values of ω obtained by using the analysis of Cooper and others are probably ωe^{-2s} values.

For open-well slug tests the skin coefficient, s ; skin permeability, K_s ; formation permeability, K ; and skin radius, r_s , are related by the following equation (Moench and Hsieh, 1985):

$$s = \frac{K}{K_s} \times \ln \frac{r_s}{r_w} \quad (4)$$

Therefore, various combinations of r_s and K_s produce similar results. Figure 3 shows the data and the three combinations of K_s and r_s shown in Table 1. As can be seen in the figure all the curves and data points superimpose upon

Figure 3. Three combinations of r_s and K_s matched with data. [XBL 902-558]

each other. If the skin effect is caused by the drilling, the skin radius is expected to be small. On the other hand, skin-like conditions also exist when a borehole intersects a low-permeability feature. In such a case the radius can be the size of the feature. If the feature is a low-permeability fracture, the skin radius is equivalent to the radius of the fracture. Although in many cases the formation permeability value is of primary interest, separate estimates of the skin permeability and the radius may be desirable in constructing a detailed model such as a fracture network model. A carefully designed constant-flow-rate test may be more effective in separating the two parameters (Karasaki, 1986).

Table 1. K_s and r_s and other parameters used in Fig. 3.

Case	1	2	3
K_s (m/s)	1.3×10^{-10}	5.0×10^{-10}	1.7×10^{-9}
r_s (cm)	1	10	50
S_{ss} (1/m)	6.9×10^{-7}	"	"
K (m/s)	4.4×10^{-8}	"	"
S_s (1/m)	6.9×10^{-7}	"	"
C_w (m ²)	7.9×10^{-3}	"	"
b (m)	24.8	"	"

CONCLUSIONS

The PTST technique was used to analyze the field data from the deep borehole in Leuggern, northern Switzerland. The analysis indicates that the formation permeability may be as much as one order of magnitude larger than previously thought. In a fractured rock, skin-like conditions can exist when a borehole intersects a low-permeability feature. Therefore, it is always important to check for the existence of a skin. The author recommends that slug tests not be used in fractured rocks. Long-term pumping tests are believed to be much more reliable. However, if slug tests must be used, it is recommended that the tests be terminated at the 50% level and that the recovery data be analyzed using the PTST technique.

REFERENCES

- Belanger, D.W., Freeze, R.A., Lolcama, J.L., and Pickens, J.F., 1987. Interpretation of hydraulic testing in crystalline rock at the Leuggern borehole—Appendices describing test analyses. NIB 87-17.
- Cooper, H.H., Jr., Bredehoeft, J.D., and Papadopoulos, I.S., 1967. Response of a finite diameter well to an instantaneous charge of water. *Water Resour. Res.*, v. 3, p. 263–269.
- Faust, C.R., and Mercer, J.W., 1984. Evaluation of slug tests in wells containing a finite radius skin. *Water Resour. Res.*, v. 20, no. 4, p. 504–506.
- Karasaki, K., 1986. Well test analysis in fractured media (Ph.D. thesis). University of California at Berkeley. Lawrence Berkeley Laboratory Report LBL-21442.
- Karasaki, K., Long, J.C.S., and Witherspoon, P.A., 1988. Analytical models of slug tests. *Water Resour. Res.*, v. 24, no. 1, p. 115–126 (LBL-23948).
- Karasaki, K., 1989. Prematurely terminated slug tests. Submitted to *Water Resour. Res.* (LBL-27528).
- Moench, A.F., and Hsieh, P.A., 1985. Evaluation of slug tests in wells containing a finite-thickness skin. *Water Resour. Res.*, v. 21, no. 9, p. 1459–1461.
- Ramey, H.J., Jr., and Agarwal, R.G., 1972. Annulus unloading rates as influenced by wellbore storage and skin effect. *Trans., A.I.M.E.*, v. 253, p. 453–462.
- Ramey, H.J., Jr., Agarwal, R.G., and Martin, I., 1975. Analysis of "slug test" or DST flow period data. *J. Can. Pet. Tech.*, p. 37–47.
- Sageev, A., 1986. Slug test analysis. *Water Resour. Res.*, v. 22, no. 8, p. 1323–1333.

Fractal Study and Simulation of Fracture Roughness and Apertures

S. Kumar and G.S. Bodvarsson

Surfaces of fractures and faults exhibit two distinct properties that make them amenable for analysis by the application of the theory of fractal geometry (Mandelbrot, 1982; Feder, 1988). The first is that roughness profiles of the surface seem to be nowhere differentiable, though they are continuous. The other is that the profile is self-similar at different scales over a large range of length scales (Brown and Scholz, 1985). Previous studies in the literature have established the fractal dimension of various geophysical surfaces but have relied on numerical simulations based on random number generators to simulate (Brown, 1989) and study these surfaces (Wang et al., 1988). The present analysis focuses on a deterministic representation of the roughness profile and the rough surface in order to reduce the computational effort as well as to derive semi-analytical expressions for various surface characteristics.

Fractal representation has the advantage that it preserves the statistics and the self-similarity exhibited by the surface roughness. It also enables the characteristics of surfaces and apertures to be predicted analytically from the profile characteristics. The analytical/deterministic expression of fractal formulation additionally offers a tremendous information compression, since the roughness can be uniquely recreated with the selection of a few constants. Other advantages of the deterministic fractal formulation are that the various values of interest (such as contact area) can be evaluated semianalytically, and profiles and surfaces exhibiting a "corner frequency" and weakly anisotropic surfaces can be easily simulated.

DETERMINISTIC REPRESENTATION OF ROUGHNESS PROFILES

The deterministic formulation selected for representing surface roughness in profile is the Weierstrass-Mandelbrot cosine fractal function (Berry and Lewis, 1980; Feder, 1988; Majumdar, 1989), which is expressed as

$$z(x) = A \sum_{n=-\infty}^{\infty} \frac{\cos(2\pi\beta^n x)}{\beta^{(2-D)n}}, \quad 1 < D < 2, \quad (1)$$

where D is the fractal dimension of the roughness profile, β is a nonintegral constant greater than unity, and A is a scaling constant. As the fractal dimension increases, heights of nearby points become more independent and the surface becomes increasingly jagged. The fractal dimension D equal to 1.5 represents a Brownian profile (Mandelbrot, 1982). The above function is continuous at all points but has no derivative at any point (Berry and Lewis, 1980; Feder, 1988). The difference between the Weierstrass-Mandelbrot function and conventional Fourier series is in the frequency modes. The discrete frequencies in a Fourier series increase in arithmetic progression as multiples of a

basic frequency, and the phases of different modes do not coincide at any non-origin point.

The power spectrum $\bar{S}(\omega)$ of $z(x)$ is equal to the square of its Fourier transform and is given as

$$\bar{S}(\omega) = \frac{A^2}{2} \sum_{n=-\infty}^{\infty} \frac{\delta(\omega - 2\pi\beta^n)}{\beta^{(4-2D)n}}, \quad (2)$$

where δ is the Dirac delta function. The discrete power spectrum (spectral density) can be approximated by a continuous spectrum given as (Berry and Lewis, 1980)

$$S(\omega) = \frac{A^2(2\pi)^{(4-2D)}}{2 \ln \beta} \frac{1}{\omega^{(5-2D)}}, \quad (3)$$

which is obtained by replacing the summation over n with an integration. Experimentally observed profiles of fracture and other rock surfaces show similar straight-line behavior on log-log plots (Brown and Scholz, 1985) indicating that the above representation is a valid one. The mean height of the distribution is zero and the standard deviation σ is the square root of $\langle z^2 \rangle$ obtained from the basic definition of mean square height

$$\langle z^2 \rangle = \frac{A^2}{2} \sum_{n=-\infty}^{\infty} \frac{1}{\beta^{(4-2D)n}} = \int_0^{\infty} \bar{S}(\omega) d\omega. \quad (4)$$

The autocorrelation function γ is given by

$$\gamma(\Delta x) = \frac{A^2}{2} \sum_{n=-\infty}^{\infty} \frac{\cos(2\pi\beta^n \Delta x)}{\beta^{(4-2D)n}}. \quad (5)$$

It is seen that if $\Delta x = 0$, the expression of $\langle z^2 \rangle$ is retrieved. By replacing the summation by integration an approximate mean behavior of the autocorrelation is obtained as ($\Delta x \neq 0$)

$$\gamma(\Delta x) \approx \frac{A^2(2\pi|\Delta x|)^{(4-2D)}}{2 \ln \beta} \int_0^{\infty} \frac{\cos \xi}{\xi^{(5-2D)}} d\xi. \quad (6)$$

Thus the autocorrelation varies as approximately $|\Delta x|^{(4-2D)}$ and matches the prediction of Wang et al. (1988). A profile simulated by the above is presented in Fig. 1.

ISOTROPIC SURFACES AND APERTURES

The statistical parameters, such as mean square height of a profile, are not expected to be identical to that of a surface, since the profile is expected to miss most of the highest peaks and deepest troughs on the surface. The requirement for an isotropic surface is that its two-dimensional autocorrelation must depend only on the distance of separation and must be independent of the coordinate system, i.e., $\gamma_s(\Delta r) = \gamma(\Delta x)$, where Δr is the separation distance $(\Delta x^2 + \Delta y^2)^{1/2}$; however, all deterministic func-

Figure 1. A profile simulated by the Weierstrass-Mandelbrot function corresponding to the parameters obtained from input profile (Brown, 1987): $D = 1.5$, $n_1 = -16$, $n_2 = -2$, $A = 0.03234$, and $\beta = 1.5$. [XBL 902-559]

tions show preferred orientations along the coordinate axes. The only way to generate an isotropic surface is to use a function that appears functionally anisotropic but whose anisotropy is very small as verified by subsequent analysis and numerical simulations. The fractal formulation coupled with the above requirements yields the following analytical prediction for the continuous power spectrum $S_s(\omega)$ of an isotropic surface (following the mathematical developments of Wang et al., 1988):

$$S_s(\omega) = \frac{(5-2D)B(3-D, 0.5)}{\pi} \frac{S(\omega)}{\omega}, \quad (7)$$

where B is the beta function.

Feder (1988, Ch. 13) has discussed different methods of generating fractal surfaces. In this study the following function based on the Weierstrass-Mandelbrot function suggested by Majumdar (1989) is examined in detail:

$$z_s(x, y) = F(D)A \sum_{n=-\infty}^{\infty} \frac{\cos(\sqrt{2}\pi\beta^n x)\cos(\sqrt{2}\pi\beta^n y)}{\beta^{(2-D)n}}. \quad (8)$$

Here $F(D)$ is a scaling function that compensates for the additional cosine term and accounts for the fact that the profile is not expected to go over the highest peaks and lowest valleys. The power spectrum of this rough surface representation is obtained by squaring its two-dimensional Fourier transform, i.e.,

$$\frac{\bar{S}_s(\omega_x, \omega_y)}{A^2 F^2(D)} = \frac{1}{4} \sum_{n=-\infty}^{\infty} \frac{\delta(\omega_x - \sqrt{2}\pi\beta^n)\delta(\omega_y - \sqrt{2}\pi\beta^n)}{\beta^{(4-2D)n}}. \quad (9)$$

Extending the relationship for converting the delta function in Cartesian coordinates to cylindrical to cover the above case, where only the first quadrant in the frequency plane is considered, yields

$$\bar{S}_s(\omega) = \frac{A^2 F^2(D)}{4\pi^2} \sum_{n=-\infty}^{\infty} \frac{\delta(\omega - 2\pi\beta^n)}{\beta^{(5-2D)n}}. \quad (10)$$

Approximating this expression by a continuous spectra (Eq. 3) and comparing with Eq. (7) gives the scaling function $F(D)$.

The autocorrelation is computed as

$$\frac{\bar{\gamma}_s(\Delta x, \Delta y)}{A^2 F^2(D)} = \frac{1}{4} \sum_{n=-\infty}^{\infty} \frac{\cos(\sqrt{2}\pi\beta^n \Delta x)\cos(\sqrt{2}\pi\beta^n \Delta y)}{\beta^{(4-2D)n}}. \quad (11)$$

Since $\Delta x = \Delta r \cos \theta$ and $\Delta y = \Delta r \sin \theta$, the autocorrelation averaged over all θ may be expressed as

$$\bar{\gamma}_s(\Delta r) = \frac{A^2 F^2(D)}{4} \sum_{n=-\infty}^{\infty} \frac{J_0(2\pi\beta^n \Delta r)}{\beta^{(4-2D)n}}, \quad (12)$$

where J_0 is a Bessel function. As before, the Fourier transform of the above yields $S_s(\omega)$ and vice versa. The above can be approximated as ($\Delta r \neq 0$)

$$\begin{aligned} \bar{\gamma}_s(\Delta r) &= \frac{A^2 F^2(D)(2\pi|\Delta r|)^{(4-2D)}}{4 \ln \beta} \int_0^{\infty} \frac{J_0(\zeta)}{\zeta^{(5-2D)}} d\zeta, \\ &= \frac{A^2 F^2(D)(2\pi|\Delta r|)^{(4-2D)}}{2 \ln \beta(5-2D)B(3-D, 0.5)} \int_0^{\infty} \frac{\cos \zeta}{\zeta^{(5-2D)}} d\zeta. \end{aligned} \quad (13)$$

Substituting the value of $F(D)$ demonstrates that $\bar{\gamma}_s(\Delta r) = \bar{\gamma}(\Delta r)$, verifying that the present formulation satisfies the criterion for isotropy on an average.

Using the above developments reveals that the mean square height ratio of the surface to that of the profile is equal to $F^2(D)/2$, which equals 2 for $D = 1$ and 1 for $D = 2$. This is consistent with physical intuition, since for a dimension D of 2 the profile does not miss even the highest peaks and lowest valleys, and thus the mean square heights of the profile and surface are the same. For a smooth undulating surface ($D = 1$) the mean square height of the surface is twice that of an average profile. Figure 2 presents a surface generated by the above scheme.

The aperture height distribution due to two opposing rough surfaces can now be evaluated by considering Fig. 3, where d is the dilatancy of the fracture. Contact areas are defined as those where $z_a \leq 0$. Letting the two surfaces be

Figure 2. Surface simulation by the Weierstrass-Mandelbrot function corresponding to the profile in Fig. 1. [XBL 902-560]

Figure 3. Schematic depiction of apertures. [XBI 902:561]

mirror images with shear displacements x_c and y_c , i.e., $z_2(x,y) = -z_1(x+x_c, y+y_c)$ gives the following expressions for the power spectrum and the autocorrelation:

$$\bar{S}_a(\omega_x, \omega_y) = 2[1 - \cos(\omega_x x_c + \omega_y y_c)] \bar{S}_s(\omega_x, \omega_y), \quad (14)$$

$$\begin{aligned} \bar{\gamma}_a(\Delta x, \Delta y) &= 2\bar{\gamma}_s(\Delta x, \Delta y) - \bar{\gamma}_s(\Delta x + x_c, \Delta y + y_c) \\ &\quad - \bar{\gamma}_s(\Delta x - x_c, \Delta y - y_c). \end{aligned} \quad (15)$$

CONCLUSIONS

The deterministic fractal scheme for generating roughness profiles and rough surfaces has tremendous advantages over conventional numerical algorithms for generating and visual rendering of random processes. The major advantages are the extreme compression of information, repeatability, saving of computer storage, and analytically extrapolating the information from profiles to generate rough surfaces. Another feature of the present scheme, not available via simple conventional algorithms, is the ease of

analyzing weakly anisotropic surfaces and surfaces and profiles that exhibit a corner frequency in their power spectra. The present method is thus a powerful tool in the study of rough surfaces and the various phenomena associated with them.

REFERENCES

- Berry, M.V., and Lewis, Z.V., 1980. On the Weierstrass-Mandelbrot fractal function. *Proc. R. Soc. London*, v. A-370, p. 459-484.
- Brown, S.R., 1987. A note on the description of surface roughness using fractal dimension. *Geophys. Res. Lett.*, v. 14, p. 1095-1098.
- Brown, S.R., 1989. Transport of fluid and electric current through a single fracture. *J. Geophys. Res.*, v. 94, p. 9429-9438.
- Brown, S.R., and Scholz, C.H., 1985. Broad bandwidth study of the topography of natural rock surfaces. *J. Geophys. Res.*, v. 90, p. 12575-12582.
- Feder, J., 1988. *Fractals*. Plenum Press, New York.
- Majumdar, A., 1989. *Fractal surfaces and their applications to surface phenomena* (Ph.D. thesis). University of California, Berkeley.
- Mandelbrot, B.B., 1982. *The Fractal Geometry of Nature*. W.H. Freeman, New York.
- Wang, J.S.Y., Narasimhan, T.N., and Scholz, C.H., 1988. Aperture correlation of a fractal fracture. *J. Geophys. Res.*, v. 93, p. 2216-2224 (LBL-22494).

Permeability of a Parallel-Walled Fracture with Cylindrical Asperities

S. Kumar, R.W. Zimmerman, and G.S. Bodvarsson

The flow of a Newtonian fluid through a rock fracture is of importance in many geophysical and geotechnical processes. For hydrological purposes, rock fractures have traditionally been modeled as two smooth parallel walls separated by a distance h , which leads to a permeability of $h^2/12$ (Bear, 1972). More recent work (Walsh, 1981; Chen et al., 1989) has attempted to account for the in-plane tortuosity caused by fluid flowing around the regions where the opposing rock faces are in contact (the asperities). Other models (Tsang, 1984; Brown, 1987) have considered the effect of variations in aperture, which causes the flow to be channeled through the paths of "least hydraulic resistance." These models do not, however, account for the increased viscous drag along the *sides* of the asperities. By assuming the simple model of a smooth-walled fracture propped open by cylindrical asperities, we have derived an estimate of the amount by which this viscous drag will reduce the hydraulic conductivity of a fracture.

THEORETICAL DEVELOPMENT

Consider a fracture that consists of two smooth parallel walls of infinite extent, separated by a distance h . Let the xy coordinate axes be parallel to the plane of the fracture and the z axis be perpendicular to the fracture walls, which are located at $z = \pm h/2$. The xy coordinates can be oriented so that the macroscopic pressure gradient and the mean flow are in the x direction (Fig. 1). For very low Reynolds numbers, such as are typically found in geological systems, the problem can be analyzed as follows. At each position z within the fracture, fluid "particles" follow a tortuous path around the cylindrical obstacles but have zero velocity in the z direction. The viscous resistance offered by these asperities can be accounted for by a "two-dimensional" permeability coefficient K_2 , defined so that the average velocity $\bar{u}$ (averaged locally over the transverse xy plane) for uniform, steady-state flow equals

Figure 1. Schematic diagram of a parallel-walled fracture propped open by cylindrical asperities. [XBL 896-7642]

$-(K_2/\mu)\nabla P$. Methods of estimating this permeability for random or periodic distributions of circular obstacles have been discussed by Hasimoto (1959), Sangani and Yao (1988), and others. The average velocities on the various planes parallel to the fracture walls will then vary with z due to the viscous drag between adjacent fluid "sheets." This effect can be treated within the framework of the Navier-Stokes equations, in the sense that the viscous drag between the various sheets is proportional to $\partial \bar{u}/\partial z$.

The time-dependent equations that govern flow within the fracture are obtained by combining the two-dimensional Navier-Stokes equations with the effective permeability concept, yielding (Brinkman, 1947)

$$\frac{\rho}{\phi^2} \frac{\partial \bar{u}(x, z, t)}{\partial t} = - \frac{d(p + \rho g \chi)}{dx} - \frac{\mu}{K_2} \bar{u}(x, z, t) + \frac{\mu}{\phi^2} \frac{\partial^2 \bar{u}(x, z, t)}{\partial z^2}, \quad (1)$$

where ρ is the density of the fluid, μ is the viscosity, g is the gravitational acceleration, χ is a coordinate measured in the direction of the gravitational field, and ϕ is the fraction of space in the xy plane that is not occupied by obstacles. The velocity $\bar{u}$ is averaged locally over the xy plane, and hence is a function only of x and z . This velocity is a "Darcy velocity," or "filter velocity," and can be related to the actual average velocity of the fluid particles by $\bar{u} = \phi^2 u(\text{actual})$. The second term on the right side of Eq. (1) represents the potential drop due to viscous drag

along the sides of the obstacles. One factor of ϕ was introduced by Vafai and Tien (1981) to account for the reduced area available for flow, and the second is introduced (Kumar et al., 1989) to account for "tortuosity," in the sense that the actual travel path of a fluid particle between two points $x = x_1$ and $x = x_2$ must exceed the distance $|x_2 - x_1|$. Although the identification of the tortuosity with $1/\phi$ is not exact, this idea has had some success in predicting the electrical conductivity of porous rocks. The potential gradient $d(p + \rho g \chi)/dx$ is averaged over the yz plane, and hence depends only on x .

For fully developed flow, the average velocity and the potential gradient will not vary in the x direction, and the flow field will not vary with time, so that the equation of motion takes the form

$$\frac{dH}{dx} = \frac{\mu}{\phi^2} \frac{\partial^2 \bar{u}(z)}{\partial z^2} - \frac{\mu}{K_2} \bar{u}(z), \quad (2)$$

where H represents the potential $p + \rho g \chi$. The no-slip boundary condition on the fracture walls requires that

$$\bar{u}(z = \pm h/2) = 0. \quad (3)$$

The governing equation (2) can be integrated, using the boundary condition (3), to yield the following velocity profile:

$$\bar{u}(z) = \frac{-K_2}{\mu} \frac{dH}{dx} \left[1 - \frac{\cosh\left[\phi z / \sqrt{K_2}\right]}{\cosh\left[\phi h / 2\sqrt{K_2}\right]} \right]. \quad (4)$$

In the limit as the concentration of obstacles goes to zero, $\phi \rightarrow 1$ and $K_2 \rightarrow \infty$. Since $\cosh \zeta \approx 1 + \zeta^2/2$ as $\zeta \rightarrow 0$, the velocity profile reduces to

$$\bar{u}(z) = \frac{-h^2}{8\mu} \frac{dH}{dx} \left[1 - \left(\frac{2z}{h} \right)^2 \right], \quad (5)$$

which is the well-known result for flow between two parallel walls.

FRACTURE PERMEABILITY

The total volumetric flux can be found by averaging the velocity again, this time over the z direction, yielding

$$\bar{u} = \frac{1}{h} \int_{-h/2}^{+h/2} \bar{u}(z) dz = \frac{-K_2}{\mu} \frac{dH}{dx} \left[1 - \frac{\tanh\left[\phi h / 2\sqrt{K_2}\right]}{\left[\phi h / 2\sqrt{K_2}\right]} \right]. \quad (6)$$

The equivalent "three-dimensional" fracture permeability can now be found by comparing Eq. (6) with Darcy's law,

$$\bar{u} = \frac{-K_3}{\mu} \frac{dH}{dx}, \quad (7)$$

to yield

$$K_3 = K_2 \left[1 - \frac{\tanh\left[\phi h / 2\sqrt{K_2}\right]}{\left[\phi h / 2\sqrt{K_2}\right]} \right] \quad (8)$$

The above expression reduces to the expected results in the two limiting cases of $\phi \rightarrow 1$ (no obstacles) and $h \rightarrow \infty$ (no side walls). In the former case, note that $K_2 \rightarrow \infty$ when $\phi \rightarrow 1$ with h held constant, so that the argument of the tanh function goes to zero. Use of the series $\tanh \zeta = \zeta - \zeta^3/3 + \dots$ in Eq. (8) leads to

$$K_3 \rightarrow \frac{h^2}{12} \text{ as } \phi \rightarrow 1, \quad (9)$$

which is the permeability for flow between parallel flat plates. In the other limit of $h \rightarrow \infty$ (with ϕ held fixed), $\tanh(\infty) = 1$, so that

$$K_3 \rightarrow K_2 \text{ as } h \rightarrow \infty. \quad (10)$$

In this case the permeability reduces to that of flow across an array of infinitely long, parallel circular cylinders.

It is clear that h/a is the important dimensionless parameter, so that the limit $h \rightarrow \infty$ actually corresponds to $h \gg a$. There is another important limit in which $h/a \rightarrow 0$ for fixed c , in which case Eq. (8) reduces to

$$K_3 = \frac{\phi^2 h^2}{12} = \frac{h^2}{12} (1-c)^2. \quad (11)$$

If the concentration of obstacles c is small but finite, Eq. (11) reduces to $(1-2c)h^2/12$, which is the result found by Walsh (1981) for a thin fracture containing a small concentration of randomly distributed circular asperities. Our analysis clarifies the fact that Walsh's result implicitly requires $h \ll a$.

In order to be more specific about the results, and to quantify what is meant by "large h ," we need to assume an expression for K_2 . In general, this is a difficult problem that is not yet completely solved. When the obstacle concentration is small, however, Hasimoto (1959) has shown that the permeability K_2 is given by

$$K_2 = \frac{a^2}{8c} (-\ln c - 1.476 + 2c + \dots), \quad (12)$$

where a is the radius of the obstacles, and $c = 1 - \phi$ is their areal concentration. For higher concentrations of randomly located asperities, Sangani and Yao (1988) used a lubrication-type approximation for the flow between near-by cylinders to derive

$$K_2 = \frac{a^2}{3.34c} \left[1 - 1.10\sqrt{c} \right]^{5/2}. \quad (13)$$

Whereas Eq. (12) is expected to be accurate for small values of c , Eq. (13) is asymptotically accurate for large values of c . If one of the K_2 expressions is used in conjunction with Eq. (8), the three-dimensional permeability K_3 can be predicted. In Fig. 2, K_3 is shown normalized

Figure 2. Fracture permeability K_3 , computed from Eq. (8) using two expressions for K_2 . [XBL 897-2860]

with respect to the "unobstructed" parallel plate value $h^2/12$. The permeability curve labeled $h/a = 0$ represents the limiting case where the viscous drag along the parallel faces of the fracture greatly exceeds the drag along the sides of the asperities. An increase in the parameter h/a increases the viscous drag along the asperities, and hence decreases the permeability below the "thin fracture" value. For example, physically reasonable values of $c = 0.30$ and $h/a = 1$ lead to a permeability that is 60% lower than that predicted by the basic "cubic law"; this effect is obviously not negligible.

ACKNOWLEDGMENT

This work was carried out in cooperation with scientists from the Nuclear Hydrology Program at the USGS, Denver.

REFERENCES

- Bear, J. 1972. Dynamics of Fluids in Porous Media. New York, Elsevier, p. 164-165.
- Brinkman, H.C., 1947. A calculation of the viscous force exerted by a flowing fluid on a dense swarm of particles. Appl. Sci. Res., v. A1, p. 27-34.
- Brown, S.R., 1987. Fluid flow through rock joints: The effect of surface roughness. J. Geophys. Res., v. 92, p. 1337-1347.
- Chen, D.W., Zimmerman, R.W., and Cook, N.G.W., 1989. The effect of contact area on the permeability of fractures. In Proceedings, 30th U.S. Symposium on Rock Mechanics. Rotterdam, Balkema, p. 81-88.
- Hasimoto, H., 1959. On the periodic fundamental solutions of the Stokes equations and their application to

viscous flow past a cubic array of spheres. *J. Fluid Mech.*, v. 5, p. 317–328.

Kumar, S., Zimmerman, R.W., and Bodvarsson, G.S., 1989. Permeability of a fracture with cylindrical asperities. Lawrence Berkeley Laboratory Report LBL-27626.

Sangani, A.S., and Yao, C., 1988. Transport processes in random arrays of cylinders. II. Viscous flow. *Phys. Fluids*, v. 31, p. 2435–2444.

Tsang, Y.W., 1984. The effect of tortuosity on fluid flow through a single fracture. *Water Resour. Res.*, v. 20, p. 1209–1215.

Vafai, K., and Tien, C.L., 1981. Boundary and inertial effects on flow and heat transfer in porous media. *Int. J. Heat Mass Transf.*, v. 24, p. 195–203.

Walsh, J.B., 1981. The effect of pore pressure and confining pressure on fracture permeability. *Int. J. Rock Mech.*, v. 18, p. 429–435.

The Hydrogeologic–Geochemical Model of Cerro Prieto Revisited

M.J. Lippmann, A.H. Truesdell,* S.E. Halfman-Dooley, and A. Manón M.†

The Cerro Prieto, Mexico, geothermal field (Fig. 1), has been extensively studied by the Comisión Federal de Electricidad (CFE) of Mexico and since 1977 by various U.S. groups participating in cooperative agreements between CFE and the U.S. Department of Energy (DOE). In mid-1987 the total installed capacity at the field reached 620 MWe, requiring a large rate of fluid production (more than 10,500 tonnes/h of a brine-steam mixture; August 1988). This significant mass extraction has led to changes in reservoir thermodynamic conditions and in the chemistry of the produced fluids. The exploration and development of the geothermal field and the changes resulting from its exploitation have been discussed in numerous papers and reports; recent summaries are given by Lippmann and Manón (1987) and Lippmann et al. (1989).

NATURAL-STATE HYDROGEOLOGIC MODEL

The hydrogeologic model of Cerro Prieto developed by Halfman et al. (1986) best describes the movement of geothermal fluids in the system under natural-state conditions. It was developed on the basis of geophysical, lithologic, and temperature well logs, as well as on information on well completion, and demonstrates the importance of lithology and faults in controlling fluid circulation.

The model shows that geothermal fluids in the Cerro Prieto system generally circulate from east to west. Hot (about 350°C) fluids enter the system from the east-southeast and are discharged in the area of surface manifestations located west of the wellfield (Fig. 2). The geothermal fluids seem to ascend from depth through the SE-dipping normal fault H. As the hot fluids rise, they tend to move laterally into the more-permeable layers (Fig. 2). An unknown amount recharges the deepest reservoir identified

Figure 1. Location of geothermal areas in the Salton Trough. Cerro Prieto is shown southeast of the city of Mexicali. [XBL 845-1692A]

so far (the γ reservoir, found below 3300 m depth; not shown in Fig. 2). The bulk of the hot fluids flow westward into sand unit Z (the β reservoir), following the general east-west gradient prevalent in the system; only a small fraction seems to penetrate sand unit Z southeast of the fault.

*U.S. Geological Survey, Menlo Park, California 94025

†Comisión Federal de Electricidad, Morelia, Michoacán, Mexico.

Figure 2. Southwest-northeast geologic cross section showing schematically the lithology, downhole temperature profiles, and flow of geothermal fluids (from Halfman et al., 1986). [XBL 828-10945D]

The westward movement of the geothermal fluids has an upward component, since the fluids follow the bottom of the less-permeable shale unit O, which dips toward the northeast. In the region of well M-10A (Fig. 2) a greater portion of the fluids manages to ascend because of the absence of a shale caprock; this region has been called the "sandy gap." The lesser portion of the fluids moves into the western continuation of the β reservoir (below 1600 m depth in the western area of the field).

As the hot fluids ascend through the gap, boiling occurs. The vertical flow of the geothermal fluids is stopped at about 1000 m depth by low-permeability sandy materials sealed by mineral precipitation. At this point, the fluids continue to flow westward through a shallower permeable layer (the α reservoir), between about 1000 and 1500 m depth. This reservoir generally corresponds to the hatched region shown in Fig. 2 at the bottom of well M-5. Under natural-state conditions the westward movement of hot fluids in the α reservoir continues somewhat west of normal fault L, shown west of well M-25 in Fig. 2. However, most of the fluids flow up this fault to reach a shallower aquifer where mixing occurs with colder groundwaters. Some of the hotter fluids leak to the surface west of the wellfield.

NATURAL-STATE GEOCHEMICAL MODEL

The original temperatures and sources of the Cerro Prieto field reservoir fluids, as well as the processes active in the system mainly after the start of fluid production, have been discussed in several papers and summarized by Truesdell et al. (1984, 1989). Initial hydrogeologic models of the Cerro Prieto field were developed mainly on the basis of geochemical information. Later models, like the one by Halfman et al. (1986), filled in details of the "sub-surface plumbing" inferred from the interpretation of the chemistry of the initially produced fluids. Thus there is general agreement between the natural-state circulation models developed for Cerro Prieto by geologists, reservoir engineers, and geochemists.

In studies of the natural state of the Cerro Prieto system, geochemistry has indicated the origin of the fluid and mineral phases through analyses of produced fluids and mineralogical study of cores and cuttings. The results of this work indicate that saline reservoir water was formed through heating (by igneous intrusions) of hypersaline brine and Colorado River water contained in the deltaic sediments of the Mexicali Valley (Fig. 3). Heated to 350–370°C, these waters mixed and rose buoyantly into the upper 3000 m, then partially boiled and mixed further with river water to form the reservoir fluids. The cation, silica, and trace-element compositions of the brine resulted from strongly temperature-dependent reactions with reservoir rocks. Gases originated from thermal metamorphism of minerals in the host sediments (CO₂, H₂S), atmospheric gases dissolved in the cold river water (N₂, most noble gases), or reactions of rock and fluid components

Figure 3. Schematic diagram of the geology and fluid flow across the Mexicali Valley (from Halfman et al., 1986). [XBL 865-10823]

(H₂, CH₄, NH₃). Only ³He was definitely introduced from the magmatic heat source.

Fluid geochemistry has also been used to follow reservoir processes and conditions during exploitation through a program of frequent sampling and analyses by CFE and other groups. These analyses have indicated the progress of cold-water entry from the margins and above the field and, used with enthalpy measurements, have indicated the mechanism and location of exploitation-induced boiling.

EXPLOITATION HISTORY OF CERRO PRIETO

Initially, the total installed electrical generating capacity at the field grew slowly, but in 1986–1987 it expanded to 620 MWe. The rate of fluid production has increased accordingly (Fig. 4). All the separated brine is being disposed of in a 16-km² evaporation pond located west of the wellfield, and to date only small-scale reinjection tests have been carried out.

Because of the large rate of fluid extraction, significant changes have been observed in the reservoirs and well discharges. The bulk of available information on reservoir changes is for the α reservoir, the first to be exploited. Even though fluid production from the β reservoir began in the late 1970s, only a few studies have dealt with the changes occurring in this reservoir. There are no data on the evolution, if any, of the γ reservoir, with only a few wells (e.g., M-112) producing from it.

Response of the α reservoir to production

As indicated earlier, the α reservoir, with hot water initially ≤ 310 °C at depths of 1000 to 1500 m, is restricted

Figure 4. Total annual fluid production at Cerro Prieto. [XBL 899-7755]

to the western part of the field. This reservoir was the main producer between 1973 and 1980. Exploitation of the α reservoir continues but on a smaller scale, as reduced production enthalpies (i.e., steam/water ratios) make some of the wells uneconomical. Since the early 1980s, the α wells are being replaced by deeper ones completed in the β reservoir ("E-wells" with total depths > 1600 m). As a consequence of production, pressures in the α reservoir have dropped, resulting in localized boiling around some of the wells and an increased influx of colder, less-saline water. With time, the boiling zones tend to expand and stabilize.

Localized reservoir boiling near some α wells has caused the deposition of large amounts of quartz and calcite, resulting in flow declines, sometimes leading to the loss of wells. On the other hand, flashing in the wellbore has also caused mineral deposition and loss of well productivity; silica and carbonate scaling dominates. If the scaling occurs above the slotted liner, reaming of the casing may result in total recovery of well output. However, the deposits formed in and behind the slots of the liner cannot be reamed out, reducing permanently the productivity of the wells.

As the α reservoir is bounded below by low-permeability rocks and above and to the west by an interface with colder waters, pressure drawdown results in cold recharge from the west and/or through fault L (Figs. 2 and 5), thus breaching the overlying shale layer. Once in the reservoir, the cooler waters tend to sweep the hot waters toward the producing wells. Because of their location near areas of natural recharge or in less-exploited parts of the field, some of the α wells do not show dilution and have never developed a boiling zone.

Fault L, which under natural-state conditions allowed the upward leakage of geothermal fluids, now acts as conduit to the downward flow of colder groundwater into the reservoir (Fig. 5). The evolution of the chemistry of the fluids produced by wells completed in the α reservoir clearly indicates the importance of this fault in the cold-water recharge of this aquifer.

Figure 5. Schematic fluid-flow model for the reservoir system at Cerro Prieto. [XBL 891-7427A]

Response of the β reservoir to production

The β reservoir was discovered in 1974 in the eastern part of the field. It extends, at depths below about 1600 m, over most of the Cerro Prieto field, deepening toward the east (unit Z in Fig. 2). It now provides the bulk of the fluids produced at Cerro Prieto.

Only a small number of studies have been made of the response of the β reservoir to production. However, a general picture of its behavior can be obtained from the available wellhead data. Because of its significant depth, and with its upper and lower boundaries sealed (Fig. 2), it has a restricted natural fluid recharge. This is especially true in the eastern areas, which are currently being heavily exploited. In the western region lateral influx from the west seems to be readily available; a similar situation could exist along the southeastern edge of the field.

Most β wells show high initial production rates and temperatures. The enthalpy of the produced fluids tends to increase immediately due to reservoir boiling (indicated by excess steam). In many β wells a decrease in flow rate has been observed that has generally been attributed to casing problems but may also result from mineral deposition in and around the well due to reservoir boiling, especially in the northeastern part of Cerro Prieto. On the other hand, the precipitation of silica in the wellbores and/or wellhead separators is a significant problem in the southeastern region of the field, indicating that in this region reservoir

boiling is not yet extensive. Not only silica and carbonate scales have been observed in production casings, but metallic sulfides (galena, sphalerite, and luzonite) have also precipitated along the casings of the hotter (up to 350°C) eastern wells.

In some of the deeper E-wells drilled in the west a decrease of fluid chloride content has been observed that could be explained by the advance of cold water entering the β reservoir from the western edge of the field (a cold-water sweep similar to the one occurring in the α reservoir; Truesdell et al., 1989).

There is a remarkable spatial correlation between the zone of general boiling in the β reservoir and fault H (Lippmann et al., 1989). There is clear evidence that the boiling β wells are located near the fault zone or in the upthrown block of fault H. A simplified model that simulates the natural recharge and response to production of the β reservoir (Fig. 6) shows that because of relative elevation, location of producing areas, and restricted recharge, the boiling in this reservoir tends to start in the upthrown block of the fault.

Figure 6. (a) Schematic vertical cross-sectional flow model of the Cerro Prieto β reservoir system. (b) Pre-exploitation (initial) flow and temperature conditions. (c) Assumed exploitation regime. (d) Temperature distribution, fluid flows, and location of boiling zone after 3 years of production. Note that since the model is two-dimensional, the flow rates are given in kg/s/m. [a and b, XBL 893-7487A; c and d, XBL 893-7487B]

Figure 6a shows a simplified, two-dimensional vertical numerical-simulation model of the Cerro Prieto β reservoir system. It extends in a general west-east direction. The natural-state hot-water discharge and cold-water recharge during exploitation that occur via the α reservoir (see Fig. 5) is part of the simulated fluid movement shown for the western part of this simplified two-dimensional model. Figure 6b describes the assumed conditions that were used to compute the pre-exploitation mass flow and temperature distributions. Note that no transfer of heat and mass was allowed between the geothermal reservoir and the surrounding formations.

For these particular conditions, 87.5% of the recharged water flows into the upthrown Zone 1 (and eventually into the α reservoir, shallower groundwater aquifers, and to the surface); only 12.5% flows into Zone 2. The computed temperatures in the β reservoir are quite uniform under these "natural-state" conditions, varying between 342 and 350°C, and no boiling is observed.

Figure 6c describes the exploitation conditions that were assumed for the model. The system is produced at a total rate 40 times the natural recharge, whereas the hot (350°C) recharge is assumed to be 10 times the natural value because of pressure drawdown. Figure 6d shows the temperature distribution and location of the general boiling zone in the system after 3 years of production. The effects of lateral cold-water recharge are reflected by the isotherms; thermal fronts are advancing toward the producing areas but have not yet reached them. The boiling is restricted to the upthrown block of the β reservoir near the fault, since this particular region is not only at lower elevation but also isolated from the recharge areas.

The model shows that the boiling zone collapses with time because of increasing system recharge and cooling. Note that at 3 years (Fig. 6d) the total (hot and cold) recharge slightly exceeds total production.

CONCLUSIONS

Even though models like the one described in Figs. 5 and 6 are very schematic, they can reproduce some of the behavior of the Cerro Prieto reservoir system. These simple models may be used to outline a production/injection program for the field that could reduce the boiling and induced cold-water recharge and the related reservoir plugging and cooling. These models can explain the behavior of individual wells and large regions of the geothermal system. Development of a reservoir management plan for this highly productive field requires more-detailed numerical simulations. This effort is being carried out in parallel by CFE and LBL scientists, who are studying the system using sophisticated three-dimensional numerical models (Halfman-Dookey et al., 1989; Ocampo et al., 1989). The basic understanding of geothermal field processes obtained here from analyzing simplified models is providing valuable guidance in the development of more-detailed numerical simulation models of Cerro Prieto.

REFERENCES

- Halfman, S.E., Manón, A., and Lippmann, M.J., 1986. Update of the hydrogeologic model of the Cerro Prieto field based on recent well log data. *Geoth. Resour. Counc. Trans.*, v. 10, p. 369–375 (LBL-20523).
- Halfman-Dooley, S.E., Lippmann, M.J., and Bodvarsson, G.S., 1989. Progress report on LBL's numerical modeling studies on Cerro Prieto. *In Proceedings, Final Symposium—Agreement US/DOE and CFE Mexico in the Field of Geothermal Energy*, San Diego, CA, April 4–5, 1989, p. 247–267 (LBL-27159).
- Lippmann, M.J., and Manón, A., 1987. The Cerro Prieto geothermal field. *Geoth. Sci. & Technol.*, v. 1, 1, p. 1–38 (LBL-21796).
- Lippmann, M.J., Truesdell, A.H., Manón, M.A., and Halfman, S.E., 1989. The hydrogeologic-geochemical model of Cerro Prieto revisited. Presented at the 14th Workshop on Geothermal Reservoir Engineering, Stanford, California, January 21–26, 1989 (LBL-26819).
- Ocampo, J.D.D., Ayuso, M.A., and Pelayo, A., 1989. Modelado del campo geotérmico de Cerro Prieto. *In Proceedings, Final Symposium—Agreement US/DOE and CFE Mexico in the Field of Geothermal Energy*, San Diego, CA, April 4–5, 1989, p. 239–245.
- Truesdell, A.H., Nehring, N.L., Thompson, J.M., Janik, C.J., and Coplen, T.B., 1984. A review of progress in understanding the fluid geochemistry of the Cerro Prieto geothermal system. *Geothermics*, v. 13, no. 1/2, p. 65–74.
- Truesdell, A.H., Terrazas, B., Hernández, L., Janik, C., Quijano, L., and Tovar, R., 1989. The response of the Cerro Prieto reservoir to exploitation as indicated by fluid geochemistry. *In Proceedings, Final Symposium—Agreement US/DOE and CFE Mexico in the Field of Geothermal Energy*, San Diego, CA, April 4–5, 1989, 123–132.

An Analytical Expression for the Permeability of Random Two-Dimensional Poisson Fracture Networks

J.C.S. Long and K. Hestir*

In cases where the matrix rock can be considered impermeable, fluid flow in fractured rock is controlled by the geometry of the fracture network. If the fractures are not interconnected, then flow will not occur. If they are highly interconnected, then fluid flow in the rock will resemble fluid flow in a porous medium. Between these two extremes, the flow system will be complex and cannot necessarily be treated as an equivalent continuum.

We can easily study the way in which the geometry of a fracture network controls the hydrologic behavior by using numerical models and a simple conceptual model for the fractures. For example, we have looked at two-dimensional Poisson systems where we assume the "fractures" are one-dimensional, finite line segments—in other words, two-dimensional pipe networks. In fact, this may not be a bad model for three-dimensional fracture networks if most of the conductance is in the intersections between fractures or the flow in the fractures is channelized. Studies of this type have been done by Long (1983), Robinson (1984), Dershowitz (1984), and Long and Witherspoon (1985). Most recently Hestir and Long (1990) have looked at Poisson models and developed an analytical expression for permeability as a function of the statistical parameters controlling the generation of the network. This work is

summarized here. These studies are a member of a class of problems known as percolation problems or equivalent-media problems. Percolation and equivalent-media theories therefore provide the basis for developing an analytical expression for permeability and the scale of the Representative Elementary Volume (REV).

Percolation theory and equivalent-media theory are usually applied to problems on regular lattices (e.g., Fig. 1a–d). Percolation theory and equivalent-media theory describe the equivalent permeability of the lattices as the bonds or sites are randomly filled with probability p . As p increases, clusters of bonds or sites are formed, and these clusters increase in size with increases in p . At the critical probability, p_{crit} , at least one cluster suddenly becomes infinite in size in what is called a critical phenomenon. Percolation theory looks at the conductance of these lattices when $p \approx p_{crit}$. Equivalent-media theory is applied to cases where p is significantly larger than p_{crit} .

As p increases, so does permeability, K . Relationships between p and K have been deduced through Monte Carlo studies. From percolation literature, Orbach (1986), for example, gives for $p \approx p_{crit}$ in bond percolation:

$$\frac{K}{K_{p=1}} \propto (p - p_{crit})^t, \quad (1)$$

where $K_{p=1}$ is the permeability at $p = 1$.

*New Mexico State University, Las Cruces, New Mexico 88003.

Figure 1. Examples of percolating networks: (a) through (d) are regular lattices that correspond to the random Poisson networks (e) through (h) below them. [XBL 896-2335]

The value of p_{crit} depends on the particular lattice and is between about 0.35 and 0.65. The exponent t is considered to be a universal constant; i.e., it is independent of the lattice type. Monte Carlo results usually indicate that t is about 1.1, but various calculations place t between 1.1 and 1.3.

From the equivalent-media literature, Kirkpatrick (1973), for example, one can find another relationship between K and p for the case where $p > p_{crit}$:

$$\frac{K}{K_{p=1}} = 1 - \frac{(1-p)}{(1-2/z)}, \quad (2)$$

where z is the coordination number defined as the number of bonds coordinated with a site. For example, on a square lattice, z is four. This expression predicts a linear relationship between p and K .

In applying these theories to fracture networks, we must resolve the following problems: What is p and what is z ? In percolation problems on a lattice, an upper bound for conductivity exists for the case where $p = 1$. For random fracture networks, there is theoretically no end to the degree of fracturing. Each time a fracture is added to the system, the permeability increases *ad infinitum*. In other words, the fracture system that corresponds to the lattice with $p = 1$ is difficult to identify. Because there is no obvious case that represents a "completely filled" lattice, we cannot determine how "relatively filled" a fracture network is.

We solve this problem by comparing systems that have the same linear fracture frequency, λ_l (the number of

fractures that intersect a line of length unity corrected for orientation bias). If λ_l is fixed, then the permeability of the fracture network will be a maximum if the fractures are of infinite length. This, in fact, is exactly the case studied by Snow (1965, 1969), where the fracture frequency was known from borehole observations and Snow made the assumption that the fractures are of infinite length. Thus Snow's permeability can be taken as the permeability equivalent to the lattice case where $p = 1$.

As we have found a way to define a maximum permeability, our work is reduced to finding a relationship between the parameters that control the geometry of the network and p and z such that the observed permeabilities can be explained with percolation and equivalent-media theories. This we do in three steps. First, we derive an expression for connectivity, ζ , in terms of the geometric parameters. Second, we propose relationships between connectivity and p and connectivity and z . Third, we use our parameter studies conducted with constant λ_l to verify that the proposed expression for p yields relationships for permeability that fit Eqs. (1) and (2).

Several authors have used the average number of intersections per fracture, ζ , as a measure of the connectivity in a random line processes (Robinson, 1984; Charlaix et al., 1986). Let $f(l)$ denote the probability density function for line length, and let $g(\theta)$ denote the probability density function for orientation. We assume that line orientation, length, and placement are statistically independent, and we take $0 \leq \theta < \pi$ and θ measured counter clockwise from horizontal. Then:

$$\zeta = \lambda_A (\bar{l})^2 H(\Theta) , \quad (3)$$

where

$$H(\Theta) = \int_0^\pi \int_0^\pi \sin \left| \theta_0 - \theta \right| g(\theta) g(\theta_0) d\theta d\theta_0 .$$

To study cases with varying ζ we note that

$$\zeta = \lambda_A (\bar{l})^2 H(\Theta) = \lambda_l \bar{l} H(\Theta) .$$

Thus we can vary ζ and still keep λ_l constant. For example, in Fig. 1e–h, we increase $\bar{l}$ by the same proportion that we decrease λ_A . As $\bar{l}$ approaches infinity, λ_l remains constant but ζ increases, and the permeability approaches the limiting case described by Snow (1965) (Fig. 1h). Further, as any value of λ_l can be rescaled to any other value, studying any one value of λ_l should allow one to predict permeability for any other value. We now present a functional form for normalized permeability, K/K_S . This requires finding expressions for p and z in terms of ζ . This expression is substituted into Eq. (1) or Eq. (2) to obtain an expression for K/K_S in terms of ζ . We test this functional form against numerical studies. The expression is not a mathematical fact but rather a guess based on analogues with other systems.

We find p as a function of ζ by finding the average length of a line in the regular lattice-bond model as a function of p and the average length of a line in the random-line model as a function of ζ and then equating the two averages (Hestir and Long, 1990):

$$p = p(\zeta) = \frac{\zeta}{\zeta + 2} . \quad (4)$$

This expression for $p(\zeta)$ yields the following expression for permeability based on percolation theory (Eq. 1):

$$\frac{K}{K_S} = \kappa \left[\frac{\zeta}{\zeta + 2} - \frac{\zeta_{crit}}{\zeta_{crit} + 2} \right] , \quad (5)$$

where κ is a constant.

To use $p(\zeta)$ in Eq. (2) for equivalent-media theory, it is necessary to calculate a modified coordination number $z(\zeta)$, for a random-line system. The coordination number of a regular lattice is the number of bonds connected to a site. In the rectangular lattice in Fig. 1a–d the coordination number is $z = 4$. In a random-line system (Fig. 1e–h) we propose an average coordination number (Hestir and Long, 1990):

$$z = z(\zeta) = 4 \left[\frac{1 - 1}{\zeta} \right] \quad (6)$$

This modified coordination number, given by Eq. (9), coupled with $p(\zeta)$ in Eq. (7), then yields

$$\frac{K}{K_S} = 1 - \frac{z(\zeta)(1 - p(\zeta))}{z(\zeta) - 2} = \frac{\zeta(\zeta - 4)}{(\zeta^2 - 4)} . \quad (7)$$

Figure 2a shows a plot of ζ versus K/K_S derived from our parameter studies for cases above the critical limit. Each point on the plot is an average permeability measured as close as possible to the scale of the REV from a realization of a random-line system (Hestir and Long, 1990). The dotted curves are calculated from the theoretical relationship between ζ and average permeability from equivalent-media theory (Eq. 10). The dashed curves are from percolation theory (Eq. (8) with a fitted value of $\kappa = 4.01$. Figure 2b and 2c show the same information plotted as a function of p . The curves in Fig. 2b and 2c have the classic shape seen in the literature.

Details of the parameter settings used for each point are given in Hestir and Long (1990). In each case a different seed was chosen for the pseudo-random number generator used to create the realization. The parameter values for the different cases were chosen to show that ζ can be used to predict permeability for a wide variety of random-line systems. We briefly describe these below.

Figure 2 shows that, on the whole, we are able to calculate permeability well with our model. From Fig. 2a and b we see that for all values of ζ significantly greater than

Figure 2. (A) Results of the parameter studies plotted against ζ . (B) and (C) show same results plotted against p . [XBL 896-2389]

ζ_{crit} , the data fit the equivalent-media model. The percolation model fits much better for values near ζ_{crit} up to values of ζ of near 10 or 12. One anomalous permeability value is for the smallest value of ζ shown. In this case, the value of permeability measured is too high for either of the models, probably because it was not possible to measure a large enough sample.

Variable-length systems are a special case because studies have shown that eliminating the shortest fractures up to some cutoff value, c , has no measurable effect on the permeability (Hestir and Long, 1990). However, eliminating all fractures shorter than a cutoff c will increase $\bar{l}$ and decrease λ_A and thus will change the value of ζ . This means that we could have many networks with the same permeability but different connectivities, which would imply a nonunique relationship between connectivity and permeability. To avoid this problem, we define the connectivity of the variable-length system to be $\zeta(c_0)$, the ζ for the system with the maximum truncation, c_0 , of short fractures that still has the same permeability as the original network. We use this value of ζ to extend the above percolation and equivalent-media models to random-line systems. We then have the model based on Eq. (10):

$$\frac{K(c_0)}{K_s(c_0)} = \frac{\zeta(c_0)(\zeta(c_0) - 4)}{\zeta^2(c_0) - 4}, \quad (8)$$

where $K(c_0)$ is the permeability of both the untruncated and the truncated system and $K_s(c_0)$ is given by Eq. (12). To find an analytical expression for c_0 in terms of ζ , Hestir and Long (1990) show that c_0 is the root of a fourth-degree polynomial in ζ .

The work summarized here allows one to calculate the value of permeability for a two-dimensional Poisson fracture system in which the fractures all have the same conductance. The model works for any distribution of fracture length, density, and orientation. It remains to extend the model to the case of variable fracture conductance. Variable conductance can also be thought of as a kind of

connectivity, in that fractures with small values of conductance form bottlenecks and thus decrease the degree of connection.

REFERENCES

- Charlaix, E., Guyon, E., and Roux, S., 1986. Permeability effects in the permeability of heterogeneous media. *In* Fragmentation, Form and Flow in Fractured Media, Annals of Israel Physical Society, v. 8, p. 316–324.
- Dershowitz, W., 1984. Rock joint systems (Ph.D. thesis). M.I.T., Cambridge, Mass.
- Hestir, K., and Long, J.C.S., 1990. Analytical expressions for the permeability of random two-dimensional Poisson fracture networks based on percolation and equivalent media theories. Submitted to J. Geophys. Res. (LBL-27625).
- Kirkpatrick, S., 1973. Percolation and conduction. *Rev. Modern Phys.*, v. 45, no. 4, p. 574–588.
- Long, J.C.S., 1983. Investigation of equivalent porous medium permeability in networks of discontinuous fractures (Ph.D. thesis). University of California at Berkeley. Lawrence Berkeley Laboratory Report LBL-16259.
- Long, J.C.S., and Witherspoon, P.A., 1985. The relationship of the degree of interconnection to permeability in fracture networks. *J. Geophys. Res.*, v. 90, no. B4, p. 3087–3097 (LBL-18446).
- Orbach, R., 1986. Dynamics of fractal networks. *Science*, 231, 814–819.
- Robinson, P., 1984. Connectivity, flow and transport in network models of fractured media (Ph.D. thesis). St. Catherine's College, Oxford.
- Snow, D.T., 1965. A parallel plate model of fractured permeable media (Ph.D. thesis). University of California at Berkeley.
- Snow, D.T., 1969. Anisotropic permeability of fractured media. *Water Resour. Res.*, v. 5, no. 6, p. 1273–1289.

Preliminary Calculations of Inflow to the D-Holes at the Stripa Mine

J.C.S. Long, K. Karasaki, A. Davey, J.E. Peterson Jr., M. Landsfeld, J.M. Kemeny, and S.J. Martel

The Site Characterization and Validation (SCV) experiment is the part of the international Stripa project sponsored by the Organization for Economic Cooperation and Development through the Swedish Nuclear Fuel and Management Co. This experiment is designed to test current abilities to characterize fractured rock before it is used for nuclear waste storage. One aim of the SCV work is to predict the inflow into five pilot boreholes (D-holes) drilled along a future drift called the Validation Drift

(Fig. 1). We present a preliminary prediction below. This article summarizes work described in Long et al. (1990).

IDENTIFICATION OF FRACTURE ZONES WITH GEOPHYSICAL METHODS

An extensive geophysical data set has been collected in the SCV block at Stripa in order to locate and character-

Figure 1. The SCV site. The D-holes are drilled along the future Validation Drift. [XBL 897-2676]

ize fracture zones. These are described in Olsson et al. (1989). Both radar and seismic methods were used, and for both techniques cross-hole tomographic and reflection data were collected.

In granitic rock, it is assumed that most rock matrix properties are relatively constant and that hydrologic features such as fracture zones and zones of increased porosity and water content will show up as anomalies. The geophysical methods allow us to "see" into the rock and predict where the major fluid conductors are. However, rock properties are not always constant, and sometimes the identified anomalies have little to do with hydrology.

An integrated analysis of all the geophysical data was used to make an interpretation of the location and extent of major features in the SCV block. This resulted in the identification of five major fracture zones called A, B, C, Ha, Hb, and I. Zones A, B, C, strike approximately N-E and dip about 45° to the S-E. The Ha, Hb, and I zones are nearly vertical and strike N-S.

THE HYDROLOGIC CONCEPTUAL MODEL

If the geophysical features are taken to have a hydraulic width of about 10 m, they account for about 60% of the measured hydraulic transmissivity measured in the boreholes. Almost all of the remaining 40% of the transmissivity is accounted for in three zones: at 80 m in borehole W2, 152 m in N2, and 80-90 m in borehole N4. By revisiting the original geophysical data, we can see that there are at least some strong radar and seismic anomalies in each of these zones. These anomalies were excluded in the process of making the geophysical interpretation because they are not substantiated in all the geophysical data. The simplest way to account for the remaining hydrologic anomalies in N4 and N2 was to add another zone, B'.

One remaining anomaly in W2 between zones H and B accounts for 21.7% of the transmissivity. If we allocate this transmissivity partly to H and partly to B, then we have accounted for 98.7% of the observed transmissivity with a zone model. The resulting hydrologic-zone model is shown in Fig. 2 in a perspective view from the N-W. Zones A, B, B', C, Ha, Hb, and I are shown. Gridding on the planes represents the hydraulic conductors of the template used for annealing. The zones are within disc-shaped planes that transect the entire block. As we do not expect the zones to be uniformly permeable, the zones are discretized into flow channels within the region of interest. The choice of grid is made with the support of geomechanical investigations of the shear zones explained below.

GEOMECHANICAL INTERPRETATION OF THE SHEAR ZONES

We have evidence that the major zones are fault zones under dip-slip motion. Associated with slip in the zones, secondary fracturing has been observed. For the NE-striking, low-dipping zones (A, B, B', C), the secondary fractures are subhorizontal, and for the N-S striking, steeply dipping zones (Ha, Hb, I), the secondary fractures strike N-S and dip 10-40° E. Numerical modeling indicates that under the present stress state in the SCV block, the subhorizontal secondary fractures could be open and have a much higher conductivity than other fractures in the SCV block. This, along with the higher fracture densities in these zones, may explain why the zones have higher conductivity than the surrounding ground. Moreover, the higher conductivity will cause flow in the zones to be anisotropic, with preferred pathways in the direction of the secondary fractures.

Figure 2. The hydrologic-zone model, shown in perspective from the northwest. Zones A, B, B', C, Ha, Hb, and I are shown. Gridding on the planes represents the hydraulic conductors of the template used for annealing. [XBL 896-2396]

SIMULATED ANNEALING

After the conceptual model, or template, has been constructed, it must be altered using inversion techniques so that the model predicts the observed hydraulic responses. Lawrence Berkeley Laboratory has been developing an inversion technique called "Simulated Annealing," which can be used to construct a system that is functionally equivalent to the observed system. The fracture network model is "annealed" by step-wise modification of the base model, or "template," such that the modified systems behave more and more like the observed system (Long et al., 1990).

The simulated annealing algorithm is used to determine an appropriate pattern of conductors among a set of possible configurations. This is achieved by methodically searching patterns to see which ones behave like those observed in the field. Simulated annealing is simply a statistical technique that controls the acceptance or rejection of trial modifications.

A synthetic example of annealing results is shown in Fig. 3. Here we have created a synthetic fracture system (Fig. 3a) and used it to create synthetic well-test data. We then create a regular grid to use as a template (Fig. 3b) and apply annealing to find a configuration that matches the synthetic well-test data (Fig. 3c). This example shows that the annealed result roughly reproduces the connection between the wells. Major gaps similar to those in the "real" system have analogous gaps in the annealed system.

PREDICTION OF INFLOW TO THE D-HOLES

At this stage in the hydraulic investigation of the SCV site, there are no formal, well-controlled cross-hole well tests available to use in annealing. To gain experience with the annealing technique and produce a preliminary estimate of the flow into the D-holes, we created a synthetic cross-hole test using a variety of data available for the SCV site. These data consisted of ad hoc cross-hole tests performed by the British Geologic Survey (BGS) and the record of heads in the boreholes as they responded to various openings and closing of holes. The BGS conducted three ad hoc cross-hole tests by opening W2 and monitoring sections in N3, N4, and W1.

Using the transient results plus the record of hydraulic heads in the holes, we fabricated a synthetic steady-state test. The steady flow rate from W2 was extrapolated to estimate the steady-state flow rate of 10 L/min. The corresponding estimation of steady-state head in N3, N4, and W1 was found by extrapolating the head values in those holes during the period when W2 was opened for a prolonged time. Wherever possible, these heads were assigned to specific zones in the boreholes on the basis of responses observed during the ad hoc test.

The choice of boundary conditions is based on head observations in the boreholes. Shut-in heads throughout

Figure 3. (a) A synthetic fracture network with pumping well A and wells B, C, D, E, F, and G. (b) A template grid. (c) Results of annealing well-test data from (a) on template in (b). [XBL 891-6142]

and around the SCV block are surprisingly consistent, averaging about 200 m. Therefore, we choose the alternative of making the boundary conditions at a constant head equal to 200 m. Although we do not expect the boundary conditions to be uniform around the edges of the zones, we have too few data to claim any more resolution than is obtained by setting the boundary conditions to one estimated figure.

The annealing program ran continuously for 931 iterations during a period of one week. Table 1 gives the heads that were calculated with the final configuration resulting from annealing. We see that the annealing routine has managed to match the observed heads very well. At the end of the annealing process, we have determined several configurations of conductors within the zones, all of which result in matching the observed head data extremely well. The match has been achieved solely by ar-

Table 1. Annealing results at the final iteration = 3749.

Hole	Zone	Observed heads	Predicted heads
N2	B,B',C	90	90
N3	A,B	80	79
	B'	none	65
	C	none	65
N4	B'	55	55
	C	none	83
	B	none	49
	A	none	49
W1	H_a ,C	65	65
	H_b	none	65
	B'	none	65
	B	none	65

ranging the conductors. As all the channels have the same conductance, k_A , any value of k_A will result in the same head distribution.

At this point we must calibrate the conductance of the channels so that the model will predict the correct value of flow from W2. To do this, we use the annealed model to calculate the flow from W2. Then we take the ratio of measured flow to calculated flow to find the conductance of the channels that would produce the correct amount of flow into W2.

Now we rearrange the numerical model, closing hole W2, adding the open D-holes, and calculating the outflow from the D-holes for seven configurations of the model. The resulting calculations of inflow to the D-holes are all between 8.8 and 9.1 L/min. It is clear from these results that the prediction of inflow to the D-holes is largely governed by the measurement of flow from hole W2. This points out that other flow data available for the SCV block would be very useful in modifying this prediction, as discussed below.

Outflows from the other N- and W-holes, ranging from 0.45 to 2.55 L/min, were measured on an ad hoc basis by BGS (Holmes, personal communication, 1989). Using the final annealed configuration of channels, we calculate the inflow into each of these holes, Q_{iM} . In each case we calibrate the channel conductance in the same manner as previously described so that the model will correctly predict the measured flow. This results in five predictions of channel conductance, which in turn results in five predictions of D-hole inflow. These predictions are given in Table 2. Our best prediction of inflow to the D-holes is 3.1 L/min.

Table 2. Predictions of D-hole inflow based on annealing and measured N- and W-hole inflows.

Hole	Resulting prediction of D-hole inflow (L/min)
N2	1.3
N3	0.6
N4	3.4
W1	1.3
W2	8.9
Mean	3.1
Standard deviation	3.1

To calculate the error associated with this prediction, we can use the five measurements of inflow. We anneal with the head data alone to get a channel configuration. Then we develop five models by calculating channel conductance with only four of the inflows at a time. In each case, we compute the flow into the hole we left out. The root mean square of the differences between predicted and observed flux for each case was 4.6 L/min, and this is the estimate of prediction error.

SUMMARY OF RESULTS AND CONCLUSIONS

On the basis of the preliminary data available at this time, the inflow predicted for the D-holes is 3.1 L/min, with a prediction error of 4.5 L/min. The actual measured value was about 1.7 L/min. The results are most sensitive to the measurements of inflow. We expect that annealing based on multiple cross-hole tests will be able to discern channel patterns much more effectively than other methods used so far.

This example should be considered preliminary at best. However, we find the approach very attractive in that the resulting models will contain more information about connectivity than an equivalent-continuum model requiring that we know all the actual details of the geometry. These new models can be considered to be "equivalent-discontinuum models." They reproduce the essential lack of connection prevalent in fracture networks without trying to reproduce every fracture. The modeling effort is concentrated on reproducing the behavior of the observed system rather than the geometry. We think this makes sense, because the reason for having a model is to predict behavior, not geometry.

REFERENCES

Long, J.C.S., Karasaki, K., Davey, A., Peterson, J., Landsfeld, M., Kemeny, J., and Martel, S., 1990. Preliminary prediction of inflow into the D-holes at the Stripa mine. Lawrence Berkeley Laboratory Re-

port LBL-27182.

Olsson, O., Black, J.H., Gale, J.E., and Holmes, D.C., 1989. Site characterization and validation. Stage 2-preliminary predictions. Swedish Geological Co. Report ID No. 88.

An Interdisciplinary Methodology for Modeling Fracture Systems, with Application to the US/BK Site, Grimsel Laboratory, Switzerland

S.J. Martel and J.E. Peterson Jr.

Fracture systems form the primary fluid flow paths in a number of rock types, including some of those being considered for high-level nuclear waste repositories. In certain situations, fracture flow must be considered explicitly as part of a site-characterization effort. We have implemented a site-characterization methodology that combines information gained from geophysical and geologic investigations to determine the 3-D geometry of the major fracture zones that might conduct water. The general philosophy is to identify and locate major structures that intersect a perimeter around the target site and then to project those structures into the site. This procedure is repeated as progressively tighter perimeters around the target site become available.

The simplest case involves four steps. First, reconnaissance information is assembled and a large-scale model of the geologic structure in the vicinity of the target site is prepared. Next, detailed geologic mapping is conducted to define the structural systematics of the major fracture zones near the site and to gain insight into how fluid might flow along the zones that might be present at the site. Site-specific geologic mapping and borehole surveys are then used to determine fracture-zone geometries on the site perimeter and to prepare a preliminary geologic model of the site. The model is refined on the basis of site-specific borehole and geophysical information. We make a special effort to use information on the systematics of the fracture systems to help link the site-specific geologic, borehole, and geophysical information.

This interdisciplinary methodology was applied at the US/BK site at the Grimsel underground rock laboratory in Switzerland; the laboratory is situated in foliated granitic rock. Previously conducted large-scale work at Grimsel (e.g., Keusen et al., 1989) revealed that northwest-striking fracture zones (K-zones), northeast-striking fracture zones (S-zones), and metamorphosed lamprophyre dikes form the major hydrologic structures in the laboratory. All of these are roughly planar features that dip steeply. The K-zones strike at high angles to the rock foliation, and the S-zones parallel it.

Detailed mapping revealed that the K-zones consist of zone-parallel faults that are linked by fractures that systematically strike at oblique angles to the faults (Fig. 1). These fractures are most abundant at echelon steps between faults. Permeability is likely to be greatest at these steps, which might function as vertical pipes. An S-zone (Fig. 1) displays a braided pattern of fractures that are subparallel to the zone as a whole, suggesting that permeability would probably be greater along the S-zones rather than across them. Fracture tortuosity appears greater along strike than downdip; horizontal permeabilities are therefore probably less than vertical permeabilities. The lamprophyres generally strike to the west or northwest, and their edges commonly are highly sheared and finely cracked. Gaping subhorizontal fissures locally extend from lamprophyre edges. Permeability along lamprophyres is likely to be greatest along their edges and least across strike.

The US/BK site (Fig. 2) itself is bounded on the north and south by two boreholes that are about 150 m long and are spaced about 150 m apart. About a dozen boreholes radiate from the BK excavation. The site is bounded on the east by the main laboratory tunnel; this

Figure 1. Schematic diagrams comparing the arrangement of fractures in a K-zone and an S-zone. The foliation in the rock dips steeply to the southeast, at a high angle to the K-zone but parallel to the S-zone. [XBL 902-623]

Figure 2. Map projection at the 1730-m level of borehole fractures (fine lines) at the US/BK site and associated major structures. Closely spaced pairs of lines mark edges of fractured zones; single lines mark prominent single fractures. Heavy symbols indicate strike and dip used for projection of fractures; these attitudes correspond to the attitudes of the major features. Feature 1 (medium screen): S-zone fractures. Feature 2 (dark screen): K-lamprophyres. Feature 3 (medium screen): S-zone fractures. Feature 4 (light screen): K-zone. Feature 5 (dark screen): Northwest-striking lamprophyres. [XBL 8911-7898]

forms the perimeter of the site, albeit a partial one. Two S-zones (feature 1, Fig. 2) and one west-striking lamprophyre-rich K-zone (feature 2) are exposed in the laboratory tunnel north of the BK room. These are the most prominent structures at the site, and they are expressed as major features at the surface. Another west-striking K-zone exposed at the entrance to the BK room would project just south of the room (feature 4). A series of northwest-striking lamprophyres (feature 5) that are exposed in a tunnel immediately south of the site and in borehole BOUS 85.003 would also project into the site. Next, we identified lamprophyres and clusters of fractures in the borehole cores. We prepared a preliminary model of the site (Fig. 2) by projecting the lamprophyre-bearing structures and S-zones exposed in the laboratory tunnel such that they intersected the lamprophyres and fracture clusters penetrated by the boreholes. The borehole data also enabled us to identify a second S-zone segment in the center of the site (feature 3) that is not on strike with the S-zone segment in the northeast corner of the site (feature 1). In accordance with our S-zone observations (Fig. 1), the fractures associated with feature 3 are subparallel to the rock foliation.

Seismic and radar tomograms identify regions of anomalous elastic and electric/dielectric properties, respec-

tively, in a rock body by using signals transmitted between boreholes and tunnels. We used seismic velocity tomograms (Westfälische Berggewerkschaftskasse, 1988) and radar attenuation tomograms (Niva and Olsson, 1988a,b) to nondestructively locate fracture zones and lamprophyres within the US/BK site; the patterns on both kinds of tomograms are broadly similar, but anomalies are most distinct on the seismic tomogram. Six anomalies (S1-S6) are defined using the 5050 m/s acoustic velocity contour on the seismic tomogram; they are compared with our preliminary model in Fig. 3. Anomaly S1 corresponds to the northernmost S-zone(s). The eastern portion of anomaly S2 matches the lamprophyre-rich K-zone. Borehole data from BOUS 85.002 suggest that the southwest arm of anomaly S2 and anomaly S4 may represent lamprophyres. Anomaly S3 corresponds to the S-zone of feature 3. Anomaly S5 reflects artifacts of the inversion process in an area traversed by relatively few signals. Anomaly S6 corresponds to an inferred step in the K-zone at the entrance to the BK room. The seismic tomogram is consistent with our preliminary model (Fig. 2).

Brine tracers were injected before the second phase and before the third phase of radar tomographic measurements. By analyzing the differences between before- and after-injection tomographic data sets one can see where the brine went. The first injection (Fig. 4) was in the middle of feature 3 (Fig. 2). Most of the brine appears to be contained within the northeast-striking S-zone segment of

Figure 3. Projection in the plane of tomography showing the features of the preliminary structural model of the US/BK site (see Fig. 2) superposed on the 5050 m/s contour of a seismic velocity tomogram of the US/BK site (WBK, 1988). [XBL 906-2066]

Figure 4. Difference tomogram of radar attenuation structure of the US/BK site from phase 1 and phase 2 measurements. The tomogram shows the increase in radar attenuation and indicates where brine has migrated between phases 1 and 2 (from Niva and Olsson, 1988a, Fig. 5.12). [XBL 8912-7902]

feature 3. This is consistent with feature 3 being bounded by low-permeability lamprophyres. The second injection (Fig. 5) was south of the intersection of features 3 and 5 (Fig. 2). The most prominent anomaly in Fig. 5 indicates that the brine migrated directly toward the borehole at the south side of the site. This is consistent with the brine being injected (1) outside of a well-defined northeast-striking S-zone and (2) south of northwest-striking lamprophyres with low across-strike permeability. The first-order results of the brine tracer tests are thus consistent with our structural model. We note, however, that minor anomalies *a* to *d* in Fig. 5 indicate that a detectable amount of brine may have flowed along fractures that are not in major fracture zones in our model.

Because of the extent and variety of information available for the US/BK site, it represents a "best case" test of our methodology. We conclude that our modeling methodology can yield a first-order model consistent with a variety of different data sets. In areas where the geology is less well understood, geophysical techniques might be relied upon more heavily than in our study, and a few points bearing on that possibility emerged in our study. The usefulness of tomograms is a function of both their resolution and how well the geology is known. Anomalies on tomograms can reflect a wide range of features (different rock types, fractures, zones of hydrothermal alteration, areas of increased porosity, etc.), so advance knowledge of the geology is essential in order for the anomalies to be inter-

Figure 5. Difference tomogram of radar attenuation structure of the US/BK site from phase 2 and phase 3 measurements. The tomogram shows the increase in radar attenuation and indicates where brine has migrated between phases 2 and 3 (from Niva and Olsson, 1988a, Figure 5.26). [XBL 8912-7903]

preted correctly. For example, borehole information at the US/BK site was instrumental in determining that seismic anomaly S3 in Fig. 3 represented fractured granitic rock and not lamprophyre. In turn, because boreholes sample relatively small volumes, the most reliable information they provide is essentially one-dimensional; advance knowledge of the fracture-zone systematics allowed us to more fully exploit the 3-D information the boreholes can provide.

There are certainly opportunities for improving our ability to identify second-order features at a site. Differences between the radar and seismic tomograms for the

US/BK site discouraged us from trying to map details of the internal structure of the major features from the tomograms, particularly for the lamprophyre-rich K-zone. Structural details probably were obscured in large part because of the high contrast between rock properties of the lamprophyre-rich K-zone and the granitic host rock. Research directed toward improving inversion techniques for bodies with large contrasts in physical properties would be especially useful. Additionally, laboratory and small-scale field research that addressed the geophysical signature of well-defined geologic structures would also increase the usefulness of the tomograms.

REFERENCES

- Keusen H.R., Ganguin, J., Schuler, P., and Buletti, M., 1989. Felslabor Grimsel: Geologie. NAGRA Technical Report 87-14.
- Niva, B., and Olsson, O., 1988a. Radar crosshole tomography results from phase 2. NAGRA Internal Report 88-31.

- Niva, B., and Olsson, O., 1988b. Radar crosshole tomography results from phase 3. NAGRA Internal Report 88-57.
- Westfälische Berggewerkschaftskasse, 1988. Felslabor Grimsel: Seismische Durchschallungs-Tomographie. NAGRA Technical Report 88-06.

First-Order Kinetics-Controlled Multiple-Species Reactive Transport of Dissolved Organic Compounds in Groundwater: A Numerical Model

W.W. McNab, Jr., and T.N. Narasimhan

Groundwater contamination from halogenated hydrocarbons has become an issue of paramount concern in recent years. Computer models used to predict the fate of such materials in the subsurface environment as a result of transport and transformation processes have largely neglected the complex chemical processes involved in the degradation of these pollutants. Often, abiotic as well biologically mediated degradation processes are represented solely by simple first-order decay constants, with no attempt made to simulate the appearance and disappearance of transient species involved in the decay schemes. This may prove to be of considerable importance in many instances where transient degradation products may themselves be highly toxic or destructive to the environment.

Bearing this in mind, we introduce a numerical model, KINETRAN (KINETically-controlled reactive chemical TRANsport), in an attempt to handle degradation processes more realistically in groundwater under environmental conditions (McNab and Narasimhan, 1990). KINETRAN contains a kinetics algorithm that allows a number of interacting aqueous species to approach their equilibrium concentrations simultaneously through a series of user-specified degradation reactions. This algorithm is dynamically coupled with a chemical transport model that is based on the Integral-Finite-Difference Method (Edwards, 1972; Narasimhan and Witherspoon, 1977). The transport model simulates solute transport due to the combined effects of advection, molecular diffusion, hydrodynamic dispersion, and adsorption. As a result of the discrete nature of the chemical transport model, we are capable of simulating conditions that involve both physical and chemical heterogeneities.

We apply KINETRAN to a hypothetical problem involving the simultaneous transport and degradation of two halogenated hydrocarbons through a one-dimensional soil column. The results of our simulation show that the model produces credible, mathematically internally consistent results given the input data.

KINETICS ALGORITHM FORMULATION

Consider a simple system in which only two aqueous species exist, A and B , either of which may be transformed into the other. At equilibrium,

$$\frac{[B]}{[A]} = K_{eq} \quad (1)$$

If the system is not at equilibrium, then, assuming first-order kinetics,

$$\frac{d[A]}{dt} = -k_1[A] ,$$

$$\frac{d[B]}{dt} = -k_2[B] .$$

By definition of a dynamic equilibrium,

$$\frac{d[A]}{dt} = \frac{d[B]}{dt} .$$

Thus, from (1),

$$k_2 = \frac{k_1}{K_{eq}} .$$

This relationship will hold for more complex reactions involving additional species, provided that equilibrium concentrations can be calculated and that reaction rates depend only on the concentrations of the principal species, A and B .

Discretization of the Rate Equations

Consider the reaction $A \rightarrow B$. Integrating the first-order rate equation yields

$$[A] = [A_0]e^{-k_1 \Delta t} \quad (2)$$

Equation (2) will describe the evolution of $[A]$ over time only for a simple system where species A participates in one reaction that is far from equilibrium. In a general system, species A will be simultaneously generated and consumed in a number of reactions, thus the quantity $[A_0]$ in (2) becomes ambiguous. Therefore, we must replace the explicit Eq. (2) with an implicit one.

The solution is as follows. First of all, we discretize the rate equation so that

$$\frac{\Delta[A]}{\Delta t} = -k_1[A] \quad (3)$$

where

$$[A] = [A_0] + \lambda \Delta[A] \quad (4)$$

The task is to choose an appropriate value for λ that will allow the discrete equation to approximate closely the differential equation.

Note that from (2) we may write

$$\Delta[A] = [A] - [A_0] = [A_0]e^{-k_1\Delta t} - [A_0] \quad (5)$$

From (3), we see that

$$\Delta[A] = -k_1 \left([A_0] + \lambda \Delta[A] \right) \Delta t$$

or

$$\Delta[A] = \frac{-k_1 A_0 \Delta t}{k_1 \lambda \Delta t + 1} \quad (6)$$

Equating (4) and (5) yields the estimate for the time-averaging factor,

$$\lambda = \frac{1}{1 - e^{-k_1\Delta t}} - \frac{1}{k_1\Delta t}$$

This will allow computation for more complex systems.

Transformation Equations for Multiple-Species Systems

We know that among all of the aqueous species present in the simulation, a certain number of reactions will take place. For any given species over a given time step, there will be sink terms, where the species is destroyed in some reactions, and source terms, where it is created in others. Thus, if we write all the reactions of interest going in initially dominant directions, then for a given species i , there will be J_r reactions in which it is a reactant and J_p reactions in which it is a product. The total effect on the concentration, including forward and reverse reactions, is given by

$$\begin{aligned} \Delta c_i = \Delta t \sum_{j=1}^{J_r} \frac{\mu_{i,j}}{\mu_{m,j}} k_{j,r} [c_{m,j}^0 + \lambda_{j,r} \Delta c_{m,j}] - k_{j,r} [c_i^0 + \lambda_{j,r} \Delta c_i] \\ + \Delta t \sum_{j'=1}^{J_p} \frac{\mu_{i,j'}}{\mu_{m,j'}} k_{j',r} [c_{m,j'}^0 + \lambda_{j',r} \Delta c_{m,j'}] - k_{j',r} [c_i^0 + \lambda_{j',r} \Delta c_i] \end{aligned} \quad (6)$$

Here, Δc_i and $\Delta c_{m,j}$ refer to the changes in concentration over time step Δt of species i and m , respectively, where m is the complementary species produced in reaction j (or destroyed in reaction j') with i . The variables c_i^0 and c_m^0 refer to the initial species concentrations at the beginning of the time step. The quantity μ represents the stoichiometry for each species in each reaction.

Equation (6) is an implicit equation, since the Δc terms are all unknowns. Thus (6) must be rewritten as a set of simultaneous linear equations and solved through the use of matrix algebra. Other species that are consumed or produced during transformation, such as free halogen ions, must have their concentrations corrected for the amount gained or lost as a result of (6) in order to maintain a mass balance. The system pH and Eh are assumed to be buffered by the local mineral assemblage, so changes in these need not be considered.

THE TRANSPORT EQUATIONS

The kinetic rate equations described above have to be incorporated in the chemical transport equations. We now present these equations for a multiple-species aqueous system. For convenience, we write these equations for a discrete elemental volume l communicating with its neighbors m , where $m = 1, 2, 3, \dots, M$. The complete equation describing chemical transport includes expressions for advection, molecular diffusion, hydrodynamic dispersion, adsorption, and source terms. Therefore, for species i ,

$$\begin{aligned} \sum_{m=1}^M q_{l,m} A_{l,m} \bar{c}_{l,m}^i + \sum_{m=1}^M n D_d^i \frac{\Delta c_{l,m}^i}{x_{l,m}} A_{l,m} \\ + \sum_{m=1}^M n D_H^i \frac{\Delta c_{l,m}^i}{x_{l,m}} A_{l,m} + G_l^i = n V_{B,l} R^i \frac{\Delta c_l^i}{\Delta t} \end{aligned} \quad (7)$$

Here, the first term on the left describes solute transport due to advection, where $q_{l,m}$ is the volumetric fluid flux per unit area (Darcy velocity) between l and m normal to the interface between them, $A_{l,m}$ is the interface area, and $\bar{c}_{l,m}^i$ is the average concentration of species i at the interface of the two volume elements.

The second and third terms on the left describe molecular diffusion and hydrodynamic dispersion, respectively. Here, D_d and D_H are the diffusion and dispersion

coefficients, and n is the porosity of the material. The expression $\Delta c_{l,m}^i/x_{l,m}$ is simply the concentration gradient of species i between l and m approximated according to the finite-difference philosophy.

The final term on the left side of (7), G_l^i , is the source/sink term, which is an expression for net generation or destruction of species i in volume element l . This quantity is generally determined directly from evaluation of (6). However, if external sources or sinks for species i exist, they must also be included in this term. This includes mass-balance corrections to account for the creation of new cell mass material for microbe populations that may participate in biodegradation processes. The source/sink term is a crucial part of the KINETRAN algorithm, as this is the variable that provides the coupling between the transport and transformation equations.

On the right-hand side of (7), the quantity $V_{B,l}$ is the bulk volume of element l . The total change in concentration of species i during Δt is given by Δc^i . This is the temporal variation of concentration of the species in volume element l and should not be confused with $\Delta c_{l,m}^i$ on the left-hand side, which represents the spatial variation. The variable R refers to the retardation coefficient, which is defined as

$$R^i = 1 + \frac{\rho_b K_d^i}{n}$$

Here, ρ_b is the dry bulk density of the matrix material, and K_d^i is the distribution coefficient for species i .

APPLICATION

We apply the KINETRAN model to a hypothetical problem involving the transport and chemical degradation of two halogenated hydrocarbons, methyl chloride and methyl bromide, through a fully saturated one-dimensional soil column, depicted in Fig. 1. Transport processes considered include advection due to infiltrating rainfall, hydrodynamic dispersion, and molecular diffusion. For simplicity, retardation due to adsorption is not considered in this simulation for any of the species present.

The pH of the system is fixed at 7.0 and the Eh at a mildly oxidizing +0.1 V. The temperature is set at 25°C. Under these conditions, possible pathways for the degradation of CH_3Cl and CH_3Br are shown in Fig. 2. We make no distinction here as to which mechanisms control the reactions, abiotic or biologically mediated. We consider only the first-order rate constants and the equilibrium thermodynamics of the reactions. Suitable rate constants were found for only a few of these reactions in the literature, hence we have used reasonable hypothetical values for the rest.

Batch-simulation results, calculated without the use of the transport model, are depicted in Figs. 3 and 4. Clearly, CH_3Cl and CH_3Br show simple exponential decay,

Figure 1. Physical configuration for the hypothetical soil or rock column used for the example simulation. [XBL 902-626]

Figure 2. Possible pathways for the degradation of methyl chloride and methyl bromide under oxidizing conditions. [XBL 902-627]

Figure 3. Batch-simulation concentrations of methyl chloride and methyl bromide, along with the free halogen ions, as a function of time. [XBL 902-628]

Figure 4. Batch-simulation concentrations over time of the secondary species produced by the degradation of the two methyl halides. [XBL 902-629]

whereas the secondary species show transient behavior that reflects the competing influences on them of degradation and generation from the parent species, as shown in Fig. 2.

The reactive transport profiles of methyl chloride and the secondary species after 100 days are shown in Figs. 5 and 6. Clearly, much of the CH_3Cl has been transformed by

Figure 5. Concentration profiles of methyl chloride in the soil column after 100 days, showing reactive and nonreactive cases. [XBL 902-630]

Figure 6. Reactive transport profiles for the secondary species after 100 days. [XBL 902-631]

this point, as shown by the comparison with the nonreactive profile. The concentrations of the subsequent daughter species reflect this as well. Note that the background concentration of total aqueous CO_2 also reflects the degradation processes, as it is the end product in the transformation chain.

REFERENCES

- Edwards, A.L., 1972. TRUMP: A computer program for transient and steady state temperature distributions in multi-dimensional systems. Lawrence Livermore National Laboratory Report UCRL-14754, Rev. 3.
- McNab, W.W., Jr., and Narasimhan, T.N., 1990. First-order kinetic-controlled multiple species reactive transport of dissolved organic compounds in groundwater: A numerical model. Submitted to Water Resour. Res. (LBL-28231).
- Narasimhan, T.N., and Witherspoon, P.A., 1977. Numerical model for saturated-unsaturated flow in deformable porous media, Part I: Theory. Water Resour. Res., v. 13, no. 3, p. 657-664.

On the Potential Importance of Transient Air Flow in Advective Radon Entry into Buildings

T.N. Narasimhan, Y.W. Tsang, and H.-Y. Holman

A necessary first step in seeking to manage radon levels in the indoor environment is to understand the phenomenon of radon entry into buildings. Studies so far (e.g., Sextro et al., 1987) have shown that the soil adjacent to a building's substructure is the major source of indoor radon. Measurements in a few houses (Nazaroff et al., 1985, 1987) seem to indicate that high concentrations of indoor radon are associated with elevated rates of radon influx, advectively transported with the bulk air inflow. Current reasoning is that the bulk soil-gas entry into buildings is driven by small, slowly changing differences between inside and outside pressures (on the order of a few pascals). This pressure differential may arise due to indoor heating (stack effect), wind, and operation of exhaust fans.

From a process point of view, it is noteworthy that bulk air inflow is dictated by pressure differences of but a few pascals, whereas it is known that barometric pressure fluctuations consist of periodic components with amplitudes ranging from a few pascals for periods of minutes to a few hundred pascals in diurnal variation. It is therefore reasonable to expect that the component of air inflow caused by the few pascals of underpressure may be masked by the transient air-flow fluctuations caused by the barometric pressure variations. In this summary, we focus on the temporal variations in air flux caused by periodic variations in barometric pressure in the presence of a persistent underpressure at the basement.

APPROACH

For our calculations we use the isothermal fluid-flow model TRUST (Narasimhan et al., 1978). TRUST is based on an Integral-Finite-Difference Method. It was developed to solve problems of transient flow of water in isothermal, variably saturated deformable media in one to three dimensions and has been extensively verified against analytical solutions and validated against experimental results for water flow in complicated systems (Narasimhan and Witherspoon, 1978). TRUST can readily be applied to air flow in so far as air can be idealized as a slightly compressible fluid.

Before applying TRUST to indoor radon problems, it is appropriate to validate the model against field observations of air flow. Accordingly, we have applied the model to a field problem investigated by Weeks (1978). Weeks developed a novel procedure by which he determined the in situ air permeability of a layered, partially saturated soil column from dynamic pressure measurements. Using Weeks' permeability estimates as input data, we validated our numerical model by closely reproducing the temporal

pressure responses that Weeks observed at various locations.

PROBLEM DEFINITION

To study the combined effects of time-dependent barometric fluctuations and time-independent underpressure on air inflow at the house basement, we define the problem as shown schematically in Fig. 1. The water table, at which a mean air pressure of $\bar{P}_{wt} = 10^5$ Pa is assumed, lies at 5 m below the land surface and 3 m below the basement floor, which is given a linear dimension of 10 m. In the initial analyses reported here, the basement has an uncovered soil floor. The soil air within the formation will be static if the gas pressure at each elevation, z , is $P_0(z) = \bar{P}_{wt} - \rho g z$, where ρ is the density of the soil air and g is the gravitation acceleration. The pressure boundary conditions for induction of air flow at the ground surface and the basement floor were chosen as follows: the fluctuations in the atmospheric pressure were assumed to be felt at both the ground surface and at the basement floor with no damping and phase lag. For our initial studies, the atmospheric pressure fluctuations were assumed to consist of only one sinusoidal component with a given amplitude and frequency. In addition to the atmospheric-fluctuation boundary conditions, the pressure at the basement floor is assumed to be always 5 Pa below that at the ground surface. Hence the pressure was allowed to vary periodically around the mean pressure corresponding to 5 m elevation at

Figure 1. Problem definition for modeling air flow in the presence of barometric fluctuations and a constant underpressure of 5 Pa at the basement. [XBL 899-3439]

the ground surface and the mean pressure corresponding to 3 m elevation at the basement floor.

Simulations of transient air flow were carried out with the above imposed boundary conditions for appropriate range of soil permeability to air: 0.153, 1.53, and $15.3 \times 10^{-12} \text{ m}^2$. Preliminary investigations of the dependence of air flow on the barometric frequency was carried out with two sets of barometric parameters: sinusoidal amplitude of 50 Pa with a period of 30 min and an amplitude of 250 Pa with a period of 24 hr.

RESULTS—TRANSIENT AIR FLOW INTO A BASEMENT

In the absence of the time-dependent sinusoidal variation of the atmospheric pressure, the constant underpressure of 5 Pa at the basement induces an air flux into the basement. The magnitude of this steady-state air flux into the half-length (5 m) of the basement varies with soil permeability, as tabulated in the second column of Table 1. As is to be expected in the case of a linear problem, the steady flux varies linearly with permeability. In response to the sinusoidal variation of atmospheric pressure, the air flow at the basement also oscillates with approximately the same period about the values given in column 2 of Table 1. In columns 3 and 4 of Table 1, we list the amplitudes of the flow oscillation for the respective permeabilities and the two frequencies of barometric pressure variation. Note that except for the last entry in column 4, these amplitudes are much larger than the magnitude of the steady-state inflow into the basement in the absence of "barometric pumping." In particular, the magnitudes of these fluxes were enhanced by almost two orders of magnitude in column 3 for the lowest-permeability case. The net result is that the dynamic system is characterized by *flux reversals*: air moves from the soil into the basement as atmospheric pressure decreases, and it moves from the basement into the soil as pressure increases.

Table 1. Air flow at basement floor with constant underpressure of 5 Pa in the absence and presence of barometric pumping.

Permeability $K (10^{-12} \text{ m}^2)$	Steady-state flow with no barometric pumping	Air flow (10^{-6} kg/s)	
		Amplitude of oscillatory flow with barometric pumping	
		$A = 50 \text{ Pa}$ $T = 0.5 \text{ hr}$	$A = 250 \text{ Pa}$ $T = 24 \text{ hr}$
0.153	0.041	2.85	1.17
1.53	0.41	10.1	1.18
15.3	4.1	16.3	1.20

To investigate further the reversal of flow directions, we also computed air fluxes (Kg/s-m^2) across the vertical plane $x = 5 \text{ m}$ at the basement edge at four depths: 0.05, 0.3, 1.0, and 1.8 m below the basement floor. These are shown in Fig. 2. Figure 2 (top) pertains to the low-permeability case of $0.153 \times 10^{-12} \text{ m}^2$, and 2 (bottom) pertains to the high-permeability case of $15.3 \times 10^{-12} \text{ m}^2$. Positive values of fluxes imply flow in the negative x direction, toward the basement. The presence of negative fluxes (Fig. 2, top) shows that in fact fluxes are periodically directed away from the basement. The increase in phase lag with depth of the fluxes in response to the oscillatory atmospheric pressure arises from longer flow paths and increased resistance (from the finite air permeability) with depth. As a result of the finite response time of the medium to the pressure-driving force, the fluxes reach "oscillatory equilibrium" (values of extrema remain invariant with cycles) beyond the third cycle. Results for the high-permeability case in Fig. 2 (bottom) show that both the phase lag and the response time to reach "oscillatory equilibrium" are negligible. Furthermore, though the fluxes across the plane $x = 5 \text{ m}$ oscillate in magnitude, they all have positive sign, indicating that the fluxes are directed toward the house at all times.

Column 4 of Table 1 shows that for the barometric pressure oscillation with an amplitude of 250 Pa and a period of 24 hr, the amplitudes of the oscillatory fluxes at

Figure 2. Air flow across vertical plane $x = 5 \text{ m}$ at basement edge for constant underpressure of 5 Pa and barometric pumping of amplitude 50 Pa and period 0.5 hr. [XBL 899-3440]

the basement exceed the steady-state fluxes in column 2 for the two smaller permeabilities. These numbers indicate that the fluxes are still alternatively flowing in and out of the basement for the two lower permeability values, but for the largest permeability value, fluxes are always directed into the basement. As to the flow directions within the soil medium, similar plots such as Fig. 2 for this low-frequency driving-pressure case show that the flow direction is exclusively toward the house across the plane $x = 5$ m.

SUMMARY

The above results show that effects of barometric fluctuation are strongest in the cases where the permeability is low and the fluctuation frequency is high. In these cases, the barometric fluctuation can greatly enhance the magnitude of fluxes as well as reverse the direction of flow from surrounding soil into the basement. This result is significant because in the absence of time-dependent barometric fluctuations, bulk flow accounts for a large amount of the total radon entry into basements only in high-permeability soils. Our calculations have identified a process by which air flow through a low-permeability medium may also be large because of time-dependent barometric fluctuations. Since a real soil system even of intrinsically high permeability is characterized by heterogeneities arising from both material property distributions as well as from variations with water saturation, these spatial variations in permeability with possible low local values will have a pronounced effect on the response of the system to periodic forcing functions and may have marked influence on radon entry.

The results of these preliminary studies show that the transient flow pattern may be complex, and the dependence on the parameters (permeability, barometric fluctuation amplitude and period) can be subtle and important. Our continuing research is directed toward refining the problem definition to resemble more closely the reality of barometric fluctuations of many frequency components, an impermeable cement basement floor with restricted open-

ings, the inclusion of effects of heterogeneities and moisture variations, and the transport of radon advected in the complex flow pattern.

ACKNOWLEDGMENT

We would like to thank R.A. Sextro, W. Fisk, A. Gadgil, and M. Modera of the Applied Science Division, Lawrence Berkeley Laboratory, for introducing us to the indoor radon problem and for many stimulating discussions.

REFERENCES

- Narasimhan, T.N., Edwards, A.L., and Witherspoon, P.A., 1978. Numerical model for saturated-unsaturated flow in deformable porous media, 2. The algorithm. *Water Resour. Res.*, v. 14, no. 2, p. 255-261.
- Narasimhan, T.N., and Witherspoon, P.A., 1978. Numerical model for saturated-unsaturated flow in deformable porous media, Part III: Applications. *Water Resour. Res.*, v. 14, no. 6, p. 1017-1034.
- Nazaroff, W.W., Feustel, H., Nero, A.V., Revzan, K.L., and Grimsrud, D.T., 1985. Radon transport into a detached one-story house with a basement. *Atmos. Environ.*, v. 19, no. 1, p. 31-46.
- Nazaroff, W.W., Lewis, S.R., Doyle, S.M., Moed, B.A., and Nero, A.V., 1987. Experiments on pollutant transport from soil into residential basements by pressure-driven airflow. *Environ. Sci. & Technol.*, v. 21, p. 459-466.
- Sextro, R.G., Moed, B.A., Nazaroff, W.W., Revzan, K.L., and Nero, A.V., 1987. Investigations of soil as a source of indoor radon. In P.L. Hopke (ed.), *Radon and Its Decay Products*. ACS Symposium Series No. 331. American Chemical Society, Washington DC.
- Weeks, E.P., 1978. Field determination of vertical permeability to air in the unsaturated zone. U.S. Geol. Survey Prof. Paper 1051, 41 pp.

Disposal of High-Level Wastes at Yucca Mountain, Nevada: A Hierarchy of Hydrological Issues Relating to the Vadose Zone

T.N. Narasimhan and J.S.Y. Wang

In December 1987 the United States Congress chose Yucca Mountain, Nevada, as the candidate site for the first U.S. nuclear waste repository. As a consequence, the site-characterization, repository-design, and performance-assessment activities for this site are expected to be intensified over the next few years to support the licensing appli-

cation from the Department of Energy (DOE) to the Nuclear Regulatory Commission (NRC). Repository evaluation and environmental assessment of the Yucca Mountain site require comprehensive scientific investigations to quantify the uncertainties inherent in the natural system between the repository and the accessible environment. A

good site, with a low fluid-flow velocity field, will most likely be difficult to characterize and to evaluate. The challenge for the earth scientists is to focus on the key issues, quantify the uncertainties, and provide credible answers that will help the public and the government decide if geological disposal at Yucca Mountain is a viable and acceptable solution to this critical national problem.

To aid the DOE in this important mission, the thrust of the report summarized here (Narasimhan and Wang, 1990) is to identify the key issues that govern the project and the tasks that are necessary for resolving the key issues. It is in the nature of the ultimate decision-making process that complex issues be digested into a set of simple measures and answers amenable to the decision-making venture. Recognizing this, we present the key issues in a hierarchical fashion; we begin with the simple elements of the unsaturated-repository concept, compile a comprehensive list of the complex issues, and end with credible and quantifiable measures to enable decision-making on the suitability of the site for geologic disposal of high-level wastes.

To analyze the problem rationally, it is desirable to start with the pros and cons of the Yucca Mountain site.

FACTORS FAVORING THE YUCCA MOUNTAIN SITE

Very low water flux. Because of the very low precipitation and very large evapotranspiration, natural recharge to the deep groundwater table is extremely small.

Rapid drainage. If the host rock in the unsaturated zone is well fractured, water will rapidly drain downward, resulting in very small residence times within the fractures.

Strong capillary retention of water. Within the porous matrix with high bulk capillarity, the vertical movement of water becomes so slow that it is questionable whether movement occurs at all.

Minimal contact with waste package. Only a fraction of the water migrating downward through the repository would actually contact the waste. This potential contact could be further reduced by suitable engineering design of the waste-package emplacement.

Geochemical retardation. An added geochemical barrier to radionuclide migration would be provided by the Calico Hills unit, which intervenes between the repository and the water table. This unit, fine-grained and rich in zeolites, possesses significant sorptive properties.

Preservation of site integrity. Because highly permeable vertical fractures may help quickly drain infrequent short pulses of flux, the presence of highly permeable channels per se within the unsaturated zone (abandoned bore holes) may not be undesirable. Therefore, site integrity may not be jeopardized by drilling a large number of exploratory holes or shafts. Moreover, faults and fracture

zones may not pose as much of a hazard as they do in the saturated zone.

Accessibility to monitoring and recovery. The accessibility of the repository above the water table has two principal advantages. First, it facilitates a systematic monitoring of site performance during construction, operation, and post-construction phases. Second, should monitoring reveal potential signs of site failure, the wastes could be recovered for alternate disposal or remediation.

CAVEATS

Perched water bodies. Possible existence of large perched water bodies within the vadose zone may provide undesirable water access to the repository. However, if shafts or boreholes intersect these, they would drain quickly, as experience would suggest. At worst, these could also be artificially drained through carefully designed boreholes.

Rise of water table. Possible rise of the water table by a few hundred meters during the next 1000 to 10,000 years, leading to flooding of the repository.

Wet Climate. Drastic change to wet climate (pluvial environment) within the next 1000 to 10,000 years.

Release of gaseous contaminants. Gas and vapor would have to be considered as transporting agents of radionuclides in addition to percolating groundwater.

A RATIONALE FOR SOLUTION

Within the constraints of the challenges, a prudent solution approach to the overall problem may contain the following elements:

1. A serial arrangement of barriers that will, in tandem, inhibit the potential migration of contaminants.
2. Continuous and systematic monitoring of the site during and after construction and operation to detect any unforeseen failures.
3. Retrievability of the wastes for alternate disposal should unforeseen failures be detected.

THE ACCESSIBLE ENVIRONMENT

The ultimate concern of the Yucca Mountain Project is the potential contamination of the human environment by radioactive contaminants if toxic radioactive constituents find their way to the biosphere. For purposes of performance assessment, the biosphere is defined in terms of the accessible environment.

At Yucca Mountain, two accessible environments are to be recognized. The first is the local land surface; this includes not only the sloping upper surface and the slopes all around the mountain but also the land surface in the general

vicinity of Yucca Mountain to an as-yet unspecified distance. The second accessible environment includes all those locations at which the groundwater may potentially come into contact with the human habitat.

FUNDAMENTAL QUESTIONS

Before we proceed to identify the key issues pertaining to unsaturated-zone hydrology, it is instructive to state the fundamental questions that dictate the achievement of the ultimate goals of the project. The following four questions serve this purpose.

1. What is the *nature of the fluid movement* within the Yucca Mountain site?
2. What is the potential for *fluid-waste contact* and mobilization of toxic constituents?
3. What is the potential for the accessible environment to be *unacceptably contaminated* over a 10,000-year period?
4. How can the potential hazard be *quantitatively represented* so as to enable decision-making on site suitability?

The fact that Yucca Mountain has been declared a candidate site is clearly an indication of the existence of strong preliminary evidence of the suitability of the Yucca Mountain site. The critical task of performance assessment is therefore to test the preliminary evidence comprehensively and quantify the results in a credible manner.

We are concerned with a multiple-barrier system in which the barriers are placed in series. In this context the fundamental questions stated above are related to each other in the following way:

Quantity of Fluids Capable
of Transporting Contaminants

Potential for Contact with
Waste Form

Potential for Transport beyond
the Unsaturated Zone

Magnitude of Impairment of
the Accessible Environment

Against the backdrop of these fundamental questions we may now proceed to consider the multitude of technical

issues that need to be addressed in order to answer the aforesaid questions.

TECHNICAL ISSUES

The accessible environment could be contaminated either by the upward migration of gaseous phases or the downward migration of liquid water through the unsaturated zone. Although the term "hydrology" is usually applicable to liquid water, we use that term in a broader sense, including transport by the gaseous phase.

DISCUSSION

The hierarchical relationships between the technical issues (see Box 1) are discussed in Narasimhan and Wang (1990), a report that is under informal and formal review among various technical and managerial personnel involved with the Yucca Mountain Project. This report is modestly perceived as a nucleus for the generation of focused discussion on critical hydrological issues that need to be addressed observationally and computationally to aid in the ultimate success of the DOE mission.

Box 1. Hierarchical Relationships of Technical Issues.

I. Nature of Hydrologic Regime

I.1 *Before Repository Construction*

I.1.1 Groundwater as the Transporting Agent

I.1.2 Vapor/Gas as the Transporting Agent

I.2 *After Repository Construction*

I.2.1 Groundwater as the Transporting Agent

I.2.2 Vapor/Gas as the Transporting Agent

II. Interaction of Fluids and Waste Package

II.1 *Groundwater and Waste Package*

II.2 *Vapor/Gas and Waste Package*

III. Migration of Contaminants

III.1 *Groundwater as the Transporting Agent*

III.2 *Vapor/Gas as the Transporting Agent*

IV. Quantification

IV.1 *Measures of Performance*

IV.2 *Mathematical Models*

IV.3 *Long-Term Validation; Monitoring the System*

REFERENCE

- Narasimhan, T.N., and Wang, J.S.Y., 1990. Conceptual, experimental, and computational approaches to support performance assessment of hydrology and chemical transport at Yucca Mountain. Lawrence Berkeley Laboratory Report LBL-28613.

Development and Verification of a Numerical Technique for Coupled Hydromechanical Phenomena in Rocks

J. Noorishad and C.F. Tsang

The physicochemical environments of geologic systems are host to natural coupled thermal-hydraulic-mechanical-chemical (THMC) events that take place at various rates, depending on the nature of the driving energies. Implementation of geotechnical projects can lead to severe alteration of the natural trend of these coupled processes (Tsang, 1987). Assessment of the influence of these various phenomena on the performance of rock structures requires the development of realistic conceptual models. The important part of such a model is conceptualization of the physicochemical phenomena and the proper choice of phenomenological solution techniques. The complexity of the multidisciplinary phenomena narrows the choice of these solution techniques to numerical methods. The hydromechanical phenomena in fractured rocks constitute one area of coupled processes that has not until recently (Barton, 1986) attracted much attention. The main reasons for this apparent neglect are the less obvious and indirect way in which this process affects rocks as opposed to soils and the difficulty of obtaining the required data for its analysis. However, as fluid transport in rocks emerges as a critical issue in a number of major problems of current interest, such as the selection, design, and operation of waste repositories in hard rocks, investigations of coupled hydromechanical phenomena have become essential. Transport of heat by water adds an additional complication, requiring thermohydromechanical consideration in rock masses (Tsang, 1987). Such complications call for the development of coupled numerical solution techniques. Earlier works (Noorishad et al., 1971; Noorishad et al., 1982) provide a starting point for such studies. This article summarizes our efforts to develop a new computational method for hydrochemical analysis that (1) overcomes some of the shortcomings of its predecessors, such as its linear joint model and nonincremental setup and (2) can easily be enhanced for application to a wider range of geotechnical problems.

INCREMENTAL FINITE ELEMENT FORMULATION FOR HYDROELASTICITY

The formulation for a general incremental law can be achieved by two different approaches. A rigorous approach involves recasting the field equations and initial and boundary conditions of hydroelasticity in rate forms and formulating an energy rate statement (Small et al., 1976). However, incremental formulation can also be obtained by simple differentiation of the nonincremental finite element matrix formulation (see Noorishad et al., 1982). Choosing the latter approach gives

$$\left. \begin{aligned} K_I \frac{\partial U}{\partial t} - L^T \frac{\partial P}{\partial t} &= \frac{\partial F}{\partial t} \\ -L \frac{\partial U}{\partial t} - E \frac{\partial P}{\partial t} - H_I P &= Q \end{aligned} \right\}, \quad (1)$$

where K_I = incremental stiffness matrix, H_I = incremental conductance matrix, L = coupling matrix, L^T = transpose of L matrix, F = nodal force vector, E = fluid storativity vector, Q = flow vector, U = displacement vector, and P = pressure vector. Equation (1) is then integrated between t_1 and $t_2 = t_1 + \Delta t$ to obtain

$$\begin{aligned} \bar{K}_I (U_2 - U_1) - L^T (P_2 - P_1) &= F_2 - F_1 \\ -L (U_2 - U_1) - E (P_2 - P_1) - \Delta t \bar{H}_I \bar{P} &= \Delta t Q(t), \quad (2) \end{aligned}$$

where

$$\bar{P} = \alpha P_2 + (1 - \alpha) P_1 \quad (3)$$

and $\bar{H}_I$ and $\bar{K}_I$ are values of H_I and K_I evaluated at $t = 1/2(t_1 + t_2)$, $U = 1/2(U_1 + U_2)$, and $P = 1/2(P_1 + P_2)$. In Eq. (3), α is the integration-rule parameter with a value between 0 and 1. In final form, the equations are

$$\begin{aligned} \bar{K}_I \quad -L^T &\left\{ \begin{array}{c} \Delta U^i \\ \Delta P^i \end{array} \right\} \\ -L \quad -E - \alpha \Delta t \bar{H}_I &= \left\{ \begin{array}{c} \Delta F^i \\ \bar{H}_I \Delta t P^{i-1} + Q \Delta t \end{array} \right\}, \quad (4) \end{aligned}$$

where

$$P^{i-1} \big|_{i=1} = \begin{cases} P_0 & \text{current level} \\ 0 & \text{excess level} \end{cases}$$

The solution is expressed in the form

$$U^i = U^{i-1} + \Delta U^i,$$

$$P_i = P^{i-1} + \Delta P^i.$$

The time-march solution technique for linear hydroelasticity is unconditionally stable for values of $\alpha \geq 1/2$ (Booker

and Small, 1975). The equations developed above can be strongly nonlinear even though they represent the hydromechanical behavior at an incremental level. The solution to these equations can therefore be obtained either by direct iteration or by one of the Newton-Raphson schemes. The direct method (variable stiffness method), though proven to be a very powerful technique, has at least two disadvantages:

1. The need for an update of the global stiffness matrix at each iteration.
2. The creation of unrealistic conditions for unloading.

Furthermore, strain-softening modeling may be difficult to achieve with the direct-iteration method. A modified Newton-Raphson method, on the other hand, offers a better alternative, though at the expense of a slower convergence rate. However, it may be possible to use this technique through the time domain. Critical nonlinear conditions, as well as demands for faster convergence, call for updating the stiffness matrices at various time periods. The latter method will be referred to as the mixed Newton-Raphson method. We should point out that conditions of large unloading and strain-softening may limit the application of this method. We first implemented the mixed method for ROCMAS II. Within this strategy we have created an option for solution with the direct-iteration method. This means that ROCMAS II has multiple linearization capacity. The stiffness perturbation scheme alone, along with the improved joint model and incremental loading, makes ROCMAS II superior to ROCMAS. In the next section we give a brief derivation of the incremental algorithm for the modified Newton-Raphson method.

NEWTON-RAPHSON LINEARIZATION

Equation (4) can be written in a more compact form as

$$\psi^i(x) = \underline{K} \delta x^i - R^i = 0 \quad (5)$$

for departure from an established equilibrium at $i - 1$ time level if we assume that

$$\delta x_0^i = 0 \rightarrow \psi_0^i = -R^i$$

we obtain

$$\delta x_1^i = \underline{K}^{-1} \psi_0^i$$

and

$$\delta x_j^i = -\underline{K}^{-1} \psi_{j-1}^i.$$

As a result, we have

$$x^i = \Sigma \delta x_j^i,$$

where

$$x^i = \begin{Bmatrix} \Delta U^i \\ \Delta P^i \end{Bmatrix}.$$

If we replace the $\bar{K}_I$ and $\bar{H}_I$ in the global stiffness matrix $\underline{K}$ above (i.e., in its expanded form, Eq. (4)) by K_E and H_E , the initial matrices, we arrive at the modified Newton-Raphson algorithm. Writing the above expressions in terms of parameters of Eq. (4), we get

$$\psi_0^i = \begin{Bmatrix} \Delta F^i \\ \Delta t \bar{H}_I P^{i-1} + Q \Delta t \end{Bmatrix}, \quad (6)$$

$$\psi_{j-1}^i = \begin{Bmatrix} (\bar{K}_{I,j-1}^i - K_E) \delta \Delta U_{j-1}^i \\ -\alpha \Delta t (\bar{H}_{I,j-1}^i - H_E) \delta \Delta P_{j-1}^i \end{Bmatrix}, \quad (7)$$

and

$$P^i = P^{i-1} + \Delta P^i = P^{i-1} + \sum_{j=1} \delta \Delta P_j^i,$$

$$U^i = U^{i-1} + \Delta U^i = U^{i-1} + \sum_{j=1} \delta \Delta U_j^i.$$

Index i indicates the time level (i). The above procedure is repeated to arrive at the next time level ($i + 1$). In the mixed method in ROCMAS II, we update the K matrix at the beginning of each time level and keep it constant throughout the rest of the iteration in that time level.

NONLINEAR MATERIAL MODELS

Although the mechanisms are in place for the implementation of general inelasticity for the continuum in the present work, we address only the nonlinear behavior of fractures in rocks. This is because of the greater and more-sensitive role fractures play in the hydroelasticity of rock masses. The joint in the new code has strain-softening shear behavior with a peak shear based on the Ladanyi and Archambault (1970) criterion. The closure behavior follows a hyperbolic compression curve (Goodman, 1975). The new shear model also allows for dilation during shear movement of the joints. This important option allows more-realistic determination of fracture apertures, and hence rock permeability in the hydromechanical simulations.

VERIFICATION ATTEMPTS

Verification of a coupled code involves systematic verification at the levels of uncoupled single and coupled multiple phenomena. Details of the comprehensive verification can be found in Noorishad and Tsang (1989). Here we describe a verification study of the fully coupled code. In calculations with the coupled code, care should be taken to ensure strategic refinement of the solution domain, since

it is essential to have sufficient discretizations in the regions of high gradients that may arise in the system response. This turns out to be of critical importance to the solution stability in nonlinear hydromechanical problems.

In this attempt the aim was to test the performance of ROCMAS II analysis of coupled hydromechanical phenomena in a saturated geological system that is perturbed by both mechanical and hydraulic forces. The motivation is provided by the geomechanical and hydrological setting in a number of underground constructions in saturated rocks. We decided on a scoping-model study of a hypothetical tunnel excavation in granitic rocks at a depth of about 300 m. To keep the system at a practical level of computing cost and complexity, we allowed only two major discontinuities to intersect the tunnel and modeled a quarter of the system. Although this is unrealistic to some degree, the exercise is sufficient for code verification, where we need to ensure that the problem fully engages all of the algorithms. The cross section of the tunnel was initially assumed to be rectangular, mainly for ease of manual mesh generation. However, after the first few runs it was found that a very high degree of spatial refinement is required near the tunnel. Thereafter, a circular cross section was used, allowing for easier automatic mesh generation. Figure 1 is a schematic diagram of the model, and Table 1 enumerates various data used in the simulations. Since the tunnel face is the location of the diffusion front—which is at least true for uncoupled fluid flow to the tunnel—it was necessary to have a geometrically refined mesh from the external boundaries toward the tunnel. The redesigned finite element mesh has 503 nodal points and 465 elements for the quarter section of the model. Inside the tunnel, the cri-

Figure 1. Schematic diagram of the tunnel model. [XBL 835-10151]

terion for mesh design is assumed to be the excavation sequence in a ten-bench excavation procedure. This assumption causes some loss of accuracy and may have created certain numerical problems very early in the solution, mostly in the immediate neighborhood of the unexcavated elements. However, in sequential excavations this problem is found to be insignificant. Considering the effectiveness of the direct-iteration method (DIR) in addressing nonlinearity, we first solved the problem with the ROCMAS approach of stiffness perturbation. Figure 2 demonstrates the early-time evolution of the pressure profile in the fracture. The propagation and attenuation of the high pressures, caused by the almost instantaneous loading as excavation is started, match our expectations. The important point in this behavior is the development of pressures with magnitudes approximately 4 times the value of the in situ fluid pressure. These effects can have significant physical implications. However, one aspect of the observed phenomena that came out of the calculations is the unexpected variation of the apertures during the development of the pressure profile. In Fig. 3 these variations are plotted for the first element of the two fractures neighboring the tunnel. Full closure and significant recovery of the apertures, in the case of the vertical fracture, is very interesting. Bundling of stress trajectories behind and in front of the pressure front and their later separation may be the cause of this phenomenon. The horizontal fracture does not experience any significant deformation until the removal of the last bench in the excavation sequence, when the reduction of fluid pressure to the atmospheric level causes some increase in the effective stress and thus slight closure of the fracture. Later-time results show rebounding and widening of this fracture above its initial value before excavation.

Intuitive analysis of the results of the direct-iteration solution confirms that a reasonably satisfactory solution had been obtained. Next the ROCMAS II, with its mixed Newton-Raphson methodology, was employed to solve the same problem. Figure 4 shows the results of this attempt; the broken lines in the figure reproduce some of the steps of the direct-iteration method for comparison. Considering the strong nonlinearity of the system in the presence of large pressures (developed as a result of the early response of the undrained fractures) and the use of rather coarse discretization with mixed quadrilateral and triangular elements, the comparison is very satisfactory. The stable oscillations of the solution can be damped and improved matching can be achieved with more refined and coherent discretization, increased iterations, and use of further damping. It is worth noting that to get this solution, we had to replace the algorithm of Eq. (3) with a damped trapezoidal time-integration form. With the shortcomings of the discretization and the existing nonlinearity, application of the trapezoidal time integration is required. Considering the fundamental differences of the two linearization schemes that were used in obtaining the two solutions, we are satisfied with the performances of ROCMAS II and ROCMAS and consider that verification of these codes has been achieved.

Table 1. Material properties used for various trial runs with ROCMAS.

Material	Property	Value
Fluid	Mass density, ρ_f	$1 \times 10^3 \text{ kg/m}^3$
	Compressibility, β_p	$5.13 \times 10^{-1} \text{ GPa}^{-1}$
	Dynamic viscosity, η_f	$1 \times 10^{-3} \text{ N-s/m}^2$
Rock	Young's modulus, E_s	69.0 GPa
	Poisson's ratio, ν_s	0.25
	Mass density, ρ_s	$2.3 \times 10^3 \text{ kg/m}^3$
	Porosity, ϵ	0.15
	Intrinsic permeability, k	10^{-18} m^2
	Biot's constant, M	130 GPa
	Biot's constant, α	1.0
Fractures	Initial normal stiffness, K_n	$3.7 \times 10^{10} \text{ N/m}^3$ for vertical fracture $1.4 \times 10^{10} \text{ N/m}^3$ for horizontal fracture
	Initial tangential stiffness, K_t	$1.2 \times 10^9 \text{ Pa/m}$
	Initial aperture, $2b$	$1 \times 10^{-3} \text{ m}$
	Wall rock compressive strength, q_u	$1 \times 10^3 \text{ GPa}$
	Ratio of tensile to compressive strength, T_o/q_u	0.1
	Ratio of residual to peak shear, τ_p/T_r	1.0
	Maximum normal closure, Vmc	0.014 m
	Seating load, ξ	$-1 \times 10^4 \text{ N/m}^2$
	Initial dilation angle, i_o	0
	Friction angle, δ	30°
	Porosity, ϵ	1.0
	Biot's constant, M	94 GPa
	Biot's constant, α	1.0, 0.0

Figure 2. Evolution of the pressure profile inside the vertical fracture during and after excavation. [XBL 8811-10530]

CONCLUSION

Limitations of the numerical hydroelasticity technique in our ROCMAS code and the lack of availability of other solution methods for nonlinear problems in this area motivated us to develop an alternative numerical technique that not only serves for cross-verification purposes but also possesses additional capabilities and a more suitable basis for further expansion. A brief account of the fundamentals of such a method in the code ROCMAS II is reported. The basic difference between ROCMAS II and its predecessor ROCMAS lies in the linearization techniques used. ROC-

Figure 3. Time variations of the aperture of the vertical and horizontal fractures at the tunnel during and after excavation. [XBL 8811-10531]

MAS employs direct iteration, whereas ROCMAS II uses mixed Newton-Raphson linearization. This fundamental difference provided the possibility of cross-verification between the two codes for their capability to handle hydromechanical nonlinearity. For this purpose we used the two methodologies to solve an excavation problem in a hypothetical deep tunnel in saturated fractured rock and obtained very similar results. This is an important step in giving us confidence that they perform properly as tools for hydromechanical analysis. The new code ROCMAS II has

Figure 4. Comparison of pressure profiles in the vertical fracture obtained by ROCMAS and ROCMAS II methodologies. Step numbers above 10 refer to post-excitation times. [XBL 894-7548]

options for both linearization techniques and embodies a host of improvements over the ROCMAS code, such as a more realistic joint model and a flexible solution strategy. The incremental setup of the code allows for straightforward implementation of various material nonlinearity models, such as plasticity, which are of importance in studying the rock mechanics of saturated rock environments.

ACKNOWLEDGMENTS

This work is jointly supported by a grant from the Swedish Nuclear Power Inspectorate (SKI), Stockholm, Sweden, and by the U.S. Department of Energy. Discussions and encouragements from Kjell Andersson, Ove Stefansson, Johan Andersson, and Alf Larsson are gratefully acknowledged.

REFERENCES

- Barton, N.R., 1986. Deformation phenomena in jointed rock. *Geotechnique*, v. 36, no. 2, p. 147-167.
- Booker, J.R., and Small, J.C., 1975. An investigation of the stability of numerical solutions of Biot's equations of consolidation. *Int. J. Solids & Struct.*, v. 11, p. 907-917.
- Goodman, R.E., 1975. *Methods of Geological Engineering*. West Publishing Co., New York.
- Ladanyi, B., and Archambault, G., 1970. Simulation of the shear behavior of a jointed rock mass. *In Proceedings, 11th Symposium on Rock Mechanics (AIME)*, p. 105-125.
- Noorishad, J., Witherspoon, P.A., and Brecke, T.L., 1971. A method for coupled stress and flow analysis of fractured rock masses. *Geotechnical Engineering Publication No. 71-6*, University of California, Berkeley.
- Noorishad, J., Ayatollahi, M.S., and Witherspoon, P.A., 1982. Coupled stress and fluid flow analysis of fractured rocks. *Int. J. Rock Mech. & Min. Sci.*, v. 19, p. 185-193.
- Noorishad J., and Tsang, C.F., 1989. Recent enhancements of the coupled hydromechanical code: ROCMAS II. *Swedish Nuclear Power Inspectorate, SKI # TR 89:4*.
- Small, J.C., Booker, J.R., and Davis, E.H., 1976. Elastoplastic consolidation of soils. *Int. J. Solids & Struct.*, v. 12, p. 431-448.
- Tsang, C.F. (ed.), 1987. *Coupled Processes Associated With a Nuclear Waste Repository*. Academic Press, San Diego, U.S.A.

Aqueous Foams for Control of Gas Migration and Water Coning in Aquifer Gas Storage

P. Persoff, C.J. Radke, K. Pruess, S.M. Benson, Y.S. Wu, and P.A. Witherspoon

Storage of natural gas in underground formations is used by utilities to ensure deliverability of gas during peak seasonal and daily demand periods. During low-demand periods gas is injected into a permeable formation overlain by an impermeable caprock with a dome-shaped structure. When needed, the gas is withdrawn through the same wells. Typically, the permeable formation is saturated with water, so the gas forms a lens-shaped gas cap or "bubble" between the caprock and the water.

Although underground gas storage is effective in meeting peak demands, in most cases only a fraction of the gas in storage—typically one-third—can be recovered during a withdrawal season. Two causes of poor recoverability are gas migration beyond the designated storage volume during the gas-injection cycle and water coning into wells during the withdrawal cycle. During the formation of the initial storage volume in an aquifer, some of the injected gas fingers away from the main bubble, sometimes for long distances, because of the adverse mobility ratio between water and gas. This migrated gas is often impossible to recover during a withdrawal season. Water coning during gas withdrawal significantly reduces the well productivity. Elimination—or significant delay—of water coning in the

production zone is thus highly desirable during the withdrawal season.

One possible solution to these problems is the use of aqueous foam as a mobility-control agent. The presence of foam in a porous medium reduces the permeability to both gas and liquid (Bernard and Holm, 1964; Bernard et al., 1965), suggesting that foam could be emplaced in a storage formation to improve the recoverability of stored gas. One idea, using the gas-blocking property of foam, is to emplace in an aquifer a suitable foam barrier that would confine the stored gas in a compact volume around the injection wells (Witherspoon et al., 1987). Two possible applications are shown in Fig. 1. Another idea, using the liquid-blocking property, is to place a foam lens strategically to reduce the permeability to water near the withdrawal well, as shown in Fig. 2, thereby delaying water coning and extending the seasonal life of the withdrawal well.

The purpose of this project was to examine the technical questions that must be answered to make the proposed applications of foam feasible. The full results are presented in Persoff et al. (1989, 1990); a major portion of this work, investigation of the durability and regenerability

Figure 1. Application of foam to improve underground gas storage by controlling gas migration (after Witherspoon et al., 1987). (a) Foam plumes formed at peripheral wells intersect to form a continuous barrier, containing stored gas in a more compact bubble near the injection-withdrawal wells. The use of foam obviates the need for natural closure. (b) A small foam barrier to cut off a spill point produces a large increase in storage capacity. [XBL 869-3258A]

Figure 2. Use of a horizontal foam lens to reduce water coning. [XBL 882-10066]

of the gas- and liquid-blocking properties of foam, is summarized here.

METHODS AND MATERIALS

The apparatus has been described in Persoff et al. (1989, 1990). The foamer solution was a synthetic brine with 1% active Steol 7N (alkylethoxysulfate surfactant, Stepan Co., Northfield IL) and 0.2% dodecyl alcohol. Foam was formed in a sandstone core by simultaneously injecting nitrogen gas and foamer solution, or only nitrogen gas, into a core initially saturated with foamer solution. Pressure and liquid saturation (by gamma-ray densitometry) were automatically measured at several locations along the sandstone core. Liquid was delivered by a constant-rate pump, and nitrogen gas was delivered at either constant mass-flow rate or constant injection pressure. Backpressure was maintained by a dome-loaded backpressure regulator. After foam was formed in the core, the gas or liquid injection was continued, and the permeability was calculated from the measured flow rates and pressures.

GAS BLOCKING BY FOAM

Experiments were conducted in a Boise sandstone core of permeability $1.3 \mu\text{m}^2$ (1.3 darcies) and porosity 0.25 and in a Berea sandstone core of permeability $0.19 \mu\text{m}^2$ (190 millidarcies) and porosity 0.19. To measure the permeability to gas, dry gas was injected through a foamed sandstone core under either constant injection pressure or constant mass-flow rate. In none of these experiments did we observe complete blocking of gas flow, as has occasionally been reported (Albrecht and Marsden, 1970; Minssieux, 1974; Hanssen, 1988). However, the permeability to gas was reduced below the intrinsic permeability of the rock by approximately three orders of magnitude, indicating that a very substantial reduction in gas leakage rate could be achieved. The permeability to gas was initially very low in all these experiments, gradually increasing to about 1 or $2 \times 10^{-3} \mu\text{m}^2$ (1 or 2 millidarcies) after 14 days.

In four experiments, the permeability to gas generally increased gradually with time as shown in Fig. 3. This behavior was observed whether the foam was formed by simultaneous injection of gas and liquid or by injection of gas alone, whether the gas was injected at constant pressure drop or constant rate, and whether the permeability of the core was 1.3 or $0.19 \mu\text{m}^2$ (1300 or 190 millidarcies). The details of each experiment are given in the caption of Fig. 3.

The increase in permeability in the first experiment, as shown in Fig. 3 (curve A), suggested that foam might need to be regenerated periodically. Therefore, a method to regenerate foam was investigated. In experiment B, gas was injected into the core at 5.17 MPa (750 psi) against a backpressure of 4.82 MPa (700 psi). Gas initially invaded rapidly, displacing liquid from the core, and as foam advanced through the core, the flow rate decreased. Gas broke through after 1 hr at a flow rate corresponding to a permeability of $1.9 \times 10^{-3} \mu\text{m}^2$ (1.9 millidarcies) or a reduction by a factor of 680 compared to the initial permeability of the core. At this point, an additional 0.03-PV

Figure 3. Gradual increase in gas permeability of foam-filled sandstone core; four experiments. In all experiments, the core was initially saturated with the foamer solution. (A) Foam generated by simultaneous injection of gas and liquid at controlled flow rates. Liquid flow stopped and gas-injection pressure reduced. Permeability measured at constant gas-injection pressure. Permeability of sandstone without foam = $1.3 \mu\text{m}^2$ (1300 millidarcies). (B) Foam generated by injection of gas at constant pressure. Additional slugs of foamer solution injected; permeability shown is after final slug. No reduction of injection pressure. Permeability of sandstone without foam = $1.3 \mu\text{m}^2$ (1300 millidarcies). (C) Foam generated by injection of gas at constant rate into $1.3 \mu\text{m}^2$ (1300-millidarcy) core. No reduction of injection pressure. (D) Foam generated by injection of gas at constant rate into $0.19 \mu\text{m}^2$ (190-millidarcy) core. No reduction of injection pressure. [XBL 8910-3663]

slug of foamer solution was injected while the inlet gas pressure was maintained. The gas flow immediately dropped to almost zero and slowly recovered. Although gas permeability through the core was $1.9 \times 10^{-3} \mu\text{m}^2$ (1.9 millidarcies) 1 hr after gas invaded the initially saturated core, it took about 36 hr for the gas permeability to regain that value after the slug was injected. Two more slugs were injected at approximately 36-hr intervals. Figure 4 shows the cumulative gas flow through the core at constant injection pressure. After each slug, the permeability dropped to almost zero and recovered gradually to less than $10^{-3} \mu\text{m}^2$ (1 millidarcy). The gradual increase in permeability after injection of the third slug is shown in Fig. 3 (curve B). After 8 days, the foam was broken by a slug of 0.09-PV foam breaker, as described in Persoff et al. (1990).

In two additional experiments, foam was formed by injection of gas at constant rate, one in $1.3\text{-}\mu\text{m}^2$ (1300-millidarcy) Boise sandstone and the other in $0.19\text{-}\mu\text{m}^2$ (190-millidarcy) Berea sandstone. Data from these experiments are plotted as curves C and D in Fig. 3. The general similarity of all the curves in Fig. 3 indicates that under foamed conditions the permeability to gas in a $0.19\text{-}\mu\text{m}^2$ core was similar to that in a $1.3\text{-}\mu\text{m}^2$ core. The degree of permeability reduction was less in the lower-permeability core, a phenomenon that was also observed by Bernard and Holm (1964).

LIQUID BLOCKING BY FOAM

Besides blocking gas flow, foam also blocks liquid flow, as first observed by Bernard et al. (1965). This property could be used to prevent upward coning of water into

Figure 4. Cumulative gas flow as a function of time; gas injected at constant pressure into core, showing effect of additional slugs of foamer solution (experiment B). [XBL 8910-3665A]

a withdrawal well. In low-permeability reservoirs, the pressure at the withdrawal well must be reduced much below the reservoir pressure to induce sufficient flow to the well. This local reduction in pressure causes water to rise in a cone and to increase the liquid saturation near the withdrawal well perforations. The result is two-phase flow in the well, with greatly reduced gas productivity. A strategically placed foam lens would reduce the permeability to water near the withdrawal well, thereby delaying water coning and extending the seasonal life of the withdrawal well.

In an experiment to measure the ability of foam to block liquid flow, foam was formed by injecting gas and liquid simultaneously into the $1.3\text{-}\mu\text{m}^2$ (1300-millidarcy) Boise sandstone core. Then the injection of gas was stopped, and liquid saturation and pressure profiles were measured while the injection of liquid (foamer solution, later changed to surfactant-free brine) was continued. Figure 5 shows the liquid saturation at two locations in the core during this experiment and the liquid permeability calculated between pairs of adjacent pressure taps. First, an amount of liquid equal to 9.5 pore volumes (based on the total pore volume of the core) was pumped through the

Figure 5. Liquid saturation at 20 and 50 cm (upper plot) and liquid permeability between pairs of adjacent pressure taps (lower plot) during injection of 27 pore volumes of liquid through a foam-filled Boise sandstone core. [XBL 8911-4348]

core. Since the liquid saturation in the core was approximately 35%, this was sufficient to replace the liquid in the core 28 times. During this part of the experiment, the liquid permeability throughout the core remained at $10^{-3} \mu\text{m}^2$ (1 millidarcy), and the liquid saturation remained at 35% throughout the core. These values agree with the relative permeability data measured for the same core using brine and nitrogen gas (for relative permeability data see Persoff et al., 1989). Next, the liquid was changed from foamer solution to brine without surfactant, and another 17 pore volumes (sufficient to replace the liquid in the core 51 times) was pumped through the core. Bubbles emerging from the exit of the backpressure regulator showed that lamellae broke and some of the trapped gas was released; Fig. 5 shows that both the liquid saturation and the liquid permeability increased as the surfactant was diluted in the foam, starting at the core inlet and progressing to the outlet. This agrees with the accepted view that low liquid permeability in a foamed core results from low liquid saturation (Bernard et al., 1965; Persoff et al., 1989).

The results of the liquid-blocking experiment indicate that the key to controlling water coning into gas withdrawal wells is to keep the liquid saturation, and the vertical liquid permeability, at a low value in the region around the wellbore. Many foam-flow experiments reported here and elsewhere (Persoff et al., 1989) show that the liquid saturation in a foam-filled core is just a few units above connate, and the relative permeability to liquid is typically about 10^{-3} . This experiment demonstrated that water saturation in a foam-filled porous medium remains low even though a large gradient of water pressure is imposed across it. This suggests that water coning could be controlled by placing a foam "lens" near the gas-water contact so as to block the upward flow of water, as shown schematically in Fig. 2.

A three-phase gas-storage reservoir simulator "MULKOM-GWF" developed for this project (Pruess and Wu, 1988) was used to study the effectiveness of a foam lens in preventing coning and to optimize its placement. This simulation study concluded that the effect of a low-permeability zone created by foam near a wellbore is not to eliminate coning but to diminish and delay it significantly. A foam lens placed above the gas-water contact was predicted to delay coning for 3 months, which is a substantial improvement in the seasonal life of a withdrawal well. Since gas withdrawal is limited to a few months of the year, permanent prevention of coning is not necessary. This application of foam appears quite promising in its economics, as the advantage may be obtained, without additional drilling, merely by emplacing a relatively small volume of foam.

DISCUSSION AND CONCLUSIONS

The technical issues to be resolved for foam application in aquifer gas storage are whether foam can be formed and emplaced in a formation, whether it will sufficiently

reduce gas or liquid permeability, and whether the reduced permeability can be maintained for months. Our experiments, although not answering all the questions, have given favorable results to suggest that foam can be applied to increase the efficiency of underground gas storage.

Although one-dimensional laboratory experiments in homogeneous media have shown large reductions in gas and liquid permeability, it is necessary to determine whether this degree of permeability reduction can be achieved in the field. Radial flow may cause gas velocities to be too slow to form a strong foam at distances from the wellbore, and natural heterogeneities may interfere with emplacement of a foam bank.

The results shown in Fig. 3 suggest that for a gas-blocking application, some provision must be made to regenerate the foam. The cost of the project will depend upon the needed frequency of regeneration. Additional slugs of liquid would be injected whenever the permeability of the foam block exceeds a certain limit, and the higher this limit is set, the less frequently regeneration would be needed. But even if the foam were allowed to decay, the gas saturation in the designated storage volume would be greater and more uniform than if foam had not been used, so that recoverability of injected gas should improve.

The rate of foam decay shown in Fig. 3 is probably pessimistic because of the test method. The gas injected in all these experiments was dry, and liquid saturations below connate measured during the later stages of each experiment near the inlet region indicate that liquid was removed from the core by evaporation. Low liquid saturation is known to be detrimental to foam stability (Khatib et al. 1988). The method used to conduct the experiment is therefore a severe test of foam-block durability.

Pilot-scale field testing is now needed to confirm our results in practice. The most promising application for a field trial appears to be control of water coning. Such a field trial could be done at a well where coning has been experienced in the past (the control experiment has already been done), and the foamer solution could be injected through the existing well and followed with gas. Another attractive prospect for a field trial would be the use of foam to seal a known leakage path of limited area, such as a fault zone or a leaky casing.

Application of foam to underground gas storage need not be limited to conventional underground storage in aquifers. Where demand is present but suitable geologic formations are absent, mined caverns in hard rock could be used as storage reservoirs. Here leakage through fractures intersecting the cavern might be controlled by foam. Another area where foam technology could be applied is compressed-air energy storage in aquifers. By controlling gas migration and water coning, foam could prevent the loss of stored energy and ensure deliverability. Because the cycle in this application would be daily, rather than annual, requirements for foam stability might be reduced.

The results presented here support the following conclusions (additional conclusions are presented in Persoff et al., 1989, 1990):

1. Foam reduces the gas permeability of a porous medium by 2 to 3 orders of magnitude. The permeability gradually increases as lamellae decay, but foam can be regenerated by injection of additional slugs of foamer solution.
2. Foam effectively blocks liquid flow because the liquid saturation is low. When liquid is pumped through a foam-filled core, the liquid saturation remains low as long as the surfactant concentration is not diluted. When the surfactant concentration is diluted, trapped gas is released, and liquid saturation and liquid permeability increase. In our experiment, approximately 17 pore volumes of water was pumped through the core before the permeability increased significantly.
3. Simulation studies indicate that a foam lens placed just above the gas-water contact significantly delays water coning into a withdrawal well.

From the results of our experimental and theoretical studies, we conclude that application of foam to improve the efficiency of aquifer gas storage appears to be technically feasible. The logical next step would be a field trial. The most promising field trial would be an attempt to control water coning by means of a relatively small foam lens emplaced beneath the feed zone of a gas-withdrawal well.

REFERENCES

- Albrecht, R.A., and Marsden, S.S., 1970. Foams as blocking agents in porous media. *Soc. Pet. Eng. J.*, March, p. 51-59.
- Bernard, G.G., and Holm, L.W., 1964. Effect of foam on permeability of porous media to gas. *Soc. Pet. Eng. J.*, September, p. 267-274.
- Bernard, G.G., Holm, L.W., and Jacobs, W.L., 1965. Effect of foam on trapped gas saturation and on permeability of porous media to water. *Soc. Pet. Eng. J.*, December, p. 295-300.
- Hanssen, J.E., 1988. A new method for testing of gas-blocking foams. Paper SPE/DOE 17362, presented at the SPE/DOE Enhanced Oil Recovery Symposium, Tulsa, Oklahoma, April 17-20.
- Khatib, Z.I., Hirasaki, G.J., and Falls, A.H., 1988. Effects of capillary pressure on coalescence and phase mobilities in foams flowing through porous media. *SPE Res. Eng.*, v. 3, no. 3, p. 919-926.
- Minssieux, L., 1974. Oil displacement by foams in relation to their physical properties in porous media. *J. Pet. Technol.*, January, p. 100-108.
- Persoff, P., Radke, C.J., Pruess, K., Benson, S.M., and Witherspoon, P.A., 1989. A laboratory investigation of foam flow in sandstone at elevated pressure. Paper SPE-18781 presented at the 1989 California Regional SPE Meeting, Bakersfield, California, April 5-7 (LBL-26639).
- P. Persoff, Pruess, K., Benson, S.M., Wu, Y.S., Radke, C.J., Witherspoon, P.A., and Shikari, Y.A., 1990. Aqueous foams for control of gas migration and water coning in aquifer gas storage. *Energy Sources*, in press (LBL-28862).
- Pruess, K., and Wu, Y.S., 1988. On PVT-data, well treatment, and preparation of input data for an isothermal gas-water-foam version of MULTKOM. Lawrence Berkeley Laboratory Report LBL-25783.
- Witherspoon, P.A., Radke, C.J., Shikari, Y., Pruess, K., Persoff, P., Benson, S.M., and Wu, Y.S., 1987. Feasibility analysis and development of foam-protected underground natural gas storage facility. American Gas Association, Proceedings Operating Section, paper #87-DT-110, p. 539-549 (LBL-23500).

Flow to Wells in Fractured Rock with Fractal Structure

*J. Polek, K. Karasaki, J.C.S. Long, and J. Barker**

Analysis of fluid flow behavior in fractured rocks is very difficult because the fracture geometry is generally unknown and complex. Furthermore, fractures exist at all scales. At one end of the spectrum, faults may be on the order of several kilometers in length, and on the other they may be no more than small microcracks at the rock-grain

level. One promising approach is to treat a fracture system as a fractal. Barton et al. (1987) observed in his pavement studies that the fracture trace-length distributions exhibit fractal characteristics.

Barker (1988) solved the generalized equation of flow to a well by letting the flow dimension be a variable. The flow dimension is therefore allowed to be fractional—e.g., a dimension of 1.6 or 2.3 (as opposed to an integral dimension, i.e., two- or three-dimensional space). He

*British Geological Survey, Oxfordshire, U.K.

showed that the head-versus-time curve plotted on log-log paper approaches a straight line with a slope of $1 - (n/2)$. This article summarizes work on the behavior of fluid flowing to wells in networks with fractal geometry. The flow dimension, n , obtained using Barker's theory is compared with two fractal dimensions calculated geometrically.

ROCK SYSTEM DESCRIPTION

Two methods were used to generate fractured rock systems with fractal properties. The first method used is a modified Sierpinski's carpet. A traditional Sierpinski's carpet has a designated number of scaled square regions that are filled in. The modified carpet places lines representing fractures within the square regions, rather than filling them in (Karasaki et al., 1988). A set of three fractures placed end to end in a straight line, without overlapping, stretches from one side of the square to the other. Four of these fracture sets were placed in a square. These sets were evenly spaced, with two sets vertical and two sets horizontal. The configuration of these fracture sets resembles the setup of a tick-tack-toe game. Figure 1 shows a modified Sierpinski carpet at the fourth construction stage. The carpet has six out of a total of nine scaled-down squares fractured at each construction stage. The location of the squares was chosen at random at each construction stage. The fractured rock system could be generated only up to the fourth construction stage because of computer-memory limitations. At the fourth stage the smallest fractures were designated to be of unit length, and the larger fractures were considered strings of unit-length fractures. At this stage the length of the side of a rock system was 243 units.

Figure 1. Modified Sierpinski carpet. [XBL 8911-4115]

The second method used to generate a rock system with fractal properties is based on the percolation theory. A lattice of equilateral triangles is used to create a percolating network. Each side of a triangle is a bond having a probability p of being an open bond and a probability $1 - p$ of being a closed bond. The rock system is generated by keeping the open bonds, which represent unit-length fractures. Of these open bonds only those constituting the backbone cluster are retained. The backbone cluster consists of any flow paths from the centrally located well to a boundary. For bond percolation on a triangular lattice the critical probability, p_c , is 0.3473. The fracture networks were all created with p close to or equal to p_c so that the network would have self-similar geometry. A network with self-similar geometry appears the same at any length scale, within a specified range, and exhibits fractal properties (Orbach, 1986).

FRACTAL AND FLOW DIMENSIONS

The geometrical fractal dimensions of the Sierpinski carpets and the percolating networks were found using a method described by Orbach (1986). The method consists of calculating the density of fractures as a function of distance from an assigned origin. The density is found by counting the number of fractures contained in a circle of radius r from the origin. The density is the ratio of the fracture mass to the area of the circle:

$$\rho(r) = \frac{M(r)}{A(r)} = \frac{Lr^D}{C \cdot r^d} \propto r^{(D-d)}, \quad (1)$$

where D is the fractal dimension, d is the Euclidean dimension, and L and C are constants. For the rock systems generated in this study, the log-log plot of the density versus the radius results in a straight line with a slope equal to $D - 2$. From this slope the fractal dimension can be calculated. By repeating the process, using many origins, an average fractal dimension is found for each rock system.

The radial fractal dimension was found using a method similar to that used to calculate the fractal dimension. However, when calculating the fracture mass of the system to get the radial fractal dimension, only the radial components of the fractures were counted. It was expected that this dimension would better describe the physical processes occurring during a well test.

The results of the well tests modeled on the two types of rock systems were used to calculate the flow dimension of the systems. A log-log plot of head versus time was constructed. The flow dimension was calculated from the value of the slope of the straight-line portion of the plot. According to Barker's generalized flow equation, the value of this slope is $1 - (n/2)$. The relationship between the flow dimension and the two geometrical fractal dimensions is discussed below.

RESULTS

Figures 1 and 2 show examples of each type of fracture system and their geometrical fractal dimensions. Both fracture systems are square. The fractured Sierpinski carpet is 243 units on a side, and the percolating fracture network is 64 units on a side. Work is currently being done on a percolating network similar in size to the Sierpinski carpet.

Table 1 shows the various dimensions for some Sierpinski carpet rock systems. The number of squares fractured at each construction stage varies from three to six, which results in dimensions between 1 and 2. The radial fractal dimension and the fractal dimension are very close to one another because of the systematic structure of the carpet. Of the two, the radial fractal dimension is closer to the flow dimension. Table 2 shows the various dimensions for percolating meshes with p ranging from 0.345 to 0.40. Again, as in Table 1, the radial fractal dimension is closer to the flow dimension than is the fractal dimension. The geometry of the percolating fracture systems results in tortuous flow paths. These crooked flow paths are "straightened" when calculating the radial fractal dimension, which accounts for the difference between these two geometrical fractal dimensions. Table 2 also shows that the probability p and the geometrical fractal dimensions are not uniquely related.

CONCLUSIONS

It was confirmed that the flow dimension obtained from the slope of a well-test pressure curve is a function of the geometrical fractal dimensions. Although the function was not defined, these geometrical fractal dimensions are

Figure 2. Percolating fracture network. [XBL 8911-4116]

Table 1. Modified Sierpinski carpets.

Number of fractured squares (N)	Backbone fractal dimension (D)	Radial fractal dimension (D_R)	Flow dimension (n)
3	1.190	1.179	1.178
4	1.382	1.379	1.274
5	1.498	1.498	1.354
6	1.620	1.616	1.508

Table 2. Percolating fracture networks.

Probability (p)	Backbone fractal dimension (D)	Radial fractal dimension (D_R)	Flow dimension (n)
0.3450	1.310	1.280	1.233
0.3473	1.152	1.108	1.070
0.3500	1.399	1.284	1.255
0.4000	1.839	1.648	1.592

always equal to or larger than the flow dimension. The reason is that, although the fractal dimensions are merely a geometric count of the fracture density, the flow dimension is a reflection of the hydraulic structure of the fracture network. It is this flow dimension that should be used to characterize a network's behavior during well tests.

REFERENCES

- Barker, J.A., 1988. A generalized radial-flow model for pumping tests in fractured rock. *Water Resour. Res.*, v. 24, no. 10, p. 1796-1804.
- Barton, C.C., Schutter, T.A., Page, W.R., and Samuel, J.K., 1987. Computer generation of synthetic fracture networks for hydrologic-flow modeling. *Trans. Am. Geophys. Union*, v. 68, no. 44, p. 1295.
- Karasaki, K., Polek, J., Long, J., and Witherspoon, P., 1988. Flow to wells in fractured reservoirs. *In* Second Berkeley Symposium on Topics in Petroleum Engineering, March 9-10, 1988 (Program and Abstracts). Lawrence Berkeley Laboratory Report LBL-24337, p. 59-64.
- Orbach, R., 1986. Dynamics of fractal networks. *Science*, v. 231, p. 814-819.

Numerical Modeling of Gas Migration at a Proposed Repository for Low- and Intermediate-Level Nuclear Wastes at Oberbauenstock, Switzerland

K. Pruess

For a number of years the Nationale Genossenschaft für die Lagerung radioaktiver Abfälle (NAGRA) has been developing a repository project for geologic disposal of low- and intermediate-level radioactive wastes. Recent investigations have focused on a site in the Oberbauenstock mountain (Resele and Tripet, 1985).

A nuclear waste repository will contain large amounts of concrete, metals, and organic materials in contact with groundwater. Detailed studies have indicated that corrosion of the metals and microbial degradation of the organic materials will evolve large amounts of gas (Rasmuson and Elert, 1986; Wiborgh et al., 1986), the chief constituents being hydrogen, methane, and carbon dioxide. Additional relatively minor amounts of gases will be generated from radiolysis of water.

The expected gas release raises several concerns. From the data given by Wiborgh et al. (1986) it can be estimated that gas pressures in the repository could build up to levels of several hundred bars unless specific design provisions are made for gas venting. Such pressures could breach the system of engineered barriers and compromise the integrity of the repository. On the other hand, gas escaping from the repository volume could alter existing groundwater flow paths in the host rock and thereby impact on the travel time of potential contaminants to the biosphere.

The study summarized here (Pruess, 1989) is a first preliminary attempt to evaluate, by means of computer simulation, the gas release from the repository and its effects on pore pressures and groundwater flow in the host rock. We define two reference cases for computer simulation of two-phase (gas-liquid) fluid flow in the host rock, which model the formations as a porous and as a fractured-porous medium, respectively. Both cases are schematic in nature; they are not necessarily expected to give realistic results, but are intended to provide guidance for future field exploration and modeling studies.

REFERENCE CASES

The present study builds on conceptual models and parameters developed by NAGRA to define a detailed numerical model for two-phase flow of groundwater and hydrogen gas in the vicinity of a potential nuclear waste repository at Oberbauenstock. The numerical model is implemented through a modified version of the simulation program "TOUGH" (Pruess, 1987), which describes non-isothermal flow of water and air in porous or fractured media. In the modified version used in the present work the air component of TOUGH was replaced by hydrogen.

We model the same two-dimensional vertical section through Oberbauenstock for which single-phase groundwater flow calculations had previously been made by NAGRA. The choice of the 2-D section was substantiated by NAGRA's three-dimensional modeling work.

For the porous-medium reference case, the flow domain is partitioned into essentially rectangular volume elements or "grid blocks." A plot of grid block locations is given in Fig. 1. For convenience grid thickness has been chosen as 1 m.

For the fractured-porous-medium case each of the volume elements of the porous-medium grid was further partitioned into two regions, corresponding to fracture and rock matrix domains, respectively. A dual-permeability formulation was used in which global flow in the system can occur in fractures as well as rock matrix, the latter permitting only vertical flow connections. In addition there is local "interporosity" flow between fractures and matrix (Fig. 2).

NAGRA has undertaken a variety of theoretical, laboratory, and field studies to estimate natural groundwater flow and large-scale permeability and porosity in the potential host formations at Oberbauenstock. Parameters obtained from NAGRA were used whenever available. Some parameters are unknown at the present time, chiefly the relative permeability and capillary pressure characteristics of the fractured rock mass. For these, "best guesses" were made on the basis of literature data. A detailed tabulation and discussion of all calculational parameters is given in Pruess (1989).

RESULTS

Simulated results for the reference cases are shown in Figs. 3 and 4. In agreement with previous analysis (Rasmuson and Elert, 1986) our simulation shows that dis-

Figure 1. Grid block locations for the model developed in the present study (shaded areas indicate the zones of higher permeability around the repository and Seelisberg tunnel). [XBL 903-706]

Figure 2. Schematic diagram of flow geometry in the fractured-porous model. [XBL 896-7654]

solution and removal of gas by flowing groundwater occurs at a rate that is smaller than the rate of gas generation. In our porous-medium model it takes approximately 2.5 years for hydrogen to exceed the solubility limit. Subsequently, a free gas phase evolves in the repository grid blocks, which is accompanied by an increase in fluid pressure (see Figs. 3 and 4).

Fluid pressure declines after a mobile gas saturation (5%) is established; for the porous medium this occurs after 20 years. At this time the rate of corrosive gas generation also is reduced because the more corrosive materials such as aluminum have been consumed; this yields a rapid pressure decline. The depressurization is accompanied by further increase in gas saturation from expansion effects.

In the fractured-porous medium, fluid pressures and gas saturations begin to rise at an earlier time, as expected. Gas saturations in the fractures are larger at all times. Overall, the behavior of the dual-permeability model is similar to the porous-medium model.

Figure 3. Simulated pore pressures (in bars) at $t = 20$ years (porous-medium model). [XBL 903-705]

Figure 4. Predicted temporal evolution of gas pressures and saturations at the repository level. The curves labeled "dual permeability" pertain to the fractured-porous-flow model. [XBL 867-10357]

DISCUSSION AND CONCLUSIONS

The results for the reference cases are to be considered illustrative and preliminary rather than quantitative. We have attempted to choose parameters that appear "reasonable" for the Oberbauenstock site, but it is recognized that some of the more important parameters, such as relative permeabilities, are not well known. The porous-medium reference case is not expected to provide a realistic outlook on gas pressurization and migration effects, whereas the fractured-porous-medium case employs highly approximate descriptions of global matrix flow and interporosity flow. Another limitation of the present simulation is that rather coarse grid blocks have been used in the repository domain.

The latest results from site investigations at Oberbauenstock indicate that a few larger fracture zones exist which could have a high permeability. Additionally, it seems that some of these features are filled with natural gas. This could diminish significantly the potential pressure build-up due to gas production in the repository.

Future work should focus on identifying the most important parameters affecting system behavior so that uncertainty in system response can be reduced to acceptable levels.

ACKNOWLEDGMENT

This work was supported by NAGRA, Baden, Switzerland, and by the U.S. Department of Energy. The author gratefully acknowledges the technical guidance obtained from NAGRA through Drs. Charles McCombie and Piet Zuidema.

REFERENCES

- Pruess, K., 1987. TOUGH user's guide. U.S. Nuclear Regulatory Commission Report NUREG/CR-4645, June 1987 (also Lawrence Berkeley Laboratory Report LBL-20700).
- Pruess, K., 1989. Numerical modeling of gas migration at a proposed repository for low and intermediate level nuclear wastes at Oberbahrenstock, Switzerland. Lawrence Berkeley Laboratory Report LBL-25413.
- Rasmuson, A., and Elert, M., 1986. The influence of gas flow on solute transport. Kemakta AB, Stockholm, Draft Report to NAGRA.
- Resele, G., and Tripet, J.P., 1985. Hydrogeologische Grundlagen für das Modellgebiet Oberbahrenstock. NAGRA Report NTB 85-29.
- Wiborgh, M., Höglund, L.O., and Pers, K., 1986. Gas formation in a L/ILW repository and gas transport in the host rock. NAGRA Report NTB 85-17.

On Two-Phase Relative Permeability and Capillary Pressure of Rough-Walled Rock Fractures

K. Pruess and Y.W. Tsang

Fluid flow in geologic media is often dominated by the highly permeable pathways provided by rock fractures and joints. Multiphase flow through fractures occurs in many subsurface flow systems that are of engineering interest in the context of energy resource recovery (petroleum, natural gas, geothermal water and steam) and environmental protection (chemical and radiation contamination in groundwater aquifers, partially saturated zones). It also plays a crucial role in petroleum migration and ore deposition and in the evolution of hydrothermal convection systems.

When several fluid phases are present simultaneously in the void space of a porous medium, or in a rock fracture, the presence of any one of the phases will interfere with the flow of all the others. Quantitatively, this permeability reduction is expressed in terms of relative permeability factors k_r , so that for a medium with absolute (intrinsic) permeability k , the effective permeability to a fluid phase β (= aqueous, gas, oil, etc.) is given by $k \cdot k_{r,\beta}$. The relative permeability functions vary between zero and one. When $k_{r,\beta} = 0$, very strong phase interference exists, with phase β completely immobile because of the presence of other phases. When $k_{r,\beta} = 1$, there is negligible phase interference, i.e., essentially single-phase flow of phase β . Experimental and theoretical work has established that the relative permeability functions are primarily dependent on the void space fraction or "saturation" S_β occupied by a fluid phase (Scheidegger, 1974). More complicated effects, including dependence on capillary number and saturation history (hysteresis), are also well documented.

Given the wide occurrence and practical importance of multiphase flow in fractures, it is surprising that very little quantitative information on fracture relative permeabilities is available. The only published experimental data that we are aware of are those of Romm (1966), who observed two-phase flow of water and kerosene in artificial parallel-

plate fractures, which were lined with strips and sheets of cellophane or polyethylene film and waxed paper. Romm obtained a linear dependence of relative permeability on saturation for the entire range of $0 < k_r < 1$, with wetting and nonwetting phase relative permeabilities given by $k_{r,w} = S_w$, $k_{r,nw} = S_{nw}$, respectively, so that $k_{r,w} + k_{r,nw} = 1$. For lack of other data Romm's relative permeabilities have been widely used in numerical simulations of fractured petroleum reservoirs (e.g., Gilman and Kazemi, 1983), although it appears unlikely that Romm's results would be applicable to relative permeabilities of real rough-walled rock fractures.

From a theoretical viewpoint the subject of multiphase flow in fractures has also received very little attention. The chief obstacle here seems to be that until recently there was a lack of credible models for the pore space geometry in natural rock fractures. Newly developed imaging techniques (Gentier, 1986; Pyrak-Nolte et al., 1987; Hakami, 1988) have led to the conceptualization of fractures as two-dimensional heterogeneous porous media, with flow taking place in intersecting channels of varying aperture (Tsang and Tsang, 1987; Wang et al., 1988). These emerging concepts open the way for new theoretical approaches to multiphase flow in fractures.

A NEW APPROACH

The approach developed in this paper for predicting two-phase relative permeability in fractures is based on the conceptualization of rough-walled rock fractures as two-dimensional porous media whose void space can be characterized by specifying the aperture as a function of position. We introduce the hypothesis that, as far as multiphase-flow properties are concerned, a rough-walled fracture with position-dependent aperture behaves locally like a parallel-plate fracture with the same average aperture. This

approximation clearly requires experimental confirmation. The approximation is expected to be applicable under conditions where the distance over which fracture apertures are correlated is large compared to the apertures themselves. The local parallel-plate approximation allows one to predict phase occupancy and permeability for any suitably small subregion of the fracture plane. The global relative permeability behavior of a rock fracture is then obtained by discretizing the fracture into a large number of connected parallel plates of different apertures. Numerical simulation is used to synthesize multiphase flow on a larger scale from the known phase occupancy and permeability characteristics of the individual parallel-plate segments.

Specifically, our procedure for calculating capillary pressures and relative permeabilities is as follows.

1. Obtain a discretized representation of fracture apertures for a finite rectangular domain, either by generating a stochastic realization of a suitable aperture distribution on a computer or by directly digitizing an image of the pore space. Figures 1 and 2 show lognormal aperture distributions with the spatial correlations used in this work.
2. Define a cutoff aperture b_c , corresponding to a capillary pressure $P_c = 2\gamma/b_c$ (γ is surface tension), and occupy all accessible apertures smaller than b_c with wetting phase, all larger apertures with nonwetting phase. Calculate the wetting-phase saturation $S_w(b_c)$ (and the nonwetting-phase saturation $S_{nw} = 1 - S_w$) corresponding to the cutoff capillary pressure P_c by directly summing the wetted pore volume.

Figure 1. A 20×20 discretized lognormal aperture distribution in a fracture plane with isotropic spatial correlation. The magnitudes of the apertures are indicated by shading, with lighter shading corresponding to larger aperture. [XBL 891-7414]

Figure 2. A 20×20 discretized lognormal aperture distribution with anisotropic spatial correlation. [XBL 891-7415]

3. Apply suitable constant-pressure conditions at the boundaries of the fracture, and simulate fluid flow in the network of occupied fracture elements. (In our simulations, flow is taking place in the x direction, with no-flow boundaries at $y = 0$ and $y = 1$; see Figs. 1 and 2.) The steady-state flow rate obtained when only apertures less than b_c are occupied will yield the effective wetting-phase permeability; a similar simulation with only apertures larger than b_c occupied will yield the effective nonwetting-phase permeability.
4. Division of the effective phase permeability by the single-phase permeability (all apertures occupied) yields the relative permeability at saturation $S_w(b_c)$. Repeat the procedure for a range of b_c to obtain the entire relative permeability and capillary pressure curves.

The procedure outlined here involves a number of approximations; further research is required to determine the conditions under which they are applicable (Pruess and Tsang, 1989, 1990).

RESULTS

We have performed simulations for a number of discretized realizations of lognormal and normal aperture distributions with different mean values and spatial correlation lengths. Figures 3 and 4 show results for wetting- and nonwetting-phase relative permeabilities, respectively, for the two aperture distributions of Figs. 1 and 2 (parameters as given in Table 1). The different data points in Figs. 3 and 4 were obtained from simulated steady-state flow rates at different cutoff apertures b_c .

Figure 3. Simulated wetting- and nonwetting-phase relative permeabilities for the lognormal aperture distribution of Fig. 1. [XBL 891-7043]

The most remarkable feature of the relative permeability curves shown in Fig. 3 is the apparent strong interference between the phases: immobile nonwetting-phase saturation is extremely large, about 84%, and a saturation "window" in which both phases would be mobile is virtually nonexistent. This contrasts with the behavior shown in Fig. 4, where immobile nonwetting saturation is a more modest (although still large) 51.5%, and there is a considerable range of saturations over which both phases can flow

Figure 4. Simulated wetting- and nonwetting-phase relative permeabilities for the lognormal aperture distribution of Fig. 2 with long-range anisotropic spatial correlation. [XBL 891-7402]

Table 1. Parameters for lognormal aperture distributions.

	Case 1	Case 2
Mean aperture (μm)	81.8	81.8
Standard deviation in log aperture	0.43	0.43
x-spatial correlation	0.20	0.60
y-spatial correlation	0.20	0.20

simultaneously. In our calculations so far we have generally found that a significant window of two-phase mobility exists only for anisotropic aperture distributions, with considerably larger spatial correlation length in the direction of flow than perpendicular to it.

Our wetting-phase relative permeabilities appear to be generally similar to experimental results for (three-dimensional) porous media, but nonwetting-phase relative permeabilities are predicted to drop off rather rapidly with increasing wetting-phase saturation.

Phase interference is generally stronger in two-dimensional than in three-dimensional porous media, because there are fewer alternative routes for bypassing inaccessible pores. Anisotropic spatial correlation, with larger correlation length in the direction of flow, tends to segregate the small-aperture and large-aperture pathways (see Fig. 2). This diminishes phase interference and broadens the saturation window for two-phase mobility (see Fig. 4). The sudden jump in nonwetting-phase relative permeability at $S_w = 48.5\%$ occurs because of a single pore throat located near $x = 0.5$, $y = 0.3$ (see Fig. 2).

For a lognormal aperture distribution, an approximate capillary pressure-saturation relationship can be obtained through direct integration in closed form. The functional relationship involves a complementary error function and is shown as the solid curve in Fig. 5 for the parameters given in Table 1. The general appearance of this curve is similar to the customary j -function (Leverett, 1941).

CONCLUSIONS

A method has been developed that allows calculation of relative permeability and capillary pressure characteristics of rough-walled rock fractures from a known or assumed void space geometry. First results indicate that interference between several fluid phases flowing simultaneously in a fracture will generally be strong. Long-range spatial correlations among apertures appear to have a profound impact on fracture relative permeability.

At the present time there are no reliable observational data with which our prediction for fracture relative permeabilities can be compared. Experimental data are needed to evaluate the various approximations made and to guide future theoretical developments.

Figure 5. Capillary pressure (in units of inverse aperture) versus saturation relationship for a fracture with lognormal aperture distribution. [XBL 896-7637]

ACKNOWLEDGMENT

In addition to support from the U.S. Department of Energy, additional funding was provided by the Nationale Genossenschaft für die Lagerung radioaktiver Abfälle (NAGRA), Baden, Switzerland.

REFERENCES

- Gentier, S., 1986. *Morphologie et Comportement Hydromécanique d'une Fracture Naturelle dans un Granite Sous Contrainte Normale* (Doctoral thesis). Université d'Orléans, Orléans, France.
- Gilman, J.R., and Kazemi, H., 1983. Improvements in simulation of naturally fractured reservoirs. *Soc. Pet. Eng. J.*, v. 23, p. 695-707.
- Hakami, E., 1988. Water flow in single rock joints (Licentiate thesis). Lulea University of Technology, Lulea, Sweden.
- Leverett, M.C., 1941. Capillary behavior in porous solids. *AIME Trans.*, v. 142, p. 152.
- Pruess, K., and Tsang, Y.W., 1989. On relative permeability of rough-walled fractures. Presented at the Fourteenth Annual Workshop on Geothermal Reservoir Engineering, Stanford University, Stanford, California, January 24-26, 1989. Lawrence Berkeley Laboratory Report LBL-26509.
- Pruess, K., and Tsang, Y.W., 1990. On two-phase relative permeability and capillary pressure of rough-walled rock fractures. *Water Resour. Res.*, in press, 1990. Lawrence Berkeley Laboratory Report LBL-27449.
- Pyrak-Nolte, L.J., Myer, L.A., Cook, N.G.W., and Witherspoon, P.A., 1987. Hydraulic and mechanical properties of natural fractures in low permeability rock. In P.G. Herget and S. Vongpaisal (eds.), *Proceedings, Sixth International Congress on Rock Mechanics*, Montreal, Canada, August 3-September 3, 1987. A.A. Balkema, Rotterdam, Netherlands. Lawrence Berkeley Laboratory Report LBL-22718.
- Romm, E.S., 1966. *Fluid Flow in Fractured Rocks*. Moscow, (trans. W.R. Blake, Bartlesville, OK, 1972).
- Scheidegger, A.E., 1974. *The physics of flow through porous media*. University of Toronto Press, Toronto and Buffalo, 3rd Edition.
- Tsang, Y.W., and Tsang, C.F., 1987. Channel model of flow through fractured media. *Water Resour. Res.*, v. 23, no. 3, p. 467-479 (LBL-21310).
- Wang, J.S.Y., Narasimhan, T.N., and Scholz, C.H., 1988. Aperture correlation of a fractal fracture. *J. Geophys. Res.*, v. 93, no. B3, p. 2216-2224 (LBL-22494).

An Exploitation Model and Performance Predictions for the Ahuachapan Geothermal Field, El Salvador

M. Ripperda, G.S. Bodvarsson, M.J. Lippmann, and C. Goranson

The Ahuachapan geothermal field in El Salvador has been producing electrical power since 1975. The field currently produces approximately 50 MWe, which is below the installed capacity of 95 MWe. We are currently investigating the possibility of significantly increasing the power generation at Ahuachapan over the next 20 to 30 years. Some of the questions addressed by this report are

1. Will injection increase the power production at Ahuachapan?
2. What is the best location for injection wells, and what percentage of the produced fluids should be injected?
3. Where should new production wells be located, and how many wells are required for the next 30 years?

4. What is the highest power-production level that can be economically maintained over a 30-year period?

To address these questions, a complex three-dimensional numerical model of the field has been developed. This model is based on all of the available data, which were analyzed by Aunzo et al. (1989). The results from this previous study, including the geologic model, the reservoir-data analysis, the conceptual model, and the natural-state models, were incorporated into the numerical model. The model was then calibrated against production data, which include the reservoir pressure decline and flow rates and enthalpies from all of the wells during the period 1975–1989. The calibration (history match) involved numerous iterations in which reservoir parameters were adjusted until a satisfactory match was obtained between calculated and observed production data.

After the history match was obtained, the model was used to predict the responses of the existing wells, hypothetical additional production (development) wells, and the overall reservoir response to various exploitation and injection scenarios. These scenarios were evaluated on the basis of the reservoir performance, the pressure decline, the returns of injected fluids, and the economic viability.

THREE-DIMENSIONAL NUMERICAL MODEL

Because of the complex thermodynamic and geologic conditions of the Ahuachapan field, it was decided that a fully three-dimensional model of the field is necessary. The important components of the model include the design of the grid, the rock and fluid properties, the initial conditions, and the boundary conditions. A three-dimensional grid with four horizontal layers was designed for the modeling. A multilayered model is necessary because (1) most of the wells have multiple feedzones, (2) a relatively shallow two-phase zone provides a significant fraction of the produced fluids, and (3) much of the recharge to the system flows through the deep Older Agglomerates.

Figure 1 is a map of the Ahuachapan area, including the field and surface thermal manifestations. Figure 2 shows an areal view of a single layer of the grid. The grid extends from the El Salitre hot springs in the north to a location about 2 km south of the Laguna Verde volcano. The total length of the grid is 14,500 m (in the north-south direction), the width is 8000 m, and the thickness is 1000 m. The AA, A, and B layers constitute the Ahuachapan Andesites and are assigned thicknesses of 30, 150 and 250 m, respectively. The C layer represents the Older Agglomerates and is assigned a thickness of 550 m.

The present wellfield at Ahuachapan is found below about 400 masl and is associated with the Ahuachapan Andesites and Older Agglomerates. The caprock is formed by a mostly impermeable layer between the Ahuachapan Andesites and Young Agglomerates. Barriers to flow are believed to exist north and west of the present wellfield. The

Figure 1. Map showing surface manifestations in the Ahuachapan and Chipilapa area. [XBL 902-642]

Figure 2. Numerical grid used in the simulations, along with the locations of the surface hot springs. [XBL 902-643]

northern barrier is indicated by the much lower temperatures found in wells AH-11 and AH-12. The western barrier is inferred from the pressure and temperature data from wells AH-17, AH-8, and AH-15. The initial temperatures in wells AH-17 and AH-8 are on the order of 220°C, whereas the temperature in AH-15 is about 120°C. Well AH-15 is located only several hundred meters west of AH-17 and AH-8.

The wellfield is located in a horst structure that has about 50 m of uplift. This shallow structure allowed a two-phase zone to develop over most of the region between wells AH-23 and AH-17 before exploitation. North and west of this structure, much cooler fluid is found. The hottest temperatures reported for the field were in well AH-14, east of the wellfield. Wells AH-18 and AH-32, which are south of the uplifted region, are also hotter than most of the other wells, but the reservoir is deeper there and those wells did not penetrate a shallow two-phase zone.

The pressure throughout the reservoir before 1975 was about 48 bars at an elevation of 75 masl. This depth corresponds to the middle of the B layer in the simulation model. The temperatures at this depth ranged from nearly 250°C around wells 32 and 18 in the southern region of the reservoir to about 140°C in well 12 just north of the reservoir. The temperatures in the reservoir increase from north to south and west to east. This is consistent with the source of hot recharge in the southeast and the location of cooler boundaries north and west of the reservoir.

HISTORY MATCHING

The primary data used for the history match of the Ahuachapán wells are the flow rate, flowing enthalpy, and static pressure. The flow rate and enthalpy data are compiled from monthly Comisión Ejecutiva Hidroeléctrica del Río Lempa (CEL) production records, and the pressure data are taken from shut-in pressure logs. Fluid production from the field began on August 27, 1968, when well AH-1 was flowed for the first time. Fluid extraction increased in the following years as new wells were completed and flow tested. Large-scale exploitation started in June 1975, when the first 30-MWe generator went on line. A second 30-MWe went on line in July 1976 and a third unit (35 MWe) in November 1980.

Numerous iterations were necessary to obtain reasonable matches with the observed flow rates and enthalpies of the wells. The parameters that were adjusted during the iteration process were (1) productivity indices, (2) permeabilities, and (3) porosities. Although the effects of these parameters are coupled, each of them affects the flow rates and enthalpies in a different way. The productivity index most strongly affects the flow rate at relatively early times; consequently, we use this parameter to fix the initial rate from a layer. The permeability primarily controls the decline of flow rate with time but also affects the enthalpy transients. Lower permeabilities cause the enthalpy to in-

crease with time. The porosity has very little effect on the flow rate but has a relatively strong effect on the enthalpy.

A sample history match for well AH-27 is shown in Fig. 3. In almost all cases there is good agreement with the late-time data, and in most cases the calculated and observed flow rates and enthalpies agree well over the entire exploitation period.

The average permeability within the wellfield is estimated to be 100 md. There are several high-permeability fault zones where the permeability ranges up to 1 darcy. The permeability in the vapor cap is estimated to range between 1 and 1.5 darcies, which is much higher than the average values for the lower layers. However, because the vapor cap is so thin (30 m) its transmissivity (permeability-thickness) is comparable to those of the other

Figure 3. Comparison between computed (solid line) and observed flow rates and enthalpies for well AH-27. [XBL 902-644]

layers (around 30 D-m). The high permeabilities in the vapor cap were necessary to support the large amounts of production from high-enthalpy wells such as AH-6, AH-17, and AH-26. With lower permeabilities, the steam mobility is too low (low steam density) and the reservoir pressures in the well elements draw down too quickly.

A contour map of the pressure distribution in the B layer at the end of the history match (1989) is shown in Fig. 4. The pressure has declined by about 16 bars within the reservoir. The pressure decline is much more pronounced at the northern edge of the field than at the southern edge, which is to be expected, given that the fluid recharge flows from the south.

Figure 4. Calculated pressure distribution in the B layer in 1989. [XBL 8910-7818]

FIELD PERFORMANCE PREDICTIONS

From the production history match we obtained a model that can be used to predict the response of the reservoir and individual wells to various exploitation schemes. The primary interest at Ahuachapan is to determine the maximum electrical power generation levels that can be economically maintained over a suitable time period. We have run numerous cases that range from letting the field continue in its present state to drilling enough wells to bring the power generation up to the full 95-MWe capacity. We also investigated the effects of injection on each case.

The results indicate that maintaining 50 MWe will require 4 new production wells over the next 30 years. Increasing the power production to 75 MWe will require 18 new wells over the next 30 years. The field can support 95 MWe for only about 15 years with the drilling of 24 new production wells. After that time the productivity of any new well is very low, so the production was allowed to decline with time for this case to a final production level of 70 MWe. Injection has a strong effect on decreasing the pressure decline for each of the cases studied.

SUMMARY

A three-dimensional numerical model of the Ahuachapan geothermal field has been developed. This model was designed on the basis of the known geology, geochemistry, and geophysics of the field. It was then calibrated against 15 years of reservoir pressure measurements and individual production rates and flowing enthalpies from 16 wells. The best-fit model indicates that hot fluid recharge to the field originates from the vicinity of the Laguna Verde volcano to the southeast. The model corroborates the location of barriers to flow identified in the conceptual flow model by Aunzo et al. (1989). There is a barrier immediately west of the field and a leaky barrier north of the field. Some cold-water recharge (in the range of 30 to 60 kg/s) enters the field from the north and from the southwest. The model was utilized to investigate the effects of different injection scenarios and to determine the level of power generation that can be sustained for 30 years. A production level of 75 MWe with 60% reinjection of the produced fluids appears to be the best option.

REFERENCES

- Aunzo, Z., Bodvarsson, G.S., Laky, C., Lippmann, M.J., Steingrimsdottir, B., Truesdell, A.H., and Witherspoon, P.A., 1989. The Ahuachapan geothermal field, El Salvador—Reservoir analysis. Lawrence Berkeley Laboratory Report LBL-26612.

A Simplified Analytical Solution for Dissolution and Transport of Nonaqueous Phase Liquids in Groundwater

C. Shan, I. Javandel, and P.A. Witherspoon

The development of contaminant plumes in groundwater systems after nonaqueous-phase liquids (NAPL) have reached the water table is a matter of great importance in attempting to select the appropriate monitoring system and remedial actions. We have developed a physical model to investigate this problem. As part of our studies, it was necessary to predict the transient concentration distribution in the experimental model due to the dissolution and transport of an organic compound. Characterization of the porous medium in the model showed that the mode of transport due to longitudinal dispersion was significantly smaller than that due to advection. As a result a simplified analytical solution was developed that could incorporate such observation. This solution considers lateral dispersion but assumes that the longitudinal dispersion is negligible. One may note that in the direction of flow, when the value of dispersivity is small, advection is the dominating mode of transport. In such cases, ignoring the effect of dispersion in the direction of flow is a reasonable assumption. A brief description of the new solution is given below. Details of the derivation are given by Javandel et al. (1989).

THEORY

Consider a body of NAPL with a given geometry resting on top of the water table, as shown in Fig. 1. Water with uniform pore velocity of u' flows horizontally through the porous medium. The concentration C'_0 of a given chemical from the NAPL at the interface of the NAPL and water is assumed to remain constant. Transport of the dissolved chemical in the water is assumed to be controlled by both advection and dispersion. Since the lens of dissolved chemical would be limited to a small portion of the upper part of the system, for the sake of simplicity the thickness

Figure 1. A schematic diagram of the mathematical model. [XBL 902-634]

of the aquifer is assumed to be infinite. The concentration on the upstream boundary of the aquifer is considered to be zero, and flux of the chemical across the rest of the upper face is assumed to be negligible. Because of the nonuniformity of the upper boundary condition, the medium is artificially divided into two regions. A Cartesian coordinate system with the origin at the downstream contact of NAPL with water is used.

Nondimensionally, the mathematical model may be presented in the form of the following initial-boundary-value problem.

DIFFERENTIAL EQUATION

$$\frac{\partial C_i}{\partial t} + \frac{\partial C_i}{\partial x} = \frac{\partial^2 C_i}{\partial z^2} \quad i = 1, 2 \quad (1)$$

INITIAL AND BOUNDARY CONDITIONS

$$C_i(x, z, 0) = 0 \quad (2)$$

$$C_1(x, 0, t) = 1 \quad (3)$$

$$C_1(-l, z, t) = 0 \quad (4)$$

$$C_i(x, \infty, t) = 0 \quad (5)$$

$$\frac{\partial C_2(x, 0, t)}{\partial z} = 0 \quad (6)$$

$$C_2(\infty, z, t) = 0 \quad (7)$$

$$C_1(0, z, t) = C_2(0, z, t) \quad (8)$$

$$\frac{\partial C_1(0, z, t)}{\partial x} = \frac{\partial C_2(0, z, t)}{\partial x} \quad (9)$$

where

$$C_i = \frac{C'_i}{C'_0}, \quad x = \frac{x'}{\alpha'_z}, \quad z = \frac{z'}{\alpha'_z},$$

$$t = \frac{u' t'}{\alpha'_z}, \quad l = \frac{l'}{\alpha'_z},$$

and where C'_i refers to the concentration of the chemical in regions 1 and 2, respectively, and α'_z is lateral dispersivity.

SOLUTION

Region 1

Applying Laplace transformation with respect to t and Fourier sine transformation with respect to z , consecutively, Eqs. (1) through (5) for region 1 may be converted to the form

$$\bar{\bar{C}}_1(x, r, s) = \frac{r}{s(s+r^2)} \left[1 - \exp[-(s+r^2)(x+l)] \right], \quad (10)$$

where s and r are Laplace and Fourier sine transform parameters, respectively, and $\bar{\bar{C}}_1(x, r, s)$ is defined as follows:

$$\bar{\bar{C}}_1(x, r, s) = \int_0^\infty \bar{C}_1(x, z, s) \sin(rz) dz \quad (11)$$

and

$$\bar{C}_1(x, z, s) = \int_0^\infty e^{-st} C_1(x, z, t) dt. \quad (12)$$

Equation (10) can be inverted first from the Laplace domain and then from the Fourier domain to give the solution for region 1:

$$C_1 = \operatorname{erfc} \left[\frac{z}{2\sqrt{t}} \right] U(x+l-t) + \operatorname{erfc} \left[\frac{z}{2\sqrt{x+l}} \right] U(t-x-l), \quad (13)$$

where $U(t-a)$ is the Heaviside unit function. Equation (13) presents a solution for concentration distribution in region 1 that satisfies the differential equation (1) and the initial and boundary conditions as specified in Eqs. (2) through (5). Using the definition of the Heaviside unit function the solution given by Eq. (13) may be split into two time periods, as shown below.

$$C_1 = \operatorname{erfc} \left[\frac{z}{2\sqrt{t}} \right] \quad \text{for } t < x+l, \quad (14)$$

$$C_1 = \operatorname{erfc} \left[\frac{z}{2\sqrt{x+l}} \right] \quad \text{for } t > x+l. \quad (15)$$

It is interesting to note that for large values of time when $t > x+l$ the solution for concentration distribution in the region 1 is independent of time.

Region 2

Applying Laplace transformation twice, first with respect to t and then with respect to x , differential equation (1), together with the initial and boundary conditions (2) and (8), yields

$$\frac{d^2 \bar{\bar{C}}_2}{dz^2} - A^2 \bar{\bar{C}}_2 = -f(z, s), \quad (16)$$

where $\bar{\bar{C}}_2$, A and $f(z, s)$ are defined as follows:

$$\bar{\bar{C}}_2(p, z, s) = \int_0^\infty e^{-px} \bar{C}_2(x, z, s) dx, \quad (17)$$

$$\bar{C}_2(x, z, s) = \int_0^\infty e^{-st} C_2(x, z, t) dt, \quad (18)$$

$$A = \sqrt{s+p}, \quad (19)$$

and

$$f(z, s) = \frac{\exp(-z\sqrt{s})}{s} - \frac{1}{2s} \left\{ e^{-z\sqrt{s}} \operatorname{erfc} \left[\sqrt{ls} - \frac{z}{2\sqrt{l}} \right] - e^{z\sqrt{s}} \operatorname{erfc} \left[\sqrt{ls} + \frac{z}{2\sqrt{l}} \right] \right\}. \quad (20)$$

The symbols s and p are Laplace transform parameters.

Solving Eq. (16) for $\bar{\bar{C}}$ and inverting from the Laplace transform domain twice yields

$$C_2(x, z, t) = \frac{1}{\pi} U(x+l-t) \int_0^t \frac{\exp(z^2/4\tau)}{\sqrt{\tau(t-\tau)}} U(l-t+\tau) d\tau \\ + \frac{1}{\pi} \int_0^t \delta(x+l-T) \int_0^T \frac{\exp(-z^2/4\tau)}{\sqrt{\tau(T-\tau)}} U(l-T+\tau) d\tau dT \\ - \frac{1}{\pi} \int_0^t \frac{\exp(-z^2/4\tau)}{\sqrt{\tau(t-\tau)}} U(l-t+\tau) U(x-\tau) d\tau, \quad (21)$$

where $\delta(x+l-T)$ is a shifted Dirac delta function. Here, too, the solution may be split into three time intervals:

$$C_2(x, z, t) = 0 \quad \text{for } t < x, \\$$

$$C_2(x, z, t) = \frac{1}{\pi} \int_x^t \frac{\exp(-z^2/4\tau)}{\sqrt{\tau(t-\tau)}} d\tau \quad \text{for } x < t < x+l, \quad (22)$$

$$C_2(x, z, t) = \frac{1}{\pi} \int_x^{x+l} \frac{\exp(-z^2/4\tau)}{\sqrt{\tau(x+l-\tau)}} d\tau \quad \text{for } t > x+l.$$

MASS TRANSFER RATES

It is very important to estimate the mass transfer rate of a specific chemical from NAPL to groundwater. Having obtained the expression for concentration distribution in groundwater below NAPL, one can easily calculate mass transfer rate as given below.

$$M_z = \frac{1}{\sqrt{\pi}} \left[\sqrt{t} + \frac{l}{\sqrt{t}} \right] \quad \text{for } t \leq l, \quad (23)$$

$$M_z = \frac{2\sqrt{l}}{\sqrt{\pi}} \quad \text{for } t > l, \quad (24)$$

where dimensionless mass transfer rate M_z is defined as

$$M_z = \frac{M_z'}{u' \alpha_z' C_0} \quad (25)$$

and M_z' is the mass transfer rate per unit width of NAPL.

The mass transfer of a given solute in groundwater can also be estimated across any vertical plane in the system under consideration. A section of particular interest is the interface between region 1 and 2, where $x = 0$. This is of great interest because one can compare the release rate of a given constituent from the NAPL to groundwater with the mass transfer rate of the same constituent leaving the source area and entering the groundwater. The mass transfer rate across the plane of $x = 0$ may be given as

$$M_x = \frac{2\sqrt{t}}{\sqrt{\pi}} \quad \text{for } t \leq l \quad (26)$$

and

$$M_x = \frac{2\sqrt{l}}{\sqrt{\pi}} \quad \text{for } t \geq l, \quad (27)$$

where M_x is dimensionless mass transfer rate and defined as

$$M_x = \frac{M_x'}{u' \alpha_z' C_0} \quad (28)$$

in which M_x' is the mass transfer rate per unit width of the aquifer perpendicular to the direction of flow. We further introduce a normalized form for the mass transfer rates and a new form of dimensionless time:

$$Q_z = \frac{\sqrt{\pi}}{2\sqrt{l}} M_z, \quad (29)$$

$$Q_x = \frac{\sqrt{\pi}}{2\sqrt{l}} M_x, \quad (30)$$

$$T_l = \frac{t}{l} = \frac{u' t'}{l'} \quad (31)$$

The expressions for normalized mass transfer rates of a given constituent from the NAPL, Q_z , and the mass transfer rate of the same substance leaving the source area, Q_x , may be written as

$$Q_z = \frac{1}{2} \left[\sqrt{T_l} + \frac{1}{\sqrt{T_l}} \right] \quad \text{for } T_l \leq 1, \quad (32)$$

$$Q_z = 1 \quad \text{for } T_l \geq 1, \quad (33)$$

and

$$Q_x = \sqrt{T_l} \quad \text{for } T_l \leq 1, \quad (34)$$

$$Q_x = 1 \quad \text{for } T_l \geq 1. \quad (35)$$

RESULTS

Figure 2 shows the variation of Q_x and Q_z as a function of new dimensionless time; note that, the release rate of the concerned contaminant from the NAPL starts from a relatively large value and will slowly decline, approaching unity when T_l becomes 1. Thereafter, the release rate remains constant. This implies that the source of pollution is unlimited, which is a direct consequence of assuming constant concentration at the interface of the NAPL with groundwater. Depending on the initial volume of the NAPL, this assumption could be valid for relatively large values of time. Strictly speaking, however, the source ultimately depletes and the mass transfer rate drops.

On the other hand, the mass transfer rate of the concerned contaminant is zero when it leaves the source area and increases with time until $T_l = 1$, when it crosses the plane $x' = 0$. Thereafter, the rate remains constant and equal to the rate of release from the NAPL. This figure suggests that for all times corresponding to $T_l > 1$ the mass entering the groundwater is equal to the mass leaving the source area. As a result, the mass of the contaminants in the source area, region 1, remains constant for all values of time corresponding to $T_l > 1$. Note that, by definition, $T_l = 1$ corresponds to the time required by the water particles to travel the length of the NAPL along the groundwater-flow direction. Also note that the area confined between the curves for Q_z and Q_x in Fig. 2 is a measure of the mass of the constituent accumulated in region 1.

We have evaluated the solution for the appropriate properties and parameters of the model. Table 1 shows the input data for which the analytical solution was evaluated.

Figure 2. Variation of vertical and horizontal mass transfer as a function of dimensionless time, $T_l = u' t' / l'$. [XBL 902-635]

Table 1. Data input for calculation.

Parameters	Values
Pore-water velocity	0.4 cm/min
Lateral dispersivity	0.009 cm
Length of the NAPL lens	9.6 cm

The value of lateral dispersivity used in this calculation was obtained from tracer tests. The pore-water velocity shown in the table is calculated from total flow rate, sand-bed cross section, and porosity of the sand. Total flow rate was measured by rotameter at the entrance and volumetrically at the exit. Pore-water velocity was also measured independently through tracer tests.

Knowing the above conditions for the model, we were interested to know the frontal position of the organic compound at various times. Figure 3 shows a cross section of the system along the flow direction. We have arbitrarily chosen contours of dimensionless concentration of 0.001 as the front of the contaminant plume. This figure shows fronts of the contaminant at 1, 2, and 3 hours after the start of the test. It should be noted that the origin of the coordinate system used in the derivation of analytical solutions was chosen to be at the downstream edge of the NAPL lens, whereas the horizontal axis in Fig. 3 refers to the distance from the upstream edge of the NAPL.

Figure 4 shows the depth of plume penetration with time below the NAPL lens and at various distances downstream from the lens. This figure consists of five frames. Frame 1 refers to the concentration distribution in a section at mid-distance below the NAPL lens. Frames 2 through 5 refer to sections at 0, 10, 20, and 30 cm downstream from the lens, respectively. Each frame refers to two values of time, and the one with the symbol > in front of it shows the concentration distribution for all values greater than the specified time. According to this figure, concentration at a specified point downstream from the source increases with time until it arrives at steady state. This figure also shows

Figure 3. A vertical section along the flow direction in the model, showing the position of toluene fronts at three values of time, 1, 2, and 3 hours. [XBL 902-636]

Figure 4. Variation of toluene concentration with depth and time at five sections, $x' = -0.5, 0, 10, 20,$ and 30 cm. [XBL 902-637]

that the depth of plume penetration increases with the distance downstream from the NAPL lens and that the steady-state concentration at shallow depths decreases with distance downstream.

REFERENCE

- Javandel, I., Holman, H., and Shan, C., 1989. Studies of dissolution and transport of nonaqueous phase liquids in groundwater. Lawrence Berkeley Laboratory Report LBL-27988, 180 p.

A Broad View of Model Validation

C F. Tsang

The safety assessment of a nuclear waste geologic repository demands much more of the scientists and engineers and their modeling results than the safety evaluation of any civil structures, such as dams, or the resource evaluation of petroleum or geothermal reservoirs. The extra demands are mainly due to two factors:

1. The safety assessment usually involves the estimation of low probability (low concentration) of radionuclides transported over kilometers and extrapolated thousands of years into the future.
2. Data that characterize the rock mass at the repository site are necessarily sparse, since too many data-

collecting boreholes may adversely impact the integrity of the rock mass. Thus there may be many uncertainties in our knowledge of the site's geometric structures, boundary conditions, and relevant processes.

There is much interest and concern in all the countries with a nuclear waste management program on the question of model validity. A number of recent international cooperative efforts—e.g., Hydrocoin (1987), Intraval (Andersson, 1987)—have been devoted to the validation of models. Model validation was also extensively discussed in various symposia, such as Geoval87 (1987) and Geoval90. Some general comments on model validation are given in Tsang (1989). Additionally, there is a wealth of literature on validation in the field of systems engineering and operations research that may be useful for our consideration. Examples include Zeigler (1976), Gass and Thompson (1980), Schruben (1980), Oren (1981), Gass (1983), Sargent (1984, 1988), Balci and Sargent (1984), and Balci (1988, 1989).

A FEW DEFINITIONS AND COMMENTS

Validation has been defined in various ways. Schlesinger et al. (1979) defined it as meaning "substantiation that a computerized model within its domain of applicability possesses a satisfactory range of accuracy consistent with the intended application of the model." The International Atomic Energy Agency (IAEA, 1982) defines validation as follows: "A conceptual model and the computer code derived from it are validated when it is confirmed that the conceptual model and the computer code provide a good representation of the actual processes occurring in the real system."

In this article the term "model" means the combination of conceptual model, computer code, and all relevant field and laboratory data and information. Only with the combination of all these elements is it possible to perform modeling studies whose results may be used as a representation of the actual processes occurring in the real system.

The computer code is a computer program that solves a given set of equations with given inputs by numerical manipulations. Thus computer codes should be certified, which means that the code is properly verified and properly documented. In other words, it is mathematically correct in the formulation and solution and is properly documented in terms of its function, accuracy, required discretization, and ranges of applicability. However, one should not be talking about *code* validation, since validation questions the appropriateness of the mathematical equations and input data and conditions, which are assumed and taken for granted in a code.

Model calibration is the process by which certain unknown parameters to be used in a code are determined by comparing modeling results with part of the observed data, which the model is required to simulate. For safety

assessment of nuclear waste repositories, the models are expected to predict data for thousands of years into the future, and calibration is done to estimate parameters with short-term data. In this paper this kind of calibration is assumed to be part of site-characterization activities, where tests and analyses (which may well include modeling calculations) are done to determine the needed model parameters for assessment of repository safety for thousands of years.

The term "conceptual model" is used to mean two main components: structure and processes. Structure refers to the geometric structure of the system, such as stratigraphy, faults, heterogeneity, fracture density and lengths, and other geometric and geologic characteristics. Processes are physical and chemical phenomena such as buoyancy flow, colloidal transport, matrix diffusion, and dissolution and precipitation. Structure is site specific and scale dependent and usually appears in modeling study as calculational mesh designs and input data. Processes, on the other hand, are usually described by mathematical equations being solved in a computer code and can often be studied in the laboratory. In practice, processes and structure are often intimately coupled.

From the above discussion it may be apparent that almost by definition one can never have a validated computer model without further qualification. One can say that a model, including the conceptualization and the code, is validated with respect to (1) a process or (2) a site-specific system. A process is first identified (e.g., buoyancy convective flow) and then conceptualized (e.g., as temperature-dependent density and viscosity), and coding is performed on this conceptualization. The model, consisting of conceptualization and code, is then applied to a buoyancy experiment and its results compared with measurements. The model can then be regarded as validated with respect to this specific process. Model validation with respect to various processes should be a significant element in any national nuclear waste management program because it establishes our capability to predict the effects of these processes at a site. This is indeed the subject of a number of current international projects.

A site-specific system may be composed of a number of processes and structures, which form the building blocks of the system. Of course it is an important and not-so-easy problem to identify the building blocks. Once the building blocks are identified, a model or group of models may be used to simulate the system and results can be compared with field observations. If successful, the group of models is said to be validated with respect to this particular site, within a range of applications determined by the range of field observations studied.

Hence there is no such thing as a validated model in the generic sense. However, one can say that "a model is validated with respect to a given process," or that "a model or group of models is validated with respect to a given site." Ranges of applicability should be given with

these statements. Though model validation with respect to processes is an important subject currently under study by many groups, this article examines model validation only with respect to a given site, since this is more relevant to the definitions of Schlesinger et al. (1979) and IAEA (1982).

THE MODELING PROCESS

This section describes the steps in a site-specific modeling exercise, or modeling process, which is distinct from the physical and chemical processes referred to previously. The first step in the modeling process (see Table 1) is to review and evaluate the available data. This involves more than just searching the data base to obtain numbers needed for a given modeling exercise. A good modeler studies the complete data base to obtain the best possible overall picture of the site and the relevant processes occurring there. Of particular interest is an evaluation of data correlation, of which there are two types. The first is the spatial or temporal correlation. This is often studied by statistical methods. The second, which may be of more importance, is the parameter correlation, which limits the range of values one parameter can have because of the value chosen for another parameter. For example, Wang and Narasimhan (1989) point out that such a correlation exists between the saturated conductivity and air-entry pressure (or radius) for the unsaturated zone at the Yucca Mountain site. Earlier studies have coupled too large a saturated conductivity value with too small an air-entry radius value as inputs to a modeling calculation, and such inputs are unphysical.

The second step is to develop a conceptual model and potential scenarios. The purpose is to abstract the essence of the data base to obtain the structure of the geometric model and to identify relevant physical and chemical processes involved in the system. Sometimes the data may be uncertain or even internally inconsistent, and

some subjective judgement will be required. Possible scenarios in time also have to be identified and evaluated according to their probabilities of occurrence.

The third step is the establishment of performance criteria. This is related to "domain of applicability" or "range of application" in the definition of validation according to Schlesinger et al. (1979). Performance criteria are the quantities of interest that the model is asked to predict. There is the possibility that a performance criterion could be defined in such a way that the quantity of interest can never be predicted with sufficient accuracy because of intrinsic uncertainties in data. For example, in a highly heterogeneous fractured porous medium, it is probably impossible to predict tracer concentration at a particular point in space and time. Thus one has to modify the performance criterion to something more plausible yet still acceptable for the problem at hand. In the same example, instead of requiring the prediction of a point value of tracer concentration, we can ask for an integrated tracer concentration over a period of time and region of space (Tsang, 1989). In the safety assessment of a nuclear waste repository, perhaps that is all that is needed.

The fourth step of the modeling process is the construction of calculational models and the determination of the associated lumped parameters. Conceptual models are usually complex and are by definition three dimensional, so that simplification is always needed before modeling can proceed. We call these simplified models the calculational models. Often it is convenient to use different simplification procedures for the calculation of different quantities of interest. Thus only a very simple calculational model may be needed for thermal-field calculation, whereas finer features might have to be added for tracer-transport calculation. By lumped parameters we mean not only those averaged over space blocks, but also those combining several more elementary parameters. For spatially lumped parameters, much consideration needs to be given to how they should be defined, especially in the case of strongly

Table 1. Steps of the modeling process and their validation.

The modeling process	Examples of issues requiring validation
1. Data review and evaluation	Spatial correlation and parameter correlation
2. Conceptual model and scenarios	Accuracy of conceptual model and probability of scenarios
3. Performance criteria	Appropriate choice of quantities of interest
4. Calculational models and lumped parameters	Simplification procedures and determination of lumped parameters from data
5. Modeling calculations and sensitivity studies	Uncertainties to data and to calculational model choices
6. Results evaluation and application to safety assessment	Application of results to performance criteria

heterogeneous systems. I believe it is still an open question how to define permeability and dispersivity for such media. An example of a lumped parameter incorporating elementary parameters is the relative permeability function for an unsaturated fractured porous medium, for which it is shown (Pruess et al., 1989) that an equivalent porous medium with a specialized relative permeability function is adequate for calculating flow in the system instead of the detailed parameters associated with liquid and gas flows in fracture networks and matrix blocks. The choice of calculational models and their associated lumped parameters is strongly dependent on the computer codes that are available. For example, if the code is capable of performing only two-dimensional calculations, the calculational model has to be two dimensional.

After the decision on calculational models has been made, calculations can proceed. Computer runs are made to yield tables of results or graphical outputs. There is a need to study the sensitivity of these results to parameter or data uncertainties. Many times stochastic modeling techniques have to be used, and results may then be given as probability-distribution functions. If ergodicity can be assumed, spatially averaged quantities can perhaps be predicted.

The final step is to evaluate the calculational results. For the safety assessment of nuclear waste repositories, these results have to be evaluated according to the performance criteria. Uncertainties in these results have to be established; they may arise not only from data uncertainties but also from every step of the modeling process discussed above. For example, a particular choice of calculational model may introduce considerable uncertainties. One could ask the question, how well can a two-dimensional model simulate a three-dimensional model? The outcome of such evaluations of results would be to revise the modeling process to better determine or reduce uncertainties or to define further data needs for measurements and site investigations.

THE BROAD VIEW OF MODEL VALIDATION

Since the goal of model validation is to ensure that the modeling results provide a good representation of the actual processes occurring in the real system (IAEA, 1982), validation should be applied to every step of the modeling process, as discussed above. Thus for the first step of data review and evaluation the methodologies of evaluation of spatial or temporal data correlation should be studied, understood, and validated. The process of evaluating parameter correlation has to be defined and properly carried out. The latter depends much on the scientific experience and knowledge of the personnel involved in the work and in the peer-review process.

Construction of the conceptual model and evaluation of various possible scenarios requires much expertise and

practice. One way to provide some confidence in this process is to involve more than one group of hydrogeologists, geochemists, geophysicists, and geologists in the performance of this step. Cross-checking of the final results and understanding the differences between the outputs from the different groups may be extremely valuable.

The step of simplifying the complex conceptual models to calculational models and their associated lumped parameters has been often overlooked in model validation. It would be useful to put this on a proper scientific basis. Each modeling team should evaluate the uncertainties involved by alternative simplifications to arrive at alternative calculational models. Sensitivity of final results on the alternative models as well as on parameter uncertainties should also be studied.

Currently the most common validation approach used by many workers in this field involves the following steps. First, a field or laboratory experiment is selected. Second, the experimental conditions are specified, including both the initial conditions and the boundary conditions. Often not all boundary conditions are known. Third, model computations are made and predictions are checked against field or laboratory data. Sargent (1984) presented a list of validation methods that includes other methods in addition to this approach:

1. *Event validity.* This represents an initial validation test of a qualitative nature, in which events of occurrences of the simulation model are compared with those of the real system.
2. *Face validity.* This may be considered as part of the peer review, and may include asking people knowledgeable in the field whether the model is reasonable. The model flow chart may be checked for its correctness, and the model input-output relationship may be checked for reasonableness.
3. *Traces.* The behavior of the different elements or entities of a model are traced or followed through the numerical model to determine if the logic and the program are correct and if the necessary accuracy is maintained.
4. *Historical methods.* A historical method may consist of three steps: (a) examining the model's assumptions on theory, observations, general knowledge, and intuition; (b) validating each of the model's assumptions, where possible, by empirically testing them; and (c) comparing the input-output relationship of the model to field behavior.
5. *Internal validity.* This is particularly important in the validation of stochastic models or models with statistical inputs. Several realizations of a stochastic model are used to determine the amount of stochastic variability in the model. A high degree of variability may cause the model's results to be questionable and may require a redefinition of appropriate quantity of interest, i.e., appropriate performance measure.

6. *Historical data validation.* If historical data exist for a given site, part of the data may be used to construct and calibrate the model and the remaining data used to check against calculated results from the model.
7. *Predictive validation.* The model is used to provide predictions for a given field or laboratory test, and further measurements are made to check these predictions.
8. *Turing tests.* This may also be considered a part of the peer review and is particularly important for stochastic models. Here people knowledgeable about the field are asked if they can discriminate between model output and field observations.

It is of interest to note that historical data validation and predictive validation are only two out of a number of validation methods. We should apply all of the above validation methods, wherever possible, to all steps of the modeling process. For example, the methods of traces and face validity have not been much used up to now in our field. Often we depend on model developers and model users to ensure the correctness of model logic and accuracy. Sometimes this is not adequate.

NEED FOR MULTIPLE ASSESSMENT GROUPS

As mentioned in the previous section, some of the modeling steps, such as the design of conceptual models and the construction of calculational models, will be difficult to validate in a nonsubjective way, since their validation depends on the depth and breadth of scientific knowledge of the modelers involved. One approach for validation is the use of multiple-assessment groups. Two or more groups studying the same geologic system independently may come up with different scenarios, different conceptual models, and different simplifications in the construction of calculational models. Discussions among these groups will clarify the reasons for the differences and stimulate new considerations and better understanding of the system to be modeled. Thus such interactions not only cross-verify the work of different groups but also promote cross-fertilization to arrive at a more "correct" solution. We may define this multiple-assessment-group approach as one of the possible validation methods. Modeling results arrived at through the study and interaction of independent groups have a better chance of being correct and will probably have greater credibility among the scientific community and the public.

Multiple-assessment groups do not necessarily imply multiple requirements of budgetary and personnel resources for the national waste management program. The repository-safety-assessment modeling studies represent only a small component of the national program. Moreover, if budgetary and personnel resources are really a problem, the multiple-assessment-group approach can be applied only to the early steps of modeling, where the usual

validation methods cannot be used easily. The later steps of detailed computation and presentation of results can be performed by one major group. International cooperation will also be helpful.

The multiple-assessment-group approach is very much needed and cannot be replaced by the expert-peer-review approach. Usually experts are requested to serve for a limited time to study a problem, and their comments may focus on the technical procedures and methodologies used by the modelers involved. More likely than not they will have no time to study the primary site-specific data and generate an independent view. Thus in most cases it is hard for them to become site-specific experts. On the other hand, the multiple-assessment-group approach allows each group to study and consider primary data in detail and develop its version of the model unbiased by the views of other groups. Once this has been accomplished, in-depth discussions among the groups can produce fruitful results. Examples of this kind of interaction may be found in some of the international cooperative projects, such as Hydrocoin and Intraval.

THE NEED FOR BASIC RESEARCH AND PUBLIC SCRUTINY

Upon examining the modeling steps and various validation methods discussed above, one quickly comes to the realization that the success with which modeling results can predict the behavior of real systems depends very much on the state of our knowledge of various physical and chemical processes that take place in complex geological systems that can be characterized only in a limited way. It also depends on the state of field-testing technologies and analysis methodologies. We should advance our state of knowledge and methodologies by short-term laboratory and field experiments and long-term natural-analog studies. Without proper understanding of physical and chemical processes and the system structure involved, there can be no validation. One can say that a thorough understanding represents the major part of validation. Thus a percentage of our nuclear waste management effort should be devoted to such basic studies to add to the general state of knowledge and methodologies in geoscience.

One of the best ways to draw on the reservoir of available knowledge is not only by the various validation methods indicated in the previous section but also by having our modeling work published in the open literature. This should be done in parallel with the usual peer-review process. Open-literature publications receive the benefits of anonymous technical review and public scrutiny. Sometimes errors may be recognized by scientists from different but related fields of research. A study whose results are in the open literature—examined by and perhaps used by the general scientific community over a number of years—has a much better chance of being correct. Eventually the decision whether a model is valid is made not only by those doing the modeling studies. The model is valid in a given

case if the modelers have done the studies correctly and have convinced other knowledgeable persons of this. Thus, in the end, it is the general scientific community that will decide the validity of models and whether they are correctly used in the right context.

ACKNOWLEDGMENTS

The ideas presented here have been developed over the last few years in discussions with a large number of colleagues in the U.S., Europe, and Japan. I have benefited greatly from presentations by participants in the Intraval project at various meetings. In particular I would like to acknowledge the inspiration of Drs. Kjell Andersson and Johan Andersson of the Secretariat of the Intraval project and the inputs from members of the Validation Overview and Integration Committee, Drs. Jesus Carrera, Neil Chapman, David Hodgkinson, Ivars Neretnieks, Shlomo Neuman, and Tom Nicholson, whose reactions and discussions have caused me much trouble but have helped me to crystallize many ideas. Acknowledgements are also due Dr. Don Alexander and others of the U.S. Department of Energy, Office of Civilian Radioactive Waste Management, for their continual support and encouragement.

REFERENCES

- Anderson, K., 1987. International cooperation in the field of verification and validation of radionuclide transport models, experiences and need for further work. *In* Proceedings, International Geoval-87 Symposium, Stockholm, Sweden, April 7-9, 1987.
- Balci, O., 1988. Credibility Assessment of Simulation Results: The State of the Art, Methodology and Validation. *Simulation Series*, Vol. 19, No. 1. The Society for Computer Simulation, p. 19-25.
- Balci, O., 1989. How to assess the acceptability and credibility of simulation results. *In* E. MacNair, K. Musselman, and P. Heidelberger (eds.), Proceedings, 1989 Winter Simulation Conference. Washington, DC.
- Balci, O., and Sargent, R.G., 1984. A bibliography on the credibility, assessment and validation of simulation and mathematical models. *Simuletter*, v. 15, no. 3, p. 15-27.
- Gass, S.I., 1983. Decision-aiding models: Validation, assessment, and related issues for policy analysis. *Operations Res.*, v. 31, no. 4, p. 601-663.
- Gass, S.I., and Thompson, B.W., 1980. Guidelines for model evaluation: An abridged version of the U.S. General Accounting Office Exposure Draft. *Operations Res.*, v. 28, no. 2, p. 431-479.
- Geoval87, 1987. Proceedings, Symposium on Verification and Validation of Cosphere Performance Assessment Models, Stockholm, Sweden, April 7-9, 1987. Swedish Nuclear Power Inspectorate, Stockholm, Sweden.
- Hydrocoin, 1987. Hydrocoin Progress Report, Swedish Nuclear Power Inspectorate, Stockholm, Sweden.
- IAEA, 1982. Radioactive waste management glossary. Report IAEA-TECDOC-264, International Atomic Energy Agency, Vienna, Austria.
- Oren, T., 1981. Concepts and criteria to assess acceptability of simulation studies. A frame of reference. *Commun. ACM*, v. 24, no. 4, p. 180-189.
- Pruess, K., Wang, J.S.Y., and Tsang, Y.W., Tsang, 1990. On thermohydrological conditions near high-level nuclear wastes emplaced in partially saturated fractured tuff. 2. Effective continuum approximation. *Water Resour. Res.*, in press (LBL-24564).
- Sargent, R.G., 1984. Simulation model validation. *In* Oren et al., *Simulation and Model-Based Methodologies: An Integrative View*. Springer-Verlag, New York.
- Sargent, R.G., 1988. A tutorial on validation and verification of simulation models. *In* M. Abrams, P. Haigh, and J. Comfort (eds.), Proceedings, Winter Simulation Conference, p. 33-39.
- Schlesinger, et al., 1979. Terminology for model credibility. *Simulation*, v. 32, no. 3, p. 103-104.
- Schruben, L.W., 1980. Establishing the Credibility of Simulations: The Art and the Science. Prentice-Hall, Englewood Cliffs, NJ.
- Tsang, C.F., 1989. A new approach to tracer transport analysis: From fracture systems to strongly heterogeneous porous media. Keynote address presented at the International Workshop on Appropriate Methodologies for Development and Management of Groundwater Resources in Developing Countries, Hyderabad, India, February 28-March 4, 1989 (LBL-27031).
- Wang, J.S.Y., and Narasimhan, T.N., 1989. Processes, mechanisms, parameters and modeling approaches for partially saturated flow in soil and rock media. Lawrence Berkeley Laboratory Report LBL-26224.
- Zeigler, B.P., 1976. Theory of Modelling and Simulation. John Wiley & Sons, Inc., New York.

Validation of a Method for Analyzing Borehole-Fluid-Conductivity Logs to Determine Fracture-Inflow Parameters

C.F. Tsang, P. Hufschmied,* and F.V. Hale

This article describes the validation of a new method involving the use of a time sequence of electric conductivity logs of borehole fluid to determine fracture-inflow parameters. The method of analysis is described in detail in Tsang and Hale (1989). In brief, the flowing fractures in an uncased section of a wellbore contain fluid with different chemical compositions, and hence different electric conductivities. If the wellbore is washed out with deionized water, there will initially be only a small residual conductivity in the fluid. As the well is produced at a small flow rate, peaks are formed in the conductivity logs near the flowing fractures. Analysis of the time series of the fluid-electric-conductivity logs yields estimates of the parameters characterizing the flow, such as the depth of the flowing fracture, the time when the fracture fluid emerges at the wellbore, the volumetric inflow rate (q_i), and the solute mass inflow rate ($q_i C_i$). A code has been developed to carry out this method of analysis and determine the inflow parameters from the time series of logs (Tsang et al., 1989). The results of the method have been validated against those of independent hydraulic measurements made with the use of packers and against those of chemical sampling and analysis of fracture fluids.

FIELD EXPERIMENT AND DATA ANALYSIS

The borehole at Leuggern is one of six boreholes studied by Nationale Genossenschaft für die Lagerung radioaktiver Abfälle (NAGRA) as part of a regional investigation program in northern Switzerland. A suite of investigations was conducted in the borehole, including core logging, geophysical logging, hydraulic-packer testing, and hydrochemical sampling. Fluid logging experiments were carried out by NAGRA in different boreholes during 1985. The borehole water was first replaced by deionized water through a downhole tubing and the fluid conductivity measured at the outflow at the welltop to stabilize at 60 $\mu\text{S}/\text{cm}$. The tubing was then pulled out of the well, a pump placed at a depth of 210 m, and background temperature and electric-conductivity logs taken. With pumping maintained at about 20 L/min a series of five complete electric-conductivity logs was taken over 2 days, after which a temperature log was again taken.

The fracture-inflow parameters resulting from the analysis are shown in Table 1. Parameters were obtained for nine inflows that form peaks on the conductivity logs. A number of features of Table 1 should be noted. First, to-

Table 1. Parameters used in final match of field data.

Peak no.	x_i (m)	t_i (hr)	$q_i C_i$ (10^{-6} kg/s)	q_i (10^{-6} m ³ /s)	C_i (kg/m ³)
1	1440	16	0.33	0.65	0.50
2	1300	15	0.27	0.60	0.45
3	1215	16	0.25	0.55	0.45
4	1200	27	0.10	0.25	0.40
5	1188	27	0.28	0.65	0.43
6	1085	24	0.074	0.20	0.37
7	1048	24	0.29	0.60	0.48
8	918	13	4.1	0.75	5.5
9	843	11	16	17	0.95

$$K = 1.0 \times 10^{-3} \text{ m}^2/\text{s}$$

$$Q = 2.1 \times 10^{-5} \text{ m}^3/\text{s}$$

tal flow rate Q is estimated to be $2.1 \times 10^{-5} \text{ m}^3/\text{s}$, which is an order of magnitude smaller than the pumping rate at the top of the well, 20 L/min (or $33 \times 10^{-5} \text{ m}^3/\text{s}$). A later review of experimental conditions showed that most of the large flow rate may be taken up by inflows between depths of 500 and 770 m and that the total flow rate from the section between 770 and 1637 m may well be much smaller. Second, the estimated flow rates q_i , with values from 0.2 to $17 \times 10^{-6} \text{ km}^3/\text{s}$ (0.01 to 1 L/min), may represent the range of sensitivity for the fluid-conductivity logging method under the particular field arrangement. Third, the salinity C_i for peak 8 is a factor of 5 larger than that for peak 9 and an order of magnitude larger than that for the others.

VALIDATION AGAINST PACKER HYDRAULIC-TESTING RESULTS

The results of fluid conductivity logging—i.e., the inflow rate produced from each fracture intersected by the borehole—are combined with other observed pressure drawdowns during the time of pumping to calculate the transmissivity of each of the fractures or fracture zones. To validate the transmissivity values thus derived from fluid-conductivity logging, a comparison is made with the transmissivities determined independently from packer hydraulic testing in the Leuggern borehole. A large number of hydraulic tests were conducted during drilling and after completion of the Leuggern borehole. All of the tests were configured in terms of either single-packer tests or double-

*National Genossenschaft für die Lagerung radioaktiver Abfälle, Switzerland.

packer tests. For the analysis of the tests, a numerical borehole simulator was used in combination with trial-and-error techniques to estimate best-guess hydraulic conductivities. On the basis of reported average hydraulic conductivity and interval length, a transmissivity was calculated for each test interval. Table 2 shows a comparison between the transmissivities derived from packer testing and from fluid logging.

The main conclusion from the comparison is that fluid-conductivity logging leads to transmissivities that are in very good agreement with conventional packer hydraulic testing. The transmissivities derived from fluid-conductivity logging are generally within half an order of magnitude of those derived from conventional packer testing. This is remarkable, considering that in the fluid-conductivity logging method inflows from fractures are estimated completely independent from the packer tests by applying a borehole-fluid advection-dispersion model to observations of electric conductivity of the borehole fluid. The overall agreement between the transmissivities derived from the different methods is remarkable.

VALIDATION AGAINST HYDROCHEMICAL SAMPLING

Water samples were collected in the Leuggern borehole at various depths to determine the chemical composition and the age of the deep groundwaters. To facilitate a proper sample analysis, tracer-marked deionized water was used during drilling of the crystalline section of the borehole. The tracers added to the drilling fluid were Na-fluorescein (uranine) and meta-trifluoromethylbenzoic acid (m-TFMBA). The tracers served to indicate the degree of contamination of the sampled formation water by drilling fluids. Water was generally produced from the formation before taking a final sample until the reduction in the tracer level indicated a negligible residual contamination of the formation water, on the order of 1–2%.

According to Wittwer (1986), four zones can be identified on the basis of formation-water composition within the section of the Leuggern borehole that was subsequently studied with fluid-conductivity logging. The zones are identical with the double-packer test intervals indicated in Table 2.

Table 2. Comparison of transmissivities derived from fluid logging and conventional packer hydraulic testing.

Test name	Packer hydraulic-testing interval				Fluid logging (Case C)	
	Bottom (m)	Top (m)	Length (m)	T ($10^{-9} \text{ m}^2/\text{s}$)	Peak no.	T ($10^{-9} \text{ m}^2/\text{s}$)
1437.0H	1449.5	1424.5	25.0	0.25	1	3.5
1433.4D	1439.4	1427.4	12.0	1.2		
1304.2S	1315.1	1293.4	21.7	0.65	2	3.2
1215.0H	1227.6	1202.6	25.0	1.3	3	2.9
1203.2D	1227.1	1179.3	47.8	4.8	3+4+5	7.6
1192.5D	1208.8	1176.2	32.6	3.3	4+5	4.7
1082.9H	1095.4	1070.4	25.0	0.75	6	0.95
1046.0H	1058.5	1033.5	25.0	0.25	7	3.2
923.0D	929.7	916.2	13.5	9.5	8	4.1
918.4H	930.9	905.9	25.0	0.75		
912.5S	919.2	905.9	13.3	0.53		
850.0S	859.5	840.5	19.0	570	9	120
847.0D	859.5	834.5	25.0	500		
837.8H	850.3	825.3	25.0	750		

S = single-packer test.

D = Double-packer tests.

H = Hydraulic reconnaissance test.

Table 3 shows a comparison of formation-water electric conductivity determined from water sampling and borehole-fluid-conductivity logging. In addition, the equivalent NaCl concentration of the formation water is calculated from the formation-water electric conductivity by dividing electric conductivity by the factor $1870 (\mu\text{S}/\text{cm}) \cdot (\text{m}^3/\text{kg})$.

The main conclusion to be drawn from Table 3 is that formation-water electric conductivities estimated from fluid-conductivity logging are generally in good agreement, within a factor of 2, with electric conductivities observed in the samples of the formation water. This is especially remarkable if one considers that the estimates of formation-water conductivity from fluid logging were made on the basis of an incomplete buildup of the electrolyte concentration in the borehole fluid.

Special attention should be given to the fact that the formation-water electric conductivity of peak 8 is predicted from fluid-conductivity logging to be 5–10 times higher than that of the other peaks. This is again closely confirmed by the water samples.

CONCLUSION AND DISCUSSION

The flow rates from each fracture obtained by the fluid-conductivity logging method are used together with other information to estimate fracture transmissivities for the Leuggern borehole in Switzerland. The method and results were validated against transmissivity obtained independently by conventional hydraulic testing using packers. The agreement is remarkable. The method and results for salinities of fracture fluids were further validated

against independent results of chemical analysis of fluid samples taken from various depths in the Leuggern borehole. The agreement is generally good. In particular, the above-average salinity at peak 8 is confirmed by the analysis of water samples.

Fluid-logging techniques have several advantages and may play a significant part in a well-planned borehole testing program. First, they allow an identification of the locations of water-conducting fractures or groups of fractures in a borehole. This is very important for subsequent core investigations aiming at a detailed geological and geochemical description of preferential flow paths through the rock mass. Second, fluid logging may be used to derive the hydraulic or flow properties, like transmissivity, of these identified water-conducting features. Such a technique would be a cost-effective alternative to the conventional hydraulic single- and double-packer testing. Even if conventional hydraulic testing were not completely eliminated, fluid logging could effectively be applied as a screening tool prior to hydraulic testing and water sampling.

ACKNOWLEDGMENTS

Discussions and cooperation with NAGRA personnel, especially M. Thury, A. Zingg, and P. Zuidema, are much appreciated. Assistance in computation and graphing from C. Doughty is acknowledged. We would also like to thank C. Doughty, N. Goldstein, and I. Javandel for reviewing and commenting on the manuscript. This work is jointly supported by the Nationale Genossenschaft für die Lagerung radioaktiver Abfälle, Switzerland, and by the U.S. Department of Energy.

Table 3. Comparison of formation-water electric conductivity (at 20°C equivalent) derived from fluid-conductivity logging and from water sampling.

Test section	Elec. cond. from water sampling ($\mu\text{S}/\text{cm}$)	Peak no.	Elec. cond. from eq. NaCl conc. (mg/L)	Elec. cond. from logging ($\mu\text{S}/\text{cm}$)
1433.4D	>2030	1	500	940
1203.2D	1290	3+4+5	430	800
923.0D	4965	8	5,500	10,000
847.0D	1437	9	950	1,800

REFERENCES

- Tsang, C.F., and Hale, F.V., 1989. A direct integral method for the analysis of borehole fluid conductivity logs to determine fracture inflow parameters. *In* Proceedings, Conference on New Field Techniques for Quantifying the Physical and Chemical Properties of Heterogeneous Aquifers, Dallas, Texas, March 20–23, 1989, National Water Well Association, p. 133–154 (LBL-27930).
- Tsang, C.F., Hufschmied, P., and Hale, F.V., 1989. Determination of fracture inflow parameters with a borehole fluid conductivity logging method. *Water Resour. Res.*, in press (LBL-24752).
- Wittwer, C., 1986. Probenahme und Chemische Analysen von Grundwassern aus den Sondierbohrungen. Sondierbohrungen Bottstein, Weiach, Riniken, Schafisheim, Kaisten, Leuggern. NAGRA Technical Report NTB 85-49, NAGRA, Baden, Switzerland.

A Permeability, Porosity, and Capillary-Radius Relationship for Rocks and Soils

J.S.Y. Wang

It is generally accepted in hydrology that flow permeability is related to pore geometry. The classical Poiseuille law for flow along circular tubes and the Bosnesq law for flow between parallel plates are the starting points for constructing microscopic conceptual models for flows through porous media and fractures. Flow permeability is a macroscopically measurable quantity. One of the difficulties involved in generalizing microscopic models to macroscopic flow laws is in choosing the proper macroscopic measures to characterize the pore geometry. Porosity is the obvious, and most easily measured, macroscopic property for estimating pore volume. However, pore volume alone is not sufficient to capture the key feature of pore geometry in controlling the flow permeability. As a result, a strong interest in the controversial permeability–porosity relationship persists in the literature.

From comparison of saturated and unsaturated properties in rocks and soils, we identify another macroscopically measurable parameter that might serve to supplement porosity in characterizing pore geometry. This parameter is the capillary scaling factor, which can be deduced from the desaturation-characteristic curve of a porous medium. A porous medium with large pores is more permeable and is also more easily desaturated than a porous medium with small pores. The suction pressure needed to initiate desaturation of a saturated porous-medium sample can be used to define a characteristic capillary radius. The Blake-Kozeny equation from chemical engineering studies of packed beds can be generalized to relate the flow permeability to both porosity and capillary radius.

CAPILLARY RADIUS

Many empirical equations have been proposed in the literature for the dependence of effective saturation S_e on suction pressure head h . For example, the Brooks and Corey (1966) model is $S_e(h) = |\alpha h|^{-\lambda}$ if $|\alpha h| \geq 1$ and

$S_e(h) = 1$ if $|\alpha h| < 1$, where λ is a pore-size distribution index and α is the capillary scaling factor. The inverse of the parameter α , $|h_{ae}| = \alpha^{-1}$, is frequently referred to as the air-entry value or bubbling pressure in the soil literature, on the basis of the following interpretation of the Brooks and Corey model. When suction pressure head h overcomes the air-entry pressure h_{ae} ($|h| \geq |h_{ae}|$), air enters the pores and water flows out of the medium to initiate desaturation. This interpretation is based on the cutoff separating the $S_e = 1$ saturated region from the $S_e = |\alpha h|^{-\lambda}$ desaturated region. Some field soil samples have no sharp and well-defined cutoff and can be fitted better with the van Genuchten (1980) model $S_e(h) = [1 + (|\alpha h|)^n]^{-(1-1/n)}$, which in the large suction range is asymptotically equivalent to the Brooks and Corey model with $\lambda = n - 1$. In the small suction region near saturation, the van Genuchten function has a sigmoidal shape in the semilog desaturation curve of S_e versus $\log(h)$ and does not have an air-entry cutoff. Both the Brooks and Corey model and the van Genuchten model, together with many empirical functions in the literature, depend on αh together and not on α and h separately. We can treat α as a scaling parameter. In Brooks and Corey (1966), van Genuchten (1980), and van Genuchten and Nielsen (1985), several measured soil-characteristic curves have been fitted with both models. Figure 1 shows that the fitted α values for these two models are consistent with each other. Other empirical functions can also be used to fit unsaturated characteristic curves and to determine the capillary scaling factor from the desaturation process.

We can define an equivalent microscopic radius r_c in terms of the macroscopic parameter α . By the capillary equation, the radius of a capillary tube that can sustain a column of water with height $|h_{ae}| = \alpha^{-1}$ is

$$r_c = -\frac{2\sigma}{\rho g h_{ae}} = \frac{2\sigma}{\rho g} \alpha \quad (1)$$

Capillary Scaling Factor, α

Figure 1. Soil capillary scaling factors; Brooks and Corey model and van Genuchten model. [XBL 902-638]

With surface tension σ , water density ρ , and gravitational acceleration g as constants, r_c is proportional to α . We can treat the capillary radius r_c as a parameter equivalent to the capillary scaling factor α and use this radius in the macroscopic flow equations.

BLAKE-KOZENY EQUATION

In the study of flow through packed columns in mass transfer operations, tube-bundle theories have been successful to relate the pressure drops through the columns with porosity ϕ (void fraction) and "particle" radius r_p . For laminar flow, the Blake-Kozeny equation, based on extension of the Hagen-Poiseuille formula and hydraulic radius concept for tubes of complicated cross section, can be found in standard chemical engineering textbooks (e.g., Bird et al., 1960). The Blake-Kozeny permeability is

$$k_s = \frac{2}{75} \frac{\phi^3}{(1-\phi)^2} r_p^2 \quad (2)$$

In the derivation of this formula, the ratio of void volume to wetted surface is assumed to be proportional to $\phi/(1-\phi)$. The empirical success of Eq. (2) for packed beds is well documented. The subscript s in the permeability k denotes the saturated condition.

GENERALIZATION

The particle radius r_p in the Blake-Kozeny equation is well defined for packed columns using man-made or well-sorted materials. For natural media, especially for

consolidated or welded rocks, we do not have a well-defined particle radius to characterize the porous solid matrix. We propose to use the capillary radius r_c to replace the particle radius r_p . To test the applicability of this hypothesis, we review a number of databases for saturated and unsaturated flow properties for soils and rocks. The databases and the correlations between k_s and α are discussed in Wang and Narasimhan (1989).

For rocks and soils, we define a permeable radius by

$$r_p = \left[\frac{75}{2} \frac{(1-\phi)^2}{\phi^3} k_s \right]^{1/2} \quad (3)$$

The permeable radius is identical to the particle radius for packed columns. For consolidated, cemented, welded, and other media, we can calculate the permeable radius from the measured values of saturated permeability k_s and porosity ϕ . Equation (1) is used to calculate the corresponding capillary radius from the α value characterizing the desaturation curve for each sample. Figures 2 to 4 compare the permeable radius with the capillary radius for three databases. All three figures have the same scale. Figure 2 shows that the soil samples and man-made samples tested by Brooks and Corey (1966) in the laboratory can be characterized by well-defined radii. The tuff samples from well USW-G4 at Yucca Mountain (Peters et al., 1984) are scattered around the equal-radius line labeled $r_p = r_c$ in Fig. 3. The soil data from a trench in Las Cruces, New Mexico (Wierenga et al., 1989), also substantiate the relation between permeable radius and capillary radius, as shown in Fig. 4.

Brooks and Corey Samples

Figure 2. Correlation between permeable radius and capillary radius for data in Brooks and Corey (1966). [XBL 902-639]

Figure 3. Correlation between permeable radius and capillary radius for welded and zeolitized tuff data in Peters et al. (1984). [XBL 902-640]

DISCUSSION

The scatteration of data points in Figs. 3 and 4 illustrates the variability of hydrological properties of samples collected in a given type of medium at a specific site. The range of variability in permeable radius r_p is mainly due to the variability in the permeability k_s , which typically can span two or more orders of magnitude in a given rock type.

Figure 4. Correlation between permeable radius and capillary radius for Las Cruces trench soil data in Wierenga et al. (1989). [XBL 902-641]

The porosity ϕ is relatively more well defined and less varied. Taking the square root in Eq. (3) reduces the number of orders of magnitude in the variability of r_p to approximately half that of k_s . The range of variability in capillary radius r_c is proportional to that of the capillary scaling factor α from the desaturation-characteristic curve. The plot of permeable radius versus capillary radius can be used to illustrate and compare the flow process with the desaturation process. A sample with data points above the $r_p = r_c$ line is more permeable and less easily desaturated than a sample with data points in the reflective region below the equal-radius line.

From comparison among Figs. 2 to 4, the simple flow law as given by Eq. (2), with the capillary radius r_c of Eq. (1) replacing particle (or permeable) radius r_p , can be useful for scaling the average hydrological properties of one medium from another, very different medium. Within a given type of medium at a specific site, this simple flow equation is probably masked by data variability and local heterogeneity. For modeling a large-scale flow field with regions of very different hydrological properties in the domain, the simple permeability-porosity-capillary radius relationship can be used to test the data compatibility among different media. It is the concern of modeling exercises in heterogeneous systems with very scanty hydrological data that prompts us to compare and evaluate soil and rock databases and deduce this simple relationship.

REFERENCES

- Bird, R.B., Stewart, W.E., and Lightfoot, E.N., 1960. Transport Phenomena. Wiley, New York, 780 p.
- Brooks, R.H., and Corey, A.T., 1966. Properties of porous media affecting fluid flow. J. Irrigation and Drainage Div., *In* Proceedings Am. Soc. Civ. Eng., 92, IR2, p. 61-88.
- Peters, R.R., Klavetter, E.A., Hall, I.J., Blair, S.C., Heller, P.R., and Gee, G.W., 1984. Fracture and matrix hydrologic characteristics of tuffaceous materials from Yucca Mountain, Nye County, Nevada. Sandia National Laboratories Report SAND84-1471, 188 p.
- van Genuchten, M.Th., 1980. A closed-form equation for predicting hydraulic conductivity of unsaturated soils. Soil Sci. Soc. Am. J., 44, p. 892-898.
- van Genuchten, M.Th., and Nielsen, D.R., 1985. On describing and predicting the hydraulic properties of unsaturated soils. Ann. Geophys. 3, p. 615-627.
- Wang, J.S.Y., and Narasimhan, T.N., 1989. Processes, mechanisms, parameters and modeling approaches for partially saturated flow in soil and rock media. Sandia National Laboratories Report SAND88-7054; Lawrence Berkeley Laboratory Report LBL-26224.
- Wierenga, P.J., Hudson, D., Vinson, J., Nash, M., Toorman, A., and Hills, R.G., 1989. Soil properties at the Las Cruces trench site. U.S. Nuclear Regulatory Commission Report NUREG/CR-5441.

Sensitivity Analysis of Partially Saturated Flow through Welded-Nonwelded Tuff Units Using a Path-Integration Technique

J.S.Y. Wang and T.N. Narasimhan

To understand the unsaturated flow processes at Yucca Mountain, a potential site for a high-level nuclear waste repository, it is important to study the relationship between saturation distribution and infiltration of water through alternating layers of welded and nonwelded tuff units. A path-integration formulation (Narasimhan, 1985) is used in the TRUST code for analyzing the sensitivity of the flow field on hydrological parameters and boundary conditions in a one-dimensional configuration. This article summarizes our systematic investigation of the sensitive dependence of saturation values in nonwelded units on the pore-size distribution indices (Wang and Narasimhan, 1986).

PATH INTEGRATION

The path-integration formulation is based on the integral form of Darcy's law for unsaturated flow along a flow tube of variable cross section. If a section of the flow tube contains a given medium, we can integrate the Darcy equation from one isopotential surface to another within the medium and obtain a complete solution. For a vertical column with five layers, as shown in Fig. 1, we have six isopotential surfaces defining the five materials treated as five volume elements. Four of these surfaces coincide with the material interfaces within the column, and the remaining two coincide with the upper and lower boundaries of the column. The material in each layer is a composite medium with a double-humped relative permeability function to account for both the fractures and the porous matrix. A piecewise exponential representation is used to discretize the relative permeability functions so that the flow integrals can be analytically evaluated (Basha, 1989).

This vertical-column problem has been studied extensively in a code-verification COVE2A benchmarking study (Narasimhan and Alavi, 1988) using an integral finite-difference method, partitioning the system into several hundred volume elements. However, with the path-integration formulation incorporated into the TRUST code, the simulation is greatly simplified. The philosophy of the path integration is such that the solution is very weakly dependent on mesh discretization for steady-state situations. Table 1 illustrates this by comparing the accuracy of the 6-node path-integration solution with a 55-node path-integration solution. With the need for the tedious task of grid refinement removed from the simulation task, our ability to perform sensitivity analysis is significantly enhanced.

Figure 1. Idealization of a vertical column through the Yucca Mountain site. [XBL 903-707]

Table 1. TRUST with path integration COVE2A-Case 1 comparison.

Elevation (m)	6-node pressure head (m)	55-node pressure head (m)
530.4 (TCw top)	-55.871	-55.869
503.6 (TCw-PTn)	-130.675	-130.660
465.5 (PTn-TSw1)	-106.574	-106.574
335.4 (TSw1-TSw2)	-105.716	-105.726
130.3 (TSw2-CHnz)	-86.368	-86.368

DATA REVIEW

The data used in COVE2A studies are based mainly on the representative values compiled by Peters et al. (1984). The Yucca Mountain data are continually updated in the reference information base (RIB) and site and engineering property database (SEPDB) being developed at Sandia National Laboratories. Figure 2 illustrates the RIB values for the ambient saturations. Although there are only a few samples (number of samples used in the averages are given in parentheses in the figure), all welded and nonwelded units have, on average, saturation values above 50%. Figure 3 compares the values of the pore-size distribution index used in the COVE2A study and in the data-bases. We will be interested mainly in the nonwelded units, which have a wider range of variation in pore-size distribution index than the welded units.

SENSITIVITY ANALYSES

Two sets of analyses were made to evaluate the sensitivity of nonwelded saturation values on the pore-size distribution index. In the original COVE2A simulation results, the saturation value in the Paintbrush nonwelded unit (PTn) is less than 20%, much less than the measured values shown in Fig. 2. Figure 4 shows that the reduction of the PTn pore-size distribution index can increase the sa-

Figure 2. Ambient saturation values of different tuff units. [XBL 903-708]

Figure 3. Pore-size distribution indices of different tuff units. [XBL 903-709]

uration value and improve the agreement between measured and predicted values. Reducing the index to one-fourth of its original value is not inconsistent with the observed range shown in Fig. 3. As can be seen from the pressure-head results, the variation in the PTn pore-size distribution index does not affect the pressure distributions in that unit by more than 10%.

Another important nonwelded tuff unit at Yucca Mountain is the Calico Hill nonwelded formation (CHN), which is altered in varying degree by the zeolitization process. If the CHN unit remains vitric (CHnv), it is also very sensitive to variation in the pore-size distribution index, as shown in Fig. 5. Only one sample value for the saturation in CHnv is included in the RIB (Fig. 2). The sensitivity analysis for CHnv demonstrates that it is possible to obtain the high saturation value with reasonable reduction of the pore-size distribution index.

DISCUSSION

The specific examples of sensitivity analyses of the dependence of saturation values of nonwelded tuff units on the pore-size distribution indices demonstrate that we can develop consistent hydrological models whose outputs agree with measured properties and whose inputs vary within the ranges of available data. To facilitate effective

Figure 4. Sensitivity of the saturation value in Paintbrush nonwelded unit on pore-size distribution index. [XBL 903-710]

sensitivity analyses, an efficient calculation tool is essential. The path-integration formulation greatly simplifies the need to adjust the mesh every time we change the material properties, boundary conditions, and flow geometry. Even more important in a fundamental sense, the path-integration formulation can be used to verify the solution accuracy in a self-consistent manner without depending on comparisons with limited analytic solutions (Wang and Narasimhan, 1989). The practical applications and theoretical ramifications of this approach are currently under investigation.

REFERENCES

- Basha, H.A., 1989. Analytical and numerical studies of unsaturated flows (Ph.D. thesis). Department of Civil Engineering, University of California at Berkeley.
- Narasimhan, T.N., 1985. Geometry imbedded Darcy's law and transient subsurface flow. *Water Resour. Res.*, v. 21, no. 8, p. 1285-1292 (LBL-17814).

Figure 5. Sensitivity of the saturation value in Calico Hill nonwelded, vitric unit on pore-size distribution index. [XBL 903-711]

- Narasimhan, T.N., and Alavi, M., 1988. COVE 2A: A benchmarking exercise using computer program TRUST. Lawrence Berkeley Laboratory Report LBL-25224.
- Peters, R.R., Klavetter, E.A., Hall, I.J., Blair, S.C., Heller, P.R., and Gee, G.W., 1984. Fracture and matrix hydrologic characteristics of tuffaceous materials from Yucca Mountain, Nye County, Nevada, 1984. Sandia National Laboratories Report SAND84-1471, 188 p.
- Wang, J.S.Y., and Narasimhan, T.N., 1986. Hydrologic mechanisms governing partially saturated fluid flow in fractured welded units and porous nonwelded units at Yucca Mountain. Sandia National Laboratories Report SAND85-7114; Lawrence Berkeley Laboratory Report LBL-21022.
- Wang, J.S.Y., and Narasimhan, T.N., 1989. Processes, mechanisms, parameters and modeling approaches for partially saturated flow in soil and rock media. Sandia National Laboratories Report SAND88-7054; Lawrence Berkeley Laboratory Report LBL-26224.

Scaling Law for Absorption of Water into Porous Blocks of Various Shapes and Sizes

R.W. Zimmerman, G.S. Bodvarsson, and E.M. Kwicklis*

Yucca Mountain in Nevada is currently being considered for the location of an underground repository for the disposal of high-level radioactive waste (U.S. DOE, 1986). The proposed repository would be constructed in the unsaturated zone above the water table in a formation consisting of highly fractured volcanic tuff. As part of the process of characterizing the site for the purpose of determining its suitability for the repository, it is necessary to develop models for studying the flow of groundwater in a fractured rock mass with low (but nonzero) matrix permeability. The complex geology of the site, along with other factors, make a purely analytical treatment impractical, and numerical analysis is constrained by limitations of computational time. Hence it is desirable to combine both approaches in order to take advantage of the benefits of each. As part of the joint LBL/USGS work on unsaturated-zone hydrology at Yucca Mountain, we have been developing a dual-porosity model for unsaturated flow in fractured media. In this model, flow along the fractures is treated numerically, and flow between the fractures and the matrix blocks is accounted for analytically. The rate at which a matrix block saturates when it is surrounded by a saturated fracture will depend on its hydraulic properties, its initial saturation, and its geometry. These factors can all be accounted for by the absorption scaling law that we have developed.

FORMULATION OF PROBLEM

Absorption of water into a porous block can be described by the following equation (Bear, 1988):

$$\text{div}[\beta k_r(\psi) \text{grad } \psi] = \frac{\partial S}{\partial t}, \quad (1)$$

where ψ is the potential of the water in the porous medium, S is the fraction of the pore space that is filled with liquid, and k_r is a dimensionless relative permeability function. The parameter β is equal to $k/\mu\phi$, where k is the permeability under conditions of full saturation, μ is the viscosity of the water, and ϕ is the porosity of the medium. Equation (1) embodies the principle of conservation of mass for the liquid phase, along with a modified form of Darcy's law to relate the volumetric flux to the potential gradient.

Each porous medium has its own characteristic functions that describe k_r and S as functions of ψ . One commonly used form of the characteristic equations is that of

van Genuchten (1980):

$$k_r(\psi) = \frac{[1 - (\alpha|\psi|)^{n-1}][1 + (\alpha|\psi|)^n]^{-m}]^2}{[1 + (\alpha|\psi|)^n]^{m/2}}, \quad (2)$$

$$S(\psi) = S_r + (S_s - S_r)[1 + (\alpha|\psi|)^n]^{-m}, \quad (3)$$

where α is a parameter that has dimensions of 1/pressure, and m and n are dimensionless parameters that are related by $m = 1 - 1/n$, $n > 1$. For the Topopah Spring welded tuff from Yucca Mountain, the estimated values of the hydraulic parameters are $k = 3.9 \times 10^{-18} \text{ m}^2$, $\phi = 0.14$, $n = 3.04$, $m = 0.671$, $S_s = 0.984$, and $S_r = 0.318$ (Rulon et al., 1986).

The basic problem to be solved involves a block that is initially at some uniform level of partial saturation, which corresponds, through Eq. (3), to some initial capillary potential ψ_i . The block occupies a region of space Ω . At some time, which can be denoted as $t = 0$, the fractures surrounding a given block become saturated, so that the outer boundary $\partial\Omega$ of the block is brought to zero potential. Since the permeability of the surrounding fractures greatly exceeds that of the matrix blocks, it is safe to assume that the entire boundary becomes saturated instantaneously. Hence the boundary and initial conditions for the problem can be stated as

$$\psi(\vec{x}, t = 0) = \psi_i \quad \text{for all } \vec{x} \in \Omega, \quad (4)$$

$$\psi(\vec{x}, t > 0) = 0 \quad \text{for all } \vec{x} \in \partial\Omega. \quad (5)$$

Equations (1) to (5), along with the block shape Ω , completely specify the problem to be solved.

SCALING LAW FOR ABSORPTION

Approximate solutions for absorption into spherical, cylindrical, and slab-like blocks have been developed using an integral technique (Zimmerman et al., 1990). These approximate solutions were made possible by the fact that for these geometries, the problem is mathematically one dimensional. The problem was also simplified by the existence of appropriate coordinate systems (spherical and cylindrical) that allowed the outer boundary of the block to be described by a single constant value of the mathematical variable, i.e., $r = r_o$ for a sphere. For irregular blocks, such as the polygonal shapes that are formed by the intersection of nonparallel fracture systems, the simplification allowed by these symmetries will not occur. Since approximate solutions are not obtainable for irregular blocks, it would be convenient to have a scaling law that allows the rate of absorption into such blocks to be predicted without requiring numerical simulation.

*Water Resources Division, U.S. Geological Survey, Denver, CO 80225

For diffusion problems with constant diffusivity, scaling laws for irregularly shaped blocks have been proposed by Barker (1985) and van Genuchten and Dalton (1986). These rules were suggested by manipulations in the Laplace transform domain that are not applicable to nonlinear absorption problems. A simple scaling rule relating the cumulative influx to the ratio of volume V to surface area A can be devised, however, by the following considerations. First, note that as $t \rightarrow \infty$, the block becomes fully saturated, so that the amount of water absorbed by a block will be proportional to its volume. For small times, on the other hand, the problem will be identical to one-dimensional absorption, since the penetration depth of the wetting front will be small enough that the curvature of the surface will not have made itself felt. This fact is demonstrated rigorously for absorption into spheres and cylinders with constant diffusivity by Crank (1975), and is discussed for unsaturated flow problems by Philip (1969). Hence for "small" times, $Q \approx A \sqrt{t}$, and $Q/Q_\infty \approx A \sqrt{t}/V = \sqrt{t}/(V/A)$. We now make the assumption that for larger times, Q/Q_∞ will continue to be a function of $\sqrt{t}/(V/A)$, and that this function is the *same* for all geometries. More specifically, we can attempt to correlate the fractional absorption to a dimensionless time τ , the form of which is suggested by the approximate solutions to the cylinder or sphere problems, with the outer radius r_o replaced by the characteristic length V/A (Zimmerman et al., 1990):

$$\tau = \frac{2(n+1)k(S_s - S_i)^{-m} t}{\alpha n \mu \phi [m(S_s - S_r)]^{1/n} (V/A)^2} \quad (6)$$

In order to test the scaling concept, we have run simulations of absorption into variously shaped blocks of Topopah Spring welded tuff using the program TOUGH (Pruess, 1987). TOUGH is an integrated-finite-difference program that is known to simulate unsaturated flow problems accurately. Figure 1 shows the fractional cumulative absorption curves for a cylinder, a sphere, and an irregularly shaped, polygonal two-dimensional block. The initial saturation in each case was 0.6765. When plotted against the normalized time τ , the absorption curves for each block very nearly coalesce into a single curve, showing that the scaling law $Q/Q_\infty = f(\tau)$ is quite accurate. Simulations carried out for varying initial conditions (Zimmerman et al., 1990) show that the scaling law also correctly accounts for the effect of initial saturation.

For incorporation into double-porosity models, similar to that carried out by Neretnieks and Rasmuson (1984) for the related problem of radionuclide transport in fractured rock masses, it would mainly be necessary to distinguish between the different time scales at which various blocks become fully saturated. Accuracy exceeding that shown by the spread of results in Fig. 1 would not be needed. For these purposes it would probably suffice to use the following empirical equation, which was fit to the numerical data for absorption into a sphere (see Fig. 1):

$$\frac{Q}{Q_\infty} = 1.79 \sqrt{\tau} - 0.79 \tau \quad (7)$$

Figure 1. Normalized cumulative flux into blocks of Topopah Spring welded tuff. The initial saturation is 0.6765. Normalized time τ is defined by Eq. (6). [XBL 903-718]

Equations (6) and (7) then give a reasonably accurate estimate of the rate of infiltration into an arbitrarily shaped block that is geometrically characterized only by its volume-to-surface ratio.

REFERENCES

- Barker, J.A., 1985. Block-geometry functions characterizing transport in densely fissured media. *J. Hydrol.*, v. 77, p. 263-279.
- Bear, J., 1988. *Dynamics of Fluids in Porous Media*. New York, Dover Publications.
- Crank, J., 1965. *The Mathematics of Diffusion*. Oxford, Clarendon Press.
- Neretnieks, I., and Rasmuson, A., 1984. An approach to modelling radionuclide migration in a medium with strongly varying velocity and block sizes along the flow path. *Water Resour. Res.*, v. 20, p. 1823-1836.
- Philip, J.R., 1969. Theory of infiltration. *Adv. Hydroscience*, v. 5, p. 215-296.
- Pruess, K., 1987. TOUGH user's guide. Lawrence Berkeley Laboratory Report LBL-20700.
- Rulon, J., Bodvarsson, G.S., and Montazer, P., 1986. Preliminary numerical simulations of groundwater flow in the unsaturated zone, Yucca Mountain, Nevada. Lawrence Berkeley Laboratory Report LBL-20553.
- U.S. Department of Energy, 1986. Final environmental assessment — Yucca Mountain site, Nevada Research and Development Area, Nevada. Office of Civilian Radioactive Waste Management Report DOE/RW-0012.

- van Genuchten, M.Th., 1980. A closed-form equation for predicting the hydraulic conductivity of unsaturated soils. *Soil Sci. Soc. Am. J.*, v. 44, p. 892-898.
- van Genuchten, M.Th., and Dalton, F.N., 1986. Models for simulating salt movement in aggregated field soils. *Geoderma*, v. 38, p. 165-183.
- Zimmerman, R.W., Bodvarsson, G.S., and Kwicklis, E.M., 1990. Absorption of water into porous blocks of various shapes and sizes. *Water Resour. Res.*, v. 26, in press (LBL-27511).

GEOLOGY AND GEOCHEMISTRY

Investigators in the Geology and Geochemistry group primarily study causes and results of chemical reactions in the earth's crust. These reactions result from interactions between subsurface aqueous fluids and the surrounding soil and rock, causing chemical alteration of the solids and changes in the chemistry of the fluids. Since many of these reactions occur during the movement of fluids, our studies are quite germane to the disposal and isolation of radioactive and toxic wastes. Successful containment of waste species depends strongly on arresting the movement of dissolved chemical species in groundwater. In this respect, specific investigations in areas of isotope geochemistry, radiochemistry, inorganic chemistry, and surface chemistry are all applicable to reactive chemical transport models. Field-oriented research pertinent to chemical transport encompasses the coupling of hydrology with isotope geology, aqueous analytical chemistry, chemical-species modeling, and hydrochemistry. Projects emphasizing geochemical and chemical modeling of nuclear waste repositories focus on how both radionuclide and major groundwater species react and migrate under near- and far-field repository conditions.

The group also conducts basic research on processes that occur in the earth's crust and oceans, including studies of the thermodynamics of high-temperature brines at mid-ocean ridges and in geothermal systems and the paleoclimatic implications of isotopic variations. Members participate in the Continental Scientific Drilling program and in studies to define the occurrence and movement of radon and its parent radioisotopes in rock and soil. Research is also in progress on interfacial chemical reactions that address both solid-liquid and solid-gas reactions on mineral surfaces.

Behavior of Isotopic Ratios during Reactive Transport in Saturated Geologic Media

D.J. DePaolo

Mathematical models for solute transport in saturated porous geologic media are well developed for nonreactive systems (e.g., Cherry et al., 1984). The primary limitations in applying the models in nature stem from difficulty in specifying the nature and scale of heterogeneity in the medium. Reactive transport is more difficult to model successfully. Thermodynamic treatment can be used to predict mineral-fluid reactions (Wolery, 1979), but reaction is limited in nature by geometrical and kinetic factors that are difficult or impossible to model quantitatively.

This article describes how isotopic ratios (e.g., $^{87}\text{Sr}/^{86}\text{Sr}$, $^{18}\text{O}/^{16}\text{O}$) in fluids and solid media respond during reactive chemical transport. The simplicity of the condition for equilibrium and the natural variability of the ratios makes it possible to use measurements of isotopic ratios in fluids, rocks, and minerals in active hydrologic and geothermal systems to obtain the effective rates of chemical reaction. Application of this capability could lead to improvement in the ability to predict solute and contaminant transport in nature.

The important characteristic of isotopic ratios that sets them apart from chemical concentrations is the condition for equilibrium. For radiogenic stable isotopes like those of Sr, Pb, Nd, Hf, Ca, and Os, two phases at equilibrium will have identical isotopic ratios. For light stable isotopes like those of H, O, C, S, and N, two phases at equilibrium will have isotopic ratios that differ by a temperature-dependent factor α . Especially for the radiogenic isotopes, no thermodynamic data are needed to understand the first-order behavior of reactive fluid-rock systems.

ONE-DIMENSIONAL MODELS

Consider a fluid moving through porous rock material and reacting by a process involving solution and precipitation of rock material. The simplest case is one in which the solid is treated as a single phase and the solution rate is equal to the precipitation rate, so that there is no net change in pore volume with time.

The equation describing the concentration (C) of an element in the fluid for a medium with uniform porosity is (Gillham and Cherry, 1982)

$$\frac{\delta C(x,t)}{\delta t} = (D_d + D_m) \frac{\delta^2 C}{\delta x^2} - V \frac{\delta C}{\delta x} - G, \quad (1)$$

where D_d = effective molecular diffusion coefficient, D_m = hydrodynamic dispersion coefficient, V = average fluid velocity, and G = source/sink term due to chemical reac-

tion. For solution-precipitation reactions involving trace elements, the source-sink term can be written

$$G = RM(KC - C_s), \quad (2)$$

where R = reaction rate (g/g of solid/time); M = $\rho_s(1 - \phi)/\rho_f \phi$ = mass ratio of solid to fluid (ρ = density, ϕ = porosity); C_s = concentration in dissolving solid; and KC = concentration in solid precipitated from solution (K = equilibrium distribution coefficient).

The equation describing an isotopic ratio (r_{ij}) composed of the isotopic species i, j can be derived using the expression for the differential of r_{ij} in terms of the concentrations of the two isotopes (C_i, C_j):

$$\delta r_{ij} = \frac{1}{C_j} (dC_i - r_{ij} dC_j). \quad (3)$$

Substituting Eqs. (1) and (2) for the time derivatives of C_i and C_j yields:

$$\frac{\delta r_{ij}(x,t)}{\delta t} = D \frac{\delta^2 r_{ij}}{\delta x^2} - \left[V - 2D \frac{\delta \ln C}{\delta x} \right] \frac{\delta r_{ij}}{\delta x} + RM_c (r_{ijs} - r_{ij}), \quad (4)$$

where $D = D_d + D_m$, r_{ijs} = isotopic ratio in the solid, and $M_c = MC_s/C$.

The solid matrix also changes concentration and isotopic ratio as a function of time. If diffusion in the solid phase is considered negligible, then the expressions for the solid (dropping the i, j indices for the ratios) are

$$\frac{\delta C_s(x,t)}{\delta t} = -R(C_s - KC), \quad (5)$$

$$\frac{\delta r_s(x,t)}{\delta t} = -RK \frac{C}{C_s} (r_s - r). \quad (6)$$

The concentration and isotopic ratio of the solid change only from exchange with the local fluid.

DIFFUSIVE LIMIT; PURE EXCHANGE

A simple but illustrative case is one in which there is no advection of fluid ($V = 0$) and no change in the concentration of the fluid with time (i.e., $KC = C_s$). The expression for the isotopic ratio in the fluid is

$$\frac{\delta r(x,t)}{\delta t} = D \frac{\delta^2 r}{\delta x^2} + 2D \frac{\delta \ln C}{\delta x} \frac{\delta r}{\delta x} + RM_c (r_s - r). \quad (7)$$

If we make $C(x, t) = \text{constant}$, then the second term is zero:

$$\frac{\delta r(x, t)}{\delta t} = D \frac{\delta^2 r}{\delta x^2} + RM_c (r_s - r) . \quad (8)$$

The solution to this equation, $r(x, t)$, varies rapidly until a local balance is attained, such that

$$D \frac{\delta^2 r}{\delta x^2} = -RM_c (r_s - r) . \quad (9)$$

Hence, a quasi-steady state difference in isotopic ratio between fluid and solid is established:

$$r_s - r = \frac{-D (\delta^2 r / \delta x^2)}{RM_c} . \quad (10)$$

Thereafter, both the solid and the fluid evolve isotopic compositions on a time scale described by Eq. (6), the time constant being the reaction rate, R .

The behavior of the isotopic ratios can be illustrated by considering a solid medium with an isotopic ratio varying sinusoidally with distance (Fig. 1):

$$r_s(x) = A \sin \omega x . \quad (11)$$

The solution for the steady state (Eq. 9) is

$$r(x) = A (1 + \frac{D \omega^2}{RM_c})^{-1} \sin \omega x . \quad (12)$$

The fluid ratio thus follows that of the solid in phase but with an attenuated amplitude (Fig. 1).

For long times, the amplitude of the isotope-ratio variations in the solid decays. Substituting Eq. (12) into (10) gives the quasi-steady-state value of $r_s - r$. Substituting this into Eq. (6) and evaluating the time derivative at the position of maximum r_s (i.e., $x = \pi/2\omega$), an expression for the decay of the amplitude of r_s is obtained

Figure 1. Pattern of isotopic ratios in one-dimensional solid and interstitial fluid for a solid with sinusoidal variation in isotopic ratio and for a stationary fluid. Numbers on fluid curves are values of $D \omega^2 / RM_c$. [XBL 903-698]

$$\frac{d \ln A}{dt} = -R \left[\frac{D \omega^2 / RM_c}{1 + D \omega^2 / RM_c} \right] . \quad (13)$$

There are two limiting cases. When $D \omega^2 / RM_c \gg 1$ (slow reaction rate or small length scales), then

$$d \ln A / dt = -R . \quad (14)$$

If $D \omega^2 / RM_c \ll 1$ (fast reaction rate or large length scales), then

$$d \ln A / dt = -D \omega^2 / M_c , \quad (15)$$

DIFFUSION AND ADVECTION

A more complex case is one that includes both diffusion in the fluid and fluid advection. If the condition of constant concentration in the fluid is retained, the equation describing the short time scale is

$$D \frac{d^2 r}{dx^2} - V \frac{dr}{dx} + RM_c (r_s - r) = 0 . \quad (16)$$

Using Eq. (11) for the isotopic variation in the solid, the steady-state solution is

$$r(x) = A \left[(1 + D \omega^2 / RM_c)^2 + (V \omega / RM_c)^2 \right]^{-1} \times [(1 + D \omega^2 / RM_c) \sin \omega x - (V \omega / RM_c) \cos \omega x] . \quad (17)$$

This function is shown in Fig. 2. The behavior of the ratios is controlled by two dimensionless parameters, $D \omega^2 / RM_c$

Figure 2. Pattern of isotopic ratios in solid and interstitial fluid for a solid with sinusoidal variation in isotopic ratio and for a fluid moving from left to right with velocity V . Numbers on fluid curves are values of $V \omega / RM_c$. $D \omega^2 / RM_c$ is equal to 0.1. [XBL 903-699]

and $V\omega/RM_c$, one that relates the diffusion time constant, $D\omega^2$, to the weighted reaction time constant RM_c , and one that relates the fluid transit time constant, $V\omega$, to RM_c .

DISCUSSION

The equations derived are applicable to a variety of problems associated with reactive fluid-rock systems in the earth. For active systems, the information gained is maximized if isotopic ratio measurements are available for both the solid matrix and the fluid. As shown in the figures, the relationship of the amplitude and phase of isotopic variations in the fluid to those in the solid is a measure of the dimensionless parameters discussed above. In nature it is often possible to measure D , ω , V , and M_c ; consequently the isotopic data determine R , the effective exchange or reaction rate (Richter and DePaolo, 1988).

Isotopic ratios of elements dissolved in fluids are often measured to determine the source of the fluids. However, only if $V\omega/RM_c \gg 1$ will the fluid isotopic composition have a long "memory" and be useful for sourcing of fluids. For smaller values of $V\omega/RM_c$ the isotopic composition of the fluid is too heavily affected by local exchange to reflect the source of the fluid.

The model presented also is applicable to understanding the time and length scales of isotopic equilibration in metamorphism and metasomatism in the lower crust and upper mantle. Reaction rates may be determinable in fossil fluid-rock systems if the fluid isotopic composition can be reconstructed from vein minerals or fluid inclusions.

REFERENCES

- Cherry, J.A., Gillham, R.W., and Barker, J.F., 1984. Contaminants in Groundwater: Chemical Processes. Groundwater Contamination, National Academy Press, Washington, D.C., p. 46-64.
- Gillham, R.W., and Cherry, J.A., 1982. Contaminant migration in saturated unconsolidated geologic deposits. Geol. Soc. Am. Special Paper 189, p. 31-62.
- Richter, F.M., and DePaolo, D.J., 1988. Diagenesis and strontium isotopic evolution of seawater using data from DSDP 590B and 575. Earth Planet. Sci. Lett., v. 90, p. 382-394.
- Wolery, T.J., 1979. Calculation of chemical equilibrium between aqueous solution and minerals: The EQ3/EQ6 software package. Lawrence Livermore National Laboratory Report UCRL-52658, 41 p.

Paleoclimatic Implications of Oceanic Strontium Isotopic Variations over the Past 2.5 Million Years

D.J. DePaolo and R.C. Capo

We have determined the variation in the $^{87}\text{Sr}/^{86}\text{Sr}$ ratio of the dissolved Sr in the oceans for the past 2.5 Ma from measurements on calcium carbonate sediment from Deep Sea Drilling Project (DSDP) Site 590. This was done to evaluate global climatic variations and to establish a reference curve for correlation of marine sediments. The $^{87}\text{Sr}/^{86}\text{Sr}$ ratio of the oceans is the only available parameter that is both globally averaged by the mixing of the oceans and sensitive to climatic effects other than ocean temperature and continental ice volume. The past 2.5 Ma is a time period in which it is possible to correlate changes in the seawater Sr isotope ratio with other proxy records of paleoclimate and paleoceanography, thereby building a more complete reconstruction of Plio-Pleistocene conditions.

The $^{87}\text{Sr}/^{86}\text{Sr}$ ratio of the oceans changed by less than 2×10^{-4} over the past 2.5 Ma. Until now it was not possible to measure the $^{87}\text{Sr}/^{86}\text{Sr}$ ratios with sufficient precision and accuracy to study the fine structure of these temporal changes. We achieved a measurement precision of approximately $\pm 0.001\%$ by using an automated data-collection procedure that minimizes inter-measurement drift, using more intense Sr^+ ion beams to improve counting statistics,

using an appropriate thermal ionization mass discrimination formulation, closely monitoring common sources of artifacts, and by performing multiple measurements on each sample.

Our results suggest that global chemical weathering rates on the continents have fluctuated by as much as $\pm 30\%$ over the past 2.5 Ma. The past 300,000 years appears to be a time of relatively low weathering rates. Some of the observed shifts in weathering rates are contemporaneous with climatic changes inferred from records of oxygen and carbon isotopes.

SAMPLES AND ANALYTICAL PROCEDURES

Site 590 was drilled in 1300 m water on the Lord Howe Rise in the Tasman Sea (31°S) (Kennett et al., 1986). Hydraulic-piston coring methods were used, which minimize drilling-related disturbance. The recovered sediment is pelagic foraminifera-nannofossil carbonate ooze; it contains a nearly continuous record of carbonate deposition

over the past 15 Ma with little terrigenous influx. The sediments contain well-preserved calcareous assemblages.

Core 590B was sampled at approximately 3-m intervals to a depth of 30 m. This corresponds to about one sample every 2×10^5 years. Three deeper samples were also measured, which extend the record back to 3.8 Ma, as well as several samples from Cores 590 and 590A. One sample from equatorial Pacific core V28-238 was also measured. Samples were assigned ages on the basis of their paleomagnetic reversal stratigraphy, and their positions within calcareous nannofossil biozones, using the time scale of Berggren et al. (1985). The sample from Core V28-238 is from the Brunhes-Matuyama Chron Boundary.

RESULTS

Figure 1 shows measured $^{87}\text{Sr}/^{86}\text{Sr}$ ratios plotted against age for the last 2.5 Ma. The $^{87}\text{Sr}/^{86}\text{Sr}$ ratio of the oceans increased by 14×10^{-5} since 2.4 Ma. During the Cenozoic, growth rates as high as those observed for the Plio-Pleistocene have occurred in five other times (~38 Ma, 23.5–22 Ma, 18–16 Ma, 11.5–11.0 Ma, and 6.2–5.5 Ma) (DePaolo and Ingram, 1985; DePaolo, 1986).

In detail, the Site 590 $^{87}\text{Sr}/^{86}\text{Sr}$ seawater curve exhibits a cyclicity with a period of about 0.8 million years. The periods of rapid growth are 2.4–1.9 Ma, 1.6–0.9 Ma, and 0.8–0.3 Ma. The remaining time periods in the last 3.0 Ma

Figure 1. Measured $^{87}\text{Sr}/^{86}\text{Sr}$ ratios age for bulk carbonate ooze from DSDP Site 590 (open circles). Samples were assigned ages on the basis of their positions within calcareous nannofossil stratigraphy (Lohman, 1986) and their paleomagnetic stratigraphy (Barton and Bloemendal, 1986). The filled square is from core V28-238. The filled circle represents our value for the Holocene EN-1 *Tridacna* bivalve standard. $\Delta^{87}\text{Sr}$ is the difference between the measured $^{87}\text{Sr}/^{86}\text{Sr}$ value and the value for EN-1, multiplied by 10^5 . [XBL 903-700]

have been times of zero growth or decreasing $^{87}\text{Sr}/^{86}\text{Sr}$; this includes the last 0.3 Ma before the present. The most noticeable discontinuity observed in the data from DSDP 590B samples (0.8–0.9 Ma) is confirmed by an analysis from drill core V28-238, which can be correlated precisely with Site 590 because of the identification of the magnetic reversal at 0.74 Ma in V28-238 and at site 590A.

DISCUSSION

The Plio-Pleistocene seawater Sr isotope curve provides a significant possibility for improving correlations and dating of marine sediments. Age resolution of 0.1 to 0.2 Ma is possible for the time periods of most rapid change of $^{87}\text{Sr}/^{86}\text{Sr}$.

The climatic significance of the Sr isotope data comes from sensitivity of the $^{87}\text{Sr}/^{86}\text{Sr}$ ratio of oceanic dissolved strontium to changes in the Sr cycle. The removal of Sr from the oceans — primarily by incorporation into the CaCO_3 of biogenic material — does not affect the $^{87}\text{Sr}/^{86}\text{Sr}$ ratio of the dissolved Sr remaining in the oceans because there is negligible fractionation in the removal process. The $^{87}\text{Sr}/^{86}\text{Sr}$ ratio in the oceans changes with time in response to changes in the Sr flux and the $^{87}\text{Sr}/^{86}\text{Sr}$ ratio of competing input sources.

We modeled the variations using three input sources. The fluxes (J_i) and the $^{87}\text{Sr}/^{86}\text{Sr}$ ratios (R_i) attributable to these sources at present are summarized in Table 1. The rapidity and magnitude of the observed shifts in the rate of change of the $^{87}\text{Sr}/^{86}\text{Sr}$ ratio of oceanic Sr argue that they result from changes in the riverine Sr input rather than changes in the seafloor basalt or sediment alteration fluxes (Hodell et al., 1989).

The most plausible explanation for the observed fluctuations in seawater $^{87}\text{Sr}/^{86}\text{Sr}$ over the last 2.5 Ma is change in the dissolved Sr flux (J_r) of rivers to the oceans. Figure 2 shows the seawater $^{87}\text{Sr}/^{86}\text{Sr}$ curve produced by varying the riverine Sr flux, keeping all other Sr cycle parameters constant. The observed time dependence of the seawater $^{87}\text{Sr}/^{86}\text{Sr}$ ratio (R_r) requires variations of about $\pm 35\%$ in J_r relative to its modern value. The deduced changes in J_r represent changes in the global chemical weathering rate, because it is chemical weathering, mainly of the minerals feldspar and calcite, that releases Sr from continental surface rocks into solution in groundwaters and eventually to the oceans. The climatic implications of the results therefore depend on the parameters that affect the global rate of chemical weathering. Qualitatively, weathering rates are believed to increase with erosion rate and with rainfall. The total amount of continental weathering is also presumably dependent on the area of the continents above sea level.

Some further insight into the significance of the Sr isotope curve can be gained by comparison with the curves for stable isotopes of oxygen. The beginnings of the first and third periods of rapid $^{87}\text{Sr}/^{86}\text{Sr}$ increase (high global

Table 1. Modern parameters for the strontium cycle.

Input source	Flux (10^{10} moles Sr/y)	$^{87}\text{Sr}/^{86}\text{Sr}$
Rivers ^a	3.0	0.7110
Submarine alteration ^b	1.2	0.7050
Diagenesis ^c	0.3	0.7085
	$\Sigma J_i = 4.5$	$R_{in} = 0.7092^d$
Mass of Sr in the ocean (N_o) = 1.21×10^{17} moles ^e		
Time constant, $N_o / \Sigma J_i (\tau) = 2.70$ Ma		

^aThe average value of riverine $^{87}\text{Sr}/^{86}\text{Sr}$ from Goldstein and Jacobsen (1985) is 0.7102; the average R_r from Palmer and Edmond (1989) is 0.7119. We choose 0.7110; if a different value were used it would change the details but not the main features of our model.

^bFlux determined by mass balance calculation, assuming steady state. Because seawater $^{87}\text{Sr}/^{86}\text{Sr}$ has apparently decreased over the last 0.3 Ma, the actual J_a may be $\sim 10\%$ higher. The $^{87}\text{Sr}/^{86}\text{Sr}$ ratio is based on values for altered Oman ophiolite, fluids from Iceland, and Troodos ophiolite epidote.

^cElderfield and Gieskes (1982); Palmer and Elderfield (1985).

^d R_{in} is the $^{87}\text{Sr}/^{86}\text{Sr}$ ratio of strontium added to the ocean ($\sim \Sigma J_i R_i / \Sigma J_i$).

^eGoldstein and Jacobsen (1987).

weathering rate) correspond to major shifts in the oceanic oxygen isotope record. At 2.4 Ma a shift in the oxygen isotope record is interpreted as the onset of permanent Northern Hemisphere glaciation (Shackleton et al., 1984). This observation in conjunction with ours implies that increased continental glaciation is correlated with increased global weathering rate. If increased continental glaciation corresponds to decreased global surface air temperatures, the observed correlation goes against the idea that weathering is more rapid during global warm periods. On the other hand, increased continental ice volume is correlated with lower eustatic sea level and greater continental area above sea level. This effect is consistent with increased global continental weathering rate. The rapid cycling between warm and cold global climatic conditions inferred for the Pleistocene from stable isotope records, and the concomitant erosion by continental glaciers interspersed with warm humid periods in the same latitudes, might produce higher mean weathering rates than prolonged warm periods.

The temporary but large decrease in J_r at 0.8 Ma corresponds to another change in climate inferred from the oxygen isotope record: a change from high-frequency, low-amplitude climatic variations to large-amplitude 100,000-year glacial-interglacial cycles (Shackleton and

Opdyke, 1973). This climatic change is associated with a period of about 100,000 years of exceptionally low weathering rates. A relatively simple explanation for the Sr isotopic data would be that 0.8 Ma was a time of small continental area caused by an exceptionally high sea level, perhaps associated with an extreme deglaciation.

The observed period of 0.8 million years for the variations in the rate of change of oceanic $^{87}\text{Sr}/^{86}\text{Sr}$ is substantially longer than the main periodicities in the oxygen isotope record. However, this period is implicit in the identification of discontinuities in these records at 2.4 and 0.8 Ma and in the fact that 1.6 Ma is an epoch boundary. Cyclic variations in climatic conditions have been attributed to changes in the pattern of solar insolation on the earth caused by changes in the earth's orbital parameters around the sun (Imbrie and Imbrie, 1980). The longest orbital variation period predicted from current models is in eccentricity and has a period of about 400,000 years. The Sr isotopic cycles have a period that is approximately twice that of the longest orbital cycle.

Figure 2. (Top) Values of riverine Sr flux (J_r) necessary to produce the observed variations in the $^{87}\text{Sr}/^{86}\text{Sr}$ of seawater, keeping all other parameters constant. (Bottom) The solid line represents the associated change in R_{in} , the mean value of the $^{87}\text{Sr}/^{86}\text{Sr}$ ratio of Sr being added to the oceans. [XBL 903-701]

REFERENCES

- Barton, C.E., and Bloemendal, J., 1986. Paleo-magnetism of sediments collected during Leg 90, Southwest Pacific. *In* J.P. Kennett, C.C. von der Borch, et al., Initial Reports. DSDP (Vol. 90). Washington, D.C. (U.S. Govt. Printing Office), p. 1273–1300.
- Berggren, W.A., Kent, D.V., Flynn, J.J., and Van Couvering, J.A., 1985. Cenozoic geochronology. *Geol. Soc. Am. Bull.*, v. 96, p. 1407–1418.
- DePaolo, D.J., 1986. Detailed record of the Neogene Sr isotopic evolution of seawater from DSDP Site 590B. *Geology*, v. 14, p. 103–106.
- DePaolo, D.J., and Ingram, B.L., 1985. High-resolution stratigraphy with strontium isotopes. *Science*, v. 227, p. 938–941.
- Elderfield, H., and Gieskes, J.M., 1982. Sr isotopes in interstitial waters of marine sediments from DSDP cores. *Nature*, v. 300, p. 493–497.
- Goldstein, S.J., and Jacobsen, S.B., 1987. The Nd and Sr isotopic systematics of river-water dissolved material: Implications for the sources of Nd and Sr in seawater. *Chem. Geol.*, v. 66, p. 245–272.
- Hodell, D.A., Mueller, P.A., McKenzie, J.A., and Mead, G.A., 1989. Strontium isotope stratigraphy and geochemistry of the late Neogene ocean. *Earth Planet. Sci. Lett.*, v. 92, p. 165.
- Imbrie, J., and Imbrie, J.Z., 1980. Modeling the climatic response to orbital variations. *Science*, v. 207, p. 943–953.
- Kennett, J.P., von der Borch, C.C., et al., 1986. Site 590: Lord Howe Rise, 31°S. *In* J.P. Kennett, C.C. von der Borch, et al., Initial Reports DSDP (Vol. 90). Washington, D.C. (U.S. Govt. Printing Office), p. 263–376.
- Lohman, W.H., 1986. Calcareous nannoplankton biostratigraphy of the southern Coral Sea, Tasman Sea, and southwestern Pacific Ocean, Deep Sea drilling Project Leg 90: Neogene and Quaternary. *In* J.P. Kennett, C.C. von der Borch, et al., Initial Reports DSDP (Vol. 90). Washington, D.C. (U.S. Govt. Printing Office), p. 763–793.
- Palmer, M.R., and Edmond, J.M., 1989. The strontium isotope budget of the modern ocean. *Earth Planet. Sci. Lett.*, v. 92, p. 11–26.
- Palmer, M.R., and Elderfield, H., 1985. Sr isotope composition of sea water over the past 75 Myr. *Nature*, v. 314, p. 526–528.
- Shackleton, N.J., and Opdyke, N.D., 1973. Oxygen isotope and paleomagnetic stratigraphy of equatorial Pacific core V28-238: Oxygen isotope temperatures and ice volumes on a 106 year scale. *Quaternary Res.*, v. 3, p. 39–55.
- Shackleton, N.J., Backman, J., Zimmerman, H., Kent, D.V., Hall, M.A., Roberts, D.G., Schnitker, D., Baldauf, J.G., Desprairies, A., Homrighausen, R., Huddlestun, P., Keene, J.B., Kaltenback, A.J., Krum-sick, K.A.O., Morton, A.C., Murray, J.W., and Westberg-Smith, J., 1984. Oxygen isotope calibration of the onset of ice-rafting and history of glaciation in the North Atlantic region. *Nature*, v. 307, p. 620–623.

The Hydrothermal Alteration and Carbonation of Oceanic Crust: Implications for Global Cycles of CO₂ and the Oxygen Isotopes

*B.M. Smith and H. Staudigel**

The submarine alteration of the oceanic crust influences the global geological cycle of greenhouse gases by fixing large amounts of seawater-derived CO₂ within the seafloor as the mineral calcite (CaCO₃). The oxygen isotopic consequences of seafloor alteration are also widely debated and poorly understood, but interactions between seawater-derived fluids and oceanic crustal rocks are sufficiently widespread and vigorous to require consideration in global-cycling models for the oxygen isotopes. It has been particularly difficult to develop a quantitative understanding of the importance of seafloor alteration to these cycles

because of (1) the heterogeneous distribution of alteration products within altered oceanic crustal rocks, (2) the limited number of deep holes drilled into oceanic basement, and (3) the poor recoveries of most DSDP holes drilled into oceanic basalts.

To provide better estimates of the amount of CO₂ removed from seawater during seafloor carbonation and the influence of seafloor alteration on the earth's oxygen isotope budget, we have studied samples of old (~118 Ma) oceanic crust taken from three DSDP sites (417A, 417D, and 418A) near the Bermuda Rise (Fig. 1). Holes 417D and 418A penetrate 500–550 m into the abyssal plains, whereas Hole 417A penetrates 267 m through a nearby 150-m-high abyssal hill (Donnelly et al., 1979). These sites

*Scripps Institute of Oceanography, University of California at San Diego, A-015, La Jolla, CA 92093.

Figure 1. Locations of DSDP Holes 417A, 417D, and 418A. [XBL 901-5703]

were selected for study because they are among the deepest holes drilled in old oceanic crust and because recoveries during drilling were uncommonly high.

COMPOSITE SAMPLING APPROACH

To minimize sampling problems related to the heterogeneous distribution of alteration products in the oceanic crust, several types of composite samples were prepared to reflect the actual proportions of materials encountered in each of the holes. "Lithology composites" were prepared separately for volcanoclastic rocks and for pillowed and massive lava flows for three depth intervals. The lithologic composites contain 40% of Holes 417D and 418A and 20% from the more intensely altered Hole 417A. Site-specific "depth composites" were prepared using 6% volcanoclastics, 25% massive flows, and 69% pillow lavas. We also produced a "super composite" by mixing the depth composites from the three sites in the same proportions as were used for the lithology composites.

Although we have already reported on the CO_2 concentration data of the composite samples (Staudigel and Smith, 1989), these results are briefly summarized here. We also present results of our oxygen isotope study of the composite samples, carried out to (1) determine the nature of temperature gradients present during silicate rock alteration and carbonation, (2) search for lithologic controls on the degree of rock alteration, and (3) provide a better estimate of the bulk oxygen isotopic composition of old oceanic crust.

CARBONATE CONCENTRATION DATA

Figure 2 shows that the CO_2 contents of the composite samples are generally higher than those estimated from analyses of individual rock specimens from these sites. Most of the introduced carbonate occurs in the uppermost 300 m of the basaltic section, where average CO_2 concentrations of 3.90, 4.06, and 3.96 wt% are calculated for the

Figure 2. CO_2 concentration versus depth for individual specimens (small black dots) and composite samples (417A depth composites = diamonds, volcanoclastic composites = unfilled circles, lava flow composites = unfilled squares). The regression line is for 417D and 418A depth composites (filled squares). [XBL 901-5702]

three sites. The total carbon inventory at these sites is estimated to be ~3.0 wt% for the uppermost 500 m, decreasing to ~0.5 wt% for the interval 500-1000 m, and then to background values of ~0.05 wt% for the remainder of the oceanic crust to depths of ~6.4 km.

STABLE-ISOTOPE DATA

Oxygen isotope compositions of the silicate and carbonate fractions of the lithologic composites are plotted against depth in Fig. 3. The silicate fractions of lava flow/pillow composites (Flows) and of pillow breccia/hyaloclastite samples (Breccias) show regular trends of decreasing $\delta^{18}\text{O}$ with depth, although all samples are enriched in ^{18}O relative to unaltered mid-ocean ridge basalt (MORB). Carbonate from both rock types has much higher $\delta^{18}\text{O}$ values, which show no apparent trend to lower values with depth. Calcite contents of the Flow composites and of the deeper Breccia composite are 10.5 to 11 wt%, whereas the shallow Breccia composite is very rich in calcite (43 wt%). The Bulk trend in Fig. 3 was calculated using the relative abundances of flows, breccias, and carbonate in the sections.

Figure 4 shows the O-isotope compositions of silicate and carbonate fractions of the depth composites plot-

Figure 3. Oxygen isotope compositions of super composite and of silicate (sloping arrays) and carbonate (vertical array) fractions of lithologic composites from Sites 417 and 418. The numbers in parentheses are calculated wt% calcite in the samples. [XBL 901-5704]

ted against elevation relative to the abyssal seafloor. The silicate fractions of the abyssal hill (417A) composites are much richer in ^{18}O than samples from the abyssal plains holes, whereas the carbonate fractions of the seamount samples are isotopically similar to those of the uppermost portions of the abyssal plains sites.

Figure 4. Oxygen isotope compositions of the super composite and of silicate and carbonate fractions of depth composites from Sites 417 and 418, plotted against elevation relative to the abyssal seafloor. [XBL 901-5705]

DISCUSSION

The trends for the stratigraphic and depth composites shown in Figs. 3 and 4 may provide information about the timing of silicate alteration and carbonation of the oceanic crust. The silicate fractions of all composite samples show decreasing $\delta^{18}\text{O}$ values with depth, implying that the silicate minerals at these sites exchanged oxygen with seawater-derived fluids under steep, vertical temperature gradients, probably relatively shortly after the basalts formed. In contrast, the uniformly higher $\delta^{18}\text{O}$ values of carbonate fractions from all composite samples indicate that carbonation took place at much lower temperatures under nearly isothermal conditions, presumably much later than the silicate alteration and far from any oceanic spreading center. Thus the carbonation of the oceanic crust appears to be a seafloor-weathering phenomenon that overprints earlier, higher-temperature silicate alteration.

The particularly high $\delta^{18}\text{O}$ values of the silicate fractions from the seamount site (417A, Fig. 4) indicate that these rocks have been more intensely altered at low temperatures than samples from the abyssal plains sites. Furthermore, the high $\delta^{18}\text{O}$ values of the silicate portions of the Breccia composites, coupled with the tendency for volcanoclastic samples to contain large amounts of high- ^{18}O carbonate, suggest that volcanoclastic-rich seamounts are especially effective sinks for ^{18}O .

GLOBAL GEOCHEMICAL CYCLES

Our earlier determination of the bulk CO_2 concentration at these sites (0.296 wt%, Staudigel et al., 1989) is substantially higher than recent estimates for the non-outgassed initial MORB carbon concentration (0.12–0.165 wt%, Gerlach, 1989). This indicates that carbonation during seafloor weathering leads to crustal uptake of carbon that exceeds carbon contributions to the hydrosphere from mantle outgassing at mid-ocean ridges. If our results can be generalized, then the oceanic crust is an important geological sink for CO_2 that must be considered in models of global cycling of carbon.

In addition to providing information on the timing of carbonation and silicate alteration, the isotope data for the composite samples show that the oceanic crust is probably much richer in ^{18}O than inferred by previous workers. Our calculated bulk $\delta^{18}\text{O}$ value for the uppermost 550 m at these sites (+11.0 ‰) is 1 to 3 per mil higher than previous estimates. If further analyses of composite samples from other DSDP sites confirm this unique observation, then models of global cycles of the oxygen isotopes must include the oceanic crust as an important sink for ^{18}O . Our evidence for preferential carbonation and ^{18}O -enrichment of volcanoclastic rocks and samples taken from the seamount site imply that the significance of seafloor carbonation and ^{18}O -uptake may depend critically on the total amount of volcanoclastic material submerged beneath the oceans. Perhaps the least known and most important factor

is the total amount of volcanoclastic material exposed to alteration by seawater in small abyssal hills and on larger seamounts, oceanic islands, and island arcs.

REFERENCES

- Donnelly, T., Francheteau, J., Bryan, W., Robinson, P.T., Flower, M.F.J., and Salisbury, M., 1979. Initial Reports DSDP 51-53, U.S. Government Printing Office, Washington, D.C.
- Gerlach, T.M., 1989. Degassing of carbon dioxide from basaltic magma at spreading centers: Mid-ocean ridge basalts. *J. Volc. Geoth. Res.* (special issue on Lake Nyos and CO₂ outgassing) in press.
- Staudigel, H., and Smith, B.M., 1989. Cretaceous ocean crust at DSDP Sites 417 and 418: Carbon uptake from weathering versus loss by magmatic outgassing. *Geochim. Cosmochim. Acta*, v. 53, p. 3091-3094.

¹⁴C Transport in a Partially Saturated Fractured Porous Medium

W.B. Light, P.L. Chambré, W.W.-L. Lee, and T.H. Pigford

Radioactive gases released from waste placed in partially saturated rock would have a direct pathway to the biosphere. This presents a new problem in assessing the potential health impacts of such releases and in complying with regulations.

We analyze the transport of ¹⁴C in an unsaturated fractured porous medium with gas-phase advection and dispersion. Gases released into a partially saturated fractured rock move in the fractures, whereas pore water is held inside the rock matrix. First we assess the interaction of ¹⁴C in CO₂ with bicarbonate ion in groundwater as a possible retardation mechanism. Then we treat the combined fracture and pore matrix as an equivalent porous medium with local carbon-distribution equilibrium between the gas and liquid phases. Our results indicate that liquid in the rock matrix between fractures will reach essentially the same equilibrium concentration as the liquid at the fracture walls when the modified Peclet number $Lq_g/\epsilon K_D D_l$ is much less than unity, where L is half the distance between fractures, q_g is the gas Darcy velocity, ϵ is the porosity, K_D is the equilibrium distribution coefficient defined as the molar concentration of liquid-phase carbon divided by the molar concentration of gas-phase carbon, and D_l is the liquid-phase diffusion coefficient.

The following equation for the transport of ¹⁴C in an equivalent porous medium has been solved analytically for a point source in a three-dimensional field, an infinite-plane source in a two-dimensional field, both for impulse and band-release source terms:

$$\epsilon((1-S) + SK_D) \left(\frac{\partial C_g}{\partial t} + \lambda C_g \right) + \vec{q}_g \cdot \nabla C_g - \epsilon((1-S)D_g + SK_D D_l) \nabla^2 C_g = f(\vec{r}, t), \quad (1)$$

where λ is the decay constant, S is the saturation, D_g is the dispersion coefficient for the gas phase and $f(\vec{r}, t)$ is the

source term. The solution is based on space-time-invariant values for ϵ , S , K_D , q_g , D_g , and D_l . With the retardation just described, the advection velocity v and dispersion coefficient D obtained for ¹⁴C are

$$v = \frac{q_g}{\epsilon((1-S) + SK_D)}, \quad (2)$$

$$D = \frac{(1-S)D_g + SK_D D_l}{(1-S) + SK_D}. \quad (3)$$

This model differs from that proposed by Ross (1988) in that we provide new support for the distribution-equilibrium assumption by solving a fracture-geometry problem, and we provide complete analytic solutions to the equivalent-porous-medium problem. We conservatively neglect calcite precipitation, thereby simplifying the equations given by Ross. In contrast with Knapp (1987), we include gas-phase dispersion and show that it is important. We obtain essentially the same results as Knapp with a simpler formulation, and our analysis reveals no ¹⁴C shock fronts.

Using parameter values from the Yucca Mountain Site Characterization Plan (USDOE, 1988), we predict peak ¹⁴C concentrations at the ground surface comparable to the USNRC limit for unrestricted areas of 10^{-7} $\mu\text{Ci}/\text{cm}^3$ -air. Figure 1 gives the concentration 350 m above the repository treated as an infinite plane source with an impulse release of 200 Ci over the total repository area of 7×10^6 m² for three values of the gas Darcy velocity as a function of time. Figure 2 gives the concentration 350 m above the repository treated as an infinite plane source with a band release of 200 Ci over 1000 yr. In Figs. 1 and 2 the effect of atmospheric dispersion has not been considered. Parameter values used for Figs. 1 and 2 also include $\epsilon = 0.1$, $S = 0.8$, $K_D = 3$, $D_g = 50$ m²/y, and $D_l = 3 \times 10^{-3}$ m²/y. Figure 3 gives the maximum concentration reached at the location 350 m above the plane

Figure 1. Gas concentration 350 m above an infinite plane source versus time for an impulse release at time zero. [XBL 903-702]

Figure 3. Peak concentration 350 m above an infinite plane source versus band-release duration. [XBL 903-704]

Figure 2. Gas concentration 350 m above an infinite plane source versus time for a band release of 1000 yr and gas Darcy velocity of 0.04 m/y. [XBL 903-703]

source for band release as a function of the release duration. It can be seen that the maximum concentration predicted at the ground surface may be independent of the period over which ^{14}C is released from the waste packages.

REFERENCES

- Knapp, R.B., 1987. An approximate calculation of advective gas phase transport of ^{14}C at Yucca Mountain, Nevada. Lawrence Livermore National Laboratory Report UCRL-97805.
- Ross, B., 1988. Gas-phase transport of carbon-14 released from nuclear waste into the unsaturated zone. In M.J. Apted and R.E. Westerman (eds.), *Scientific Basis for Nuclear Waste Management XI* (Materials Research Society Symposium Proceedings, Vol. 112). Materials Research Society, Pittsburgh, Pennsylvania, p. 273.
- U.S. Department of Energy, 1988. Site Characterization Plan, Yucca Mountain Site, Nevada Research and Development Area, Nevada.

Analytic Solution of Pseudocolloid Migration in Fractured Rock

Y. Hwang, T.H. Pigford, W.W.-L. Lee, and P.L. Chambre

A form of colloid migration that can enhance or retard the migration of a dissolved contaminant in groundwater is the sorption of the contaminant onto the moving colloidal particulate to form pseudocolloids. This article summarizes our analytical solutions for the interactive migration of radioactive species dissolved in groundwater and sorbed as pseudocolloids.

The solute and pseudocolloids are assumed to undergo advection and dispersion in a one-dimensional flow field in planar fractures in porous rock. Interaction between pseudocolloid and dissolved species is described by equilibrium sorption. Sorbed species on the pseudocolloids undergo radioactive decay, and pseudocolloids can sorb onto fracture surfaces and sediments. Filtration is neglected. The solute can decay and sorb onto pseudocolloids, fracture surfaces, and sediments and can diffuse into the porous rock matrix.

The mass balance for the pseudocolloid, per unit volume of fracture, is

$$\begin{aligned} \epsilon_1 \xi_1 \frac{\partial C_1(x,t)}{\partial t} + \epsilon_1 \xi_1 v_1 \frac{\partial C_1(x,t)}{\partial x} + \epsilon_1 S_1(x,t) + \epsilon_1 S_2(x,t) \\ - \epsilon_1 \xi_1 D_1 \frac{\partial^2 C_1(x,t)}{\partial x^2} + \epsilon_1 \xi_1 \lambda C_1 = 0, \quad x > 0, t > 0, \quad (1) \end{aligned}$$

where $C_1(x,t)$ is the amount of species sorbed onto the colloid per unit volume of solid colloid, v_1 is the colloid pore velocity, D_1 is the colloid dispersion coefficient, λ is the decay constant, ϵ_1 is the porosity within the fracture, ξ_1 is the constant-volume fraction of pseudocolloids in fracture liquid, $\epsilon_1 S_1(x,t)$ is the rate of sorption to stationary solid, $\epsilon_1 S_2(x,t)$ is the rate of desorption from the pseudocolloid.

For the same species as solute in liquid in the fracture,

$$\begin{aligned} \epsilon_1 \frac{\partial C_2(x,t)}{\partial t} + \epsilon_1 v_2 \frac{\partial C_2(x,t)}{\partial x} - \epsilon_1 S_2(x,t) + \epsilon_1 S_3(x,t) \\ - \epsilon_1 D_2 \frac{\partial^2 C_2(x,t)}{\partial x^2} + \epsilon_1 \lambda C_2 + \frac{q(x,t)}{b} = 0, \quad x > 0, t > 0, \quad (2) \end{aligned}$$

where $C_2(x,t)$ is the solute concentration in the fracture liquid, v_2 is the solute pore velocity, $\epsilon_1 S_3(x,t)$ is the rate of solute sorption onto stationary fracture solids, b is the fracture half-width, and $q(x,t)$ is the diffusive solute flux into the rock matrix, given by

$$q(x,t) = -\epsilon_p D_p \frac{\partial N(x,y,t)}{\partial y} \Big|_{y=b}, \quad x > 0, t > 0, \quad (3)$$

ϵ_p is the rock porosity, D_p is the solute diffusion coefficient in rock, and $N(x,y,t)$ is the solute concentration in pore water in the rock.

For solute species sorbed onto stationary fracture solids,

$$(1 - \epsilon_1) \frac{\partial C_3(x,t)}{\partial t} - \epsilon_1 S_3 + (1 - \epsilon_1) \lambda C_3(x,t) = 0, \quad x > 0, t > 0, \quad (4)$$

where $C_3(x,t)$ is the concentration of sorbed solute species.

For species sorbed as pseudocolloids onto the stationary fracture solids,

$$(1 - \epsilon_1) \xi_2 \frac{\partial C_1(x,t)}{\partial t} - \epsilon_1 S_1(x,t) + (1 - \epsilon_1) \xi_2 \lambda C_1(x,t) = 0, \quad x > 0, t > 0, \quad (5)$$

where ξ_2 is the constant volume fraction of the sorbed colloid per unit volume of the stationary fracture solid.

Inside the rock matrix,

$$R_p \frac{\partial N(x,t)}{\partial t} - D_p \frac{\partial^2 N(x,t)}{\partial y^2} + R_p \lambda N(x,t) = 0, \quad x > 0, t > 0, y > 0, \quad (6)$$

where R_p is the solute retardation coefficient in the rock matrix.

We assume linear sorption equilibrium between the solute species in the fracture liquid and the same species sorbed onto the colloid. Both the solute species and the colloids in the fracture liquid are assumed to undergo linear sorption equilibrium with the fracture solids

$$K_{d1} = \frac{C_1(x,t)}{C_2(x,t)}, \quad K_{d2} = \frac{\xi_2}{\xi_1}, \quad K_{d3} = \frac{C_3(x,t)}{C_2(x,t)}. \quad (7)$$

From Eqs. (1)–(5), we can obtain the equation for C_1 in terms of the effective retardation factor R , dispersion coefficient D , and velocity v :

$$\begin{aligned} R \frac{\partial C_1(x,t)}{\partial t} + v \frac{\partial C_1(x,t)}{\partial x} - D \frac{\partial^2 C_1(x,t)}{\partial x^2} \\ + R \lambda C_1(x,t) + \frac{q(x,t)}{\epsilon_1 b} = 0, \quad x > 0, t > 0, \quad (8) \end{aligned}$$

where

$$R = \left[\xi_1 \left(1 + \frac{1 - \varepsilon_1}{\varepsilon_1} K_{d1} \right) \right] + \left[1 + \frac{1 - \varepsilon_1}{\varepsilon_1} K_{d1} \right] \frac{1}{K_{d1}}, \quad (9)$$

$$v = v_1 \left[\xi_1 + \frac{v_2}{K_{d1} v_1} \right], \quad (10)$$

$$D = D_1 \left[\xi_1 + \frac{D_2}{D_1 K_{d1}} \right]. \quad (11)$$

The initial and boundary conditions are

$$N(x, \infty, t) = 0, \quad x > 0, \quad t > 0, \quad (12)$$

$$N(x, b, t) = \frac{1}{K_{d1}} C_1(x, t), \quad x > 0, \quad t > 0, \quad (13)$$

$$N(x, y, 0) = 0, \quad x > 0, \quad y > 0, \quad (14)$$

$$C_1(0, t) = K_{d1} C_o, \quad t > 0, \quad (15)$$

$$C_1(\infty, t) = 0, \quad t > 0, \quad (16)$$

$$C_1(x, 0) = 0, \quad x > 0, \quad (17)$$

where C_o is the inlet solute concentration.

The solution is

$$C_1 = \frac{2K_{d1}C_o}{\sqrt{\pi}} \int_{(x/2)\sqrt{R/Dt}}^{\infty} \exp \left\{ -\frac{\sqrt{v^2 + 4R\lambda D} - v}{2D} x \right\} \\ \times \operatorname{erfc} \left[\frac{x^2 \varepsilon_p \sqrt{D_p} R_p}{8Dh \varepsilon_1 \eta^2 \sqrt{t - \frac{Rx^2}{4D\eta^2}}} \right] \exp \left[-\left(\eta - \frac{xv}{4D\eta} \right)^2 \right] d\eta \\ x \geq 0, \quad t \geq 0. \quad (18)$$

Figure 1. Relative concentrations of pseudocolloid and solute, fracture flow, and matrix diffusion of solute. [XBL 903-689]

Figure 1 shows the concentration profiles of species as solute and pseudocolloid for assumed parameters and for a step release. Matrix diffusion of the solute, together with dispersion in fracture flow, results in a monotonic decrease in the concentrations of solute and pseudocolloids, approaching zero concentration at the front. Solute and pseudocolloid remain in constant ratio within the fracture liquid.

Preliminary Derivation of a Gas-Flow Source Term from a Nuclear Waste Container

E.D. Zwahlen, T.H. Pigford, P.L. Chambre, and W.W.-L. Lee

We have analyzed the flow of gases out of and into a high-level-waste container in the unsaturated tuff of Yucca Mountain and have made a preliminary estimate of the release of gaseous radionuclides. Containers are expected to fail eventually by the formation of localized cracks and penetrations. Even though the penetrations may be small,

argon gas initially in the hot container can leak out. When a waste package cools, the gas pressure inside the container can become less than atmospheric and air can leak in. Carbon-14 released from the hot fuel-cladding surface can leak out of penetrations, and air that leaks in can mobilize additional ^{14}C and other volatile radioactive species as it

oxidizes the fuel cladding and the spent fuel. This article summarizes our analysis of the flow of gas for various penetration sizes, assuming the penetration occurs at the time of emplacement, at 300 yr, and at 1000 yr.

The Yucca Mountain Site Characterization Plan (SCP) (USDOE, 1988) proposes that a waste container will have failed if the product of gas pressure and volumetric leakage rate exceeds 10^{-4} atm-cm³/s (ASME, 1986). This value divided by RT , where R is the gas constant and T the absolute temperature, gives the allowable molar flow rate, above which the container would be considered failed. We assume that this criterion applies to both outleakage and inleakage.

The penetrations are modeled as a single equivalent hole of radius r and length l , the container wall thickness. The gas flow is analyzed using isothermal viscous flow through a tube:

$$Q = \frac{\pi r^4 (P^2 - P_0^2)}{16\mu l RT} \quad (1)$$

Here Q is the mass of gas flowing per unit time, P and P_0 are the gas pressures within and outside the container, and μ is the gas viscosity. Using this equation to predict flow from a waste container requires careful consideration of the temperatures and pressures to use in (1). In a waste container of volume V containing n moles of ideal gas ($P = nRT/V$), the equation becomes

$$\frac{dn(t)}{dt} = - \frac{\pi r^4 [(nRT/V)^2 - P_0^2]}{16\mu l RT_w} \quad (2)$$

with the initial quantity of gas given by

$$n(0) = \frac{P(0)V}{RT(0)} \quad (3)$$

Here, $\bar{T}$, the average internal temperature, and T_w , the wall temperature, are known functions of time (USDOE, 1988), and μ is a function of T_w . $\bar{T}$ is approximated as the arithmetic average of the peak fuel-cladding temperature and T_w (Fig. 1).

At penetration, we assume viscous flow through a single equivalent hole of radius 5μ or 10μ or larger. Using the time-temperature history for a waste package from the SCP, we calculate the time-dependent inventory of gas within the waste container (Fig. 2). Curves are for a fill pressure of 1 atm and fill temperatures of 298 K or 558 K, the maximum internal gas temperature predicted to occur after emplacement. The time to reach the maximum temperature is neglected. The magnitude of the leakage rate is shown as a function of these parameters in Fig. 3, together with the SCP leakage-rate limit. The container gas volume is 1 m³, and the wall thickness is 1 cm.

Figure 2 shows that for penetration at emplacement, a $5\text{-}\mu$ hole, and a fill temperature of 298 K, argon slowly leaks out for about 800 yr, after which repository cooling causes the internal pressure to fall below atmospheric, and air leaks in. For a $10\text{-}\mu$ hole or larger, the internal pressure

Figure 1. Waste package gas and wall temperature. [LBL 903-690]

Figure 2. Quantity of gas in a container as a function of time. [LBL 903-691]

Figure 3. Gas flow rate through penetrations of various sizes and initial conditions. [LBL 903-692]

rapidly falls to atmospheric, as early as 1 yr for a 30- μ hole. The rate of subsequent air leakage is determined by the cooling rate and is not affected by the size of holes. Figure 3 shows that the leakage-rate limit is not exceeded by a 5- μ hole, and it is exceeded only briefly by larger holes at a 298 K fill temperature.

For a 558 K fill temperature, penetration results only in inleakage of air. Because the fill temperature is the same as the temperature at penetration time, the pressure gradient and flow are zero at the time of penetration. Had the penetration occurred later, the SCP leakage-rate limit would be exceeded only briefly for holes 10 μ or larger.

These data are important in assessing waste container performance, but ultimately we are interested in radionuclide release rates. Assuming that early heating of the waste package volatilizes 1% of the ^{14}C inventory, primarily from the cladding surfaces, a 5- μ hole and 298 K fill temperature result in an initial argon leak rate of 0.06 mole/y and a ^{14}C fractional leak rate of $2 \times 10^{-5}/\text{y}$. For a 10- μ hole, the leak rate would be 16-fold larger. Also from Fig. 2 we find that for a 298 K fill temperature and 5- μ holes, about one-fourth of the gas and volatilized radionuclides leaks from the container. For 10- μ holes or larger, almost half of the gas leaks out before air begins to leak in.

After air begins to flow into the waste container, volatilized radionuclides cannot be released by advection. However, radionuclides can escape by diffusion against the flow. We analyze advective-diffusive release in the penetration as a tube, with quasi-steady-state flow and diffusion. Neglecting radial diffusion, assuming slug flow and constant-concentration boundary conditions at the tube ends, the mass balance equation for the radionuclide concentration c is

$$\bar{v} \frac{\partial c}{\partial z} = D \frac{\partial^2 c}{\partial z^2}, \quad (4)$$

with boundary conditions $c(0) = c_0 = M/V$, $c(l) = 0$. Here z is the direction of flow along the tube, M is the initial inventory of volatilized radionuclide in the container, D is the gas diffusion coefficient, and $\bar{v}$ is the average gas velocity in the tube. For countercurrent diffusion, $\bar{v}$ is negative. The fractional release rate is given by

$$f = \begin{cases} \pi r^2 \bar{v} / V \frac{e^\alpha - 1}{e^\alpha - 1}, & \bar{v} < 0; \\ \pi r^2 D / V l, & \bar{v} = 0, \end{cases} \quad (5)$$

where $\alpha = \bar{v} l / D$.

Because countercurrent flow is a resistance to diffusion, assuming $\bar{v} = 0$ will give an upper bound to the countercurrent release rate. The upper curve in Fig. 4 shows the diffusive fractional release rate as a function of penetration radius for $D = 0.27 \text{ cm}^2/\text{s}$, the diffusion coefficient for

Figure 4. Fractional release rate of a gaseous species as a function of hole size, with countercurrent diffusion. [LBL 903-693]

CO_2 -air at 400 K. Multiplying these values by the fraction of the total radionuclide inventory that is volatilized gives the inventory-based fractional release. For a 5- μ hole and 1% ^{14}C volatilized, the diffusive fractional release rate is $7 \times 10^{-8}/\text{y}$ based on total ^{14}C inventory.

The lower curve in Fig. 4 shows the fractional release with a molar flow rate of $5 \times 10^{-3} \text{ mole/y}$, which is the late-time inflow rate from Fig. 3. This corresponds to a volumetric flow rate, $\pi r^2 \bar{v}$, of $5 \times 10^{-6} \text{ cm}^3/\text{s}$ at 390 K. For holes smaller than 30 μ there is a reduction in the release rate, but for larger holes the flow is slow and diffusion is the dominant release mode.

We also studied the effect of initial fill pressure, which along with the fill temperature gives the initial argon inventory. Qualitatively, the curves are the same as those in Figs. 2 to 4 for 1 atm. For fill pressures greater than 1 atm, the fractional release rates are greater than for 1 atm. For 2 atm and a 5- μ hole, about 60% of the volatile radionuclides is released with the outflow. For 10- μ holes or larger, 70% is released. For higher initial pressures, the air inleakage time is delayed a few hundred years for 5- μ holes, but it is not affected for 10- μ holes or larger. If the pressure at penetration is less than 1 atm, air leaks in immediately. Pressurizing the container increases the release of volatile radionuclides, but an initial vacuum allows more air to leak in.

In conclusion, we have studied the gas flow out of and into a waste container for various fill conditions and hole sizes. For holes of 5 μ or less, the flow rates are much less than the failure criterion. For holes 10 μ or larger, the long-term flow rates are controlled by the cooling rate and are about the same as for 10- μ holes. We found that the flow rate through a 5- μ hole is below the SCP leakage rate criterion, but for 10- μ holes or larger the leakage rate is exceeded briefly. For holes 30 μ or larger, countercurrent diffusive release is important because the resistance due to

inflow of air is small. We also obtained some insights for designers, such as whether to prepressurize and preheat the waste containers at assembly. From this model, at least the qualitative effects of these important parameters can be seen, and to a first approximation, the quantitative effects can also be seen. Gas flow through a hole in an "unfailed" container may still be important.

Simulation of Reactive Chemical Transport in a Varying Thermal Field with Reaction-Flow Coupling

C.L. Carnahan

An aspect of geochemical behavior that can have important consequences in numerical studies of subsurface migration of chemically reactive solutes is the effect of a variable thermal field on (1) the movement of major solution components and dissolved trace contaminants and (2) the stabilities of minerals exposed to the changing thermohydrochemical environment. Variable thermal fields can arise in the near vicinity of heat sources and from mixing of fluids having different temperatures. Such fields imposed on previously stable or metastable minerals can induce dissolution of existing minerals, transport of dissolved chemical species, and precipitation of new solid phases. Redistribution of materials by chemical reactions and transport can produce changes of physical properties, such as porosity, mass diffusivity, and permeability. Changes of these parameters can affect transport of both trace contaminants and major components of subsurface fluids.

THE COMPUTER PROGRAM THCVP

The reactive chemical transport simulator THCVP is an extension of the simulator THCC (Carnahan, 1987a,b; 1988) and is being used to study effects on mass transport of precipitation-dissolution reactions in the presence of varying thermal fields. The THCVP computer program is a thermodynamically based simulator of multicomponent, reactive chemical transport that couples mass transport directly to chemical reactions. The program simulates transport of reactive chemical species by advection and hydrodynamic dispersion or mass diffusion in one-dimensional linear or cylindrically symmetric geometry. Chemical reactions are assumed to be in a state of local equilibrium. The reactions simulated are complexation, oxidation-reduction, ionization of water, and reversible precipitation of solid phases. Chemical reactions are described by mass-action relations among thermodynamic activities of participating species. Temperature variations during transport and reaction of chemical components are simulated by numerical solution of a heat-transport equation within THCVP. Three kinds of thermal variations can be simulated:

REFERENCES

- U.S. Department of Energy, 1988. Site Characterization Plan, Yucca Mountain Site, Nevada Research and Development Area, Nevada, DOE/RW-0199.
American Society of Mechanical Engineers, 1986. Boiler and Pressure Vessel Code, Sec. V, Art. 10, App. IV.

ed: (1) mixing of advecting fluids having different temperatures, (2) diffusion of heat from a constant-temperature boundary, and (3) a constant linear gradient of temperature between two boundaries.

COUPLING BETWEEN CHEMICAL REACTIONS, POROSITY, AND FLUID FLOW

The THCVP program obtains numerical solutions of differential equations of mass transport and nonlinear algebraic equations describing chemical equilibria. The primary unknowns are the concentrations of dissolved chemical species and reactive solids. Changes in the concentrations of solids are converted to changes in porosity through the known molar volumes of the solids. The current local values of porosity are then used to compute local values of hydraulic conductivity. A number of empirical relations are available for this purpose; currently, THCVP uses a relation similar to the Kozeny-Carmen equation.

The program assumes a constant hydraulic head drop across a finite one-dimensional domain divided into segments by a set of finite-difference nodes. Associated with each node and adjacent segment are the current values of porosity and hydraulic conductivity. Because there are no sources or sinks of fluid flow in the domain, the Darcy flux at any time must be constant throughout the spatial domain. Knowledge of the total head drop and local hydraulic conductivities allows computation of the Darcy flux, which enters into the advective and dispersive terms of the mass transport equations. This procedure provides the feedback from heterogeneous chemical reactions to fluid flow.

EXAMPLE SIMULATION

A simple chemical reaction, the precipitation of quartz from saturated solution of silicic acid, illustrates the effect of varying temperature on porosity, hydraulic conductivity, and fluid flow. A constant temperature gradient

is imposed on a finite spatial domain, the temperature varying from 90°C at $x = 0$ to 50°C at $x = 1$ m. The domain has initial porosity of 0.05 and is saturated with silicic acid at the local temperature. The variation with temperature of the equilibrium constant, K_{SP} , for the reaction

is given by

$$\log K_{SP} = 1.881 - \frac{1560}{T} - 2.028 \times 10^{-3}T, \quad (1)$$

where T is the absolute temperature in kelvins (Phillips et al., 1988). The molar volume of quartz is $0.0227 \text{ dm}^3/\text{mole}$ (Robie et al., 1967). At the simulated initial porosity of 0.05, the initial hydraulic conductivity is computed to be $6.2 \times 10^{-6} \text{ m/s}$. A constant hydraulic head gradient of unity is imposed on the system, the head dropping from 1 m at $x = 0$ to zero at $x = 1$ m. Under the influence of the head gradient, fluid saturated with silicic acid at 90°C enters the domain at $x = 0$ and is advected in the direction of increasing x . Due to decreasing temperature and the decreasing solubility of silicic acid, quartz is deposited in the region near $x = 0$; the "concentrations" (moles of quartz per cubic decimeter of matrix) of deposited solid are shown in Fig. 1 as functions of time for nodes located at $x = 0$ and $x = 0.05$ m. Figure 2 shows values of porosity at the same two nodes. The deposited solid concentration rises to a steady-state value of about 2.2 moles/dm^3 at time 2.7×10^7 s, whereas the porosity drops to about 0.0004 at this time. Figure 3 shows the Darcy flux with time, plotted semilogarithmically to emphasize the sudden decrease of fluid flow near 2.5×10^7 s and the non-zero steady-state value of about $6.7 \times 10^{-11} \text{ m/s}$, a decrease of about five orders of

Figure 2. Porosity versus time at $x = 0$ and $x = 0.05$ m. [XBL 903-695]

magnitude from the initial value. Finally, Fig. 4 shows spatial profiles of hydraulic head at various times, indicating the effect of accumulation of solid quartz near the fluid inlet.

CONCLUSION

The computer program THCVF provides a capability to simulate coupling and feedback among processes of sa-

Figure 1. Moles of quartz precipitated per cubic decimeter of matrix versus time at $x = 0$ and $x = 0.05$ m. [XBL 903-694]

Figure 3. Flow rate (Darcy flux) of water versus time. [XBL 903-696]

Figure 4. Hydraulic head versus distance for various simulated times. [XBL 903-697]

turated fluid flow, transport of reactive solutes, and chemical reactions under conditions of varying temperature. Reduction of flow by mineralization involving major solution components can result in decreased migration rates of trace contaminants as well as major components.

Nonsteady-State Simulation of Coupled Transport Processes in Geological Materials

C.L. Carnahan and J.S. Jacobsen

A large body of experimental and field observations indicates that certain low-permeability geological materials, notably argillaceous media, exhibit coupling among flows of heat and matter, a property known as permselectivity. These couplings give rise to contributions to the flows driven by seemingly unrelated forces in addition to the usual conjugate forces. For example, volume flux in such media is observed to be driven not only by the gradient of hydraulic potential (Darcy's law) but also by gradients of solute chemical potentials (chemical osmosis), electrical potential (electro-osmosis), and temperature (thermal osmosis). Obviously, advective fluxes of solutes can be affected also by these coupled fluid flows. In addition, other coupled processes (ultrafiltration and electrophoresis), as well as ordinary chemical diffusion (Fick's law), can influence migration of solutes relative to motion of the fluid. Because permselective geological materials

REFERENCES

- Carnahan, C.L., 1987a. Simulation of chemically reactive solute transport under conditions of changing temperature. *In* C.-F. Tsang (ed.), *Coupled Processes Associated with Nuclear Waste Repositories*. Academic Press, Orlando, Florida, p. 249-257.
- Carnahan, C.L., 1987b. Simulation of uranium transport with variable temperature and oxidation potential: The computer program THCC. *In* J.K. Bates and W.B. Seefeldt (eds.), *Scientific Basis for Nuclear Waste Management X (Materials Research Society Symposia Proceedings, Vol. 84)*. Materials Research Society, Pittsburgh, Pennsylvania, p. 713-721.
- Carnahan, C.L., 1988. Simulation of effects of redox and precipitation on diffusion of uranium solution species in backfill. *In* M.J. Apted and R.E. Westerman (eds.), *Scientific Basis for Nuclear Waste Management XI (Materials Research Society Symposia Proceedings, Vol. 112)*. Materials Research Society, Pittsburgh, Pennsylvania, p. 293-302.
- Phillips, S.L., Hale, F.V., Silvester, L.F., and Siegel, M., 1988. Thermodynamic tables for nuclear waste isolation. Lawrence Berkeley Laboratory LBL-22860, Vol. 1.
- Robie, R.A., Bethke, P.M., and Beardsley, K.M., 1967. Selected X-ray Crystallographic Data, Molar Volumes, and Densities of Minerals and Related Substances. Bulletin 1248, U.S. Geological Survey.

usually exhibit very low fluid permeability and mass diffusivity, the coupled fluxes of fluids and solutes may be significant relative to the Darcian and Fickian fluxes.

The thermodynamics of irreversible processes provides a theoretical basis for quantitative description of coupled transport processes (Carnahan and Jacobsen, 1990). The linear phenomenological equations relating coupled fluxes and forces, postulated by this theory, have been experimentally validated for many systems in temporal steady states. Analysis of transient behavior of coupled systems according to this theory has not been accomplished in a rigorous sense because of the nonlinear nature of the governing conservation equations. However, the transient states of geological and engineered systems may be of considerable interest, and a capability for simulating transient behavior of such systems has been needed.

The computer program TIP was developed to simulate transient behavior of systems supporting irreversible processes with coupling among flows of mass and energy (Jacobsen and Carnahan, 1990). Here we present results of example calculations using the TIP program to simulate transient phenomena associated with two coupled processes: chemical osmosis in bentonite and thermal osmosis in kaolinite.

CHEMICAL OSMOSIS IN BENTONITE

This example illustrates the effects of chemical osmosis on solute fluxes and concentrations and on pressure changes in a system with no net volume flow. A one-dimensional domain has spatial extent of 1 m, initial solute concentration of 10 kg/m^3 , and initial pressure of 10^7 Pa .

At one end of the domain, solute concentration and pressure are maintained at their initial values; at the other end, a constant small flux of solute enters the domain. At both boundaries, the net volume (water plus solute) flux is constrained to be zero. The system evolves to a steady state at which the solute concentration at the inlet attains a value of 40 kg/m^3 and the flux of solute everywhere in the domain equals the inlet flux. Two cases are compared: the case with no coupling and the case with active chemical osmosis. Phenomenological coefficients for bentonite were obtained from the experimental results reported by Letey and Kemper (1969).

With no coupling and no net volume flux, the pressure field remains unchanged and solute migrates away from the inlet boundary by diffusion only. Figure 1 shows the evolution of the solute flux in time and space after the

Figure 1. Solute flux in bentonite versus distance at several simulated times with no coupling. [XBL 903-684]

initiation of the inlet flux. It is seen that the flux reaches a steady value of $4.3 \times 10^{-12} \text{ kg/(m}^2\text{s)}$, the inlet value for this case.

In the case with chemical osmosis, coupling among volume fluxes (with net volume flux held at zero) produces pressure changes (osmotic pressure) in the domain. These changes are small relative to the initial pressure; their evolution is shown in Fig. 2. In this case, solute can migrate by both advection and diffusion, but migration away from the inlet is opposed by ultrafiltration and osmosis. The result is that the inlet flux required to achieve a steady-state concentration of 40 kg/m^3 at the inlet is smaller in this case than in the case without coupling. Figure 3 shows the evolution of the solute flux in this case. The flux reaches a steady value of $2.6 \times 10^{-12} \text{ kg/(m}^2\text{s)}$, equal to the inlet flux.

Figure 4 shows the evolution of solute concentrations for the two cases considered. Transient concentrations are lower in the presence of coupling, as expected. The gradient of concentration at the steady state is variable, contrary to the prediction of practical diffusion theory. In the thermodynamics of irreversible processes, the correct driving force for chemical diffusion is the gradient of chemical potential, and this quantity is constant at the steady state of the system under consideration here.

THERMAL OSMOSIS IN KAOLINITE

This example illustrates the effect of thermal osmosis on flow of water in a system undergoing active heat transport. A one-dimensional domain has spatial extent of 1 m, initial temperature of 325 K , and initial pressure of 10^7 Pa . At one end of the domain, temperature and pressure are

Figure 2. Osmotic pressure changes in bentonite versus distance at several simulated times. [XBL 903-685]

Figure 3. Solute flux in bentonite versus distance at several simulated times in the presence of chemical osmosis. [XBL 903-686]

maintained at their initial values; at the other end, a constant flux of heat (1.6 W/m^2) enters the domain and a pressure gradient of 10^4 Pa/m is maintained. The system evolves to a steady state at which the temperature at the inlet attains a value of 327 K , establishing a temperature gradient of -2 K/m , and a pressure gradient of 10^4 Pa/m is es-

Figure 4. Solute concentration profiles in bentonite at several simulated times with no coupling and with active chemical osmosis. [XBL 903-687]

tablished throughout the domain. Two cases are compared: the case with no coupling and the case with active thermal osmosis. Phenomenological coefficients for kaolinite were obtained from the experimental results reported by Srivastava and Avasthi (1975).

With no coupling, the pressure gradient creates a volume (Darcy) flux of water equal to $-5.00 \times 10^{-10} \text{ m/s}$ throughout the domain. This volume flux remains invariant in time while the heat flux and temperature evolve to the steady state.

In the case with thermal osmosis, the advective Darcian (pressure-driven) volume flux is opposed by the thermo-osmotic (temperature-driven) flux, and the net volume flux at steady state is only $-9 \times 10^{-12} \text{ m/s}$. In this example, the latter value is imposed as a boundary condition; then, at steady state, the contribution of the advective flux is the same as that without coupling, $-5.00 \times 10^{-10} \text{ m/s}$, and the thermo-osmotic flux is $4.91 \times 10^{-10} \text{ m/s}$. Transiently, the volume fluxes evolve in response to the migration of heat from the inlet boundary. Figure 5 shows the spatial distribution of the flux contributions at two times; the volume flux for the case with no coupling is indicated also. Progression of the flux profiles toward the steady-state values is evident. In this case, in the presence of opposing gradients of pressure and temperature, thermal osmosis causes a reduction of total volume flux by a factor of more than 500 relative to the case without coupling.

CONCLUSION

The computer program TIP is a useful tool for simulation and analysis of the effects of coupling among transport processes in both transient and steady states. Possible areas of application of this tool to geological problems include the origins of anomalous pressure differences across permselective materials (e.g., clay and shale aquitards) separating groundwaters of different salinities, the role of

Figure 5. Volume fluxes in kaolinite versus distance at simulated times of 1 yr and 100 yr in the presence of thermal osmosis and with no coupling. [XBL 903-688]

osmotic pressure in facilitation of thrust faulting, the origins of deep brines in sedimentary basins, and the hydrothermal and magmatic segregation of minerals.

REFERENCES

- Carnahan, C.L., and Jacobsen, J.S., 1990. Coupled transport processes in semipermeable media. Part I: Theoretical basis. Lawrence Berkeley Laboratory Report LBL-25618.
- Jacobsen, J.S., and Carnahan, C.L., 1990. Coupled transport processes in semipermeable media. Part II: Numerical method and results. Lawrence Berkeley Laboratory Report LBL-25619.
- Letey, J., and Kemper, W.D., 1969. Movement of water and salt through a clay-water system: Experimental verification of Onsager reciprocal relation. *Soil Sci. Soc. Am. Proc.*, v. 33, p. 25-29.
- Srivastava, R.C., and Avasthi, P.K., 1975. Non-equilibrium thermodynamics of thermo-osmosis of water through kaolinite. *J. Hydrology*, v. 24, p. 111-120.

Development of UTHCC — A Computer Program for Simulating Reactive Chemical Transport through Unsaturated Media

J.S. Jacobsen, C.L. Carnahan, and K. Pruess

UTHCC, a computer program capable of simulating reactive chemical transport through partially saturated media has been developed by linking two existing computer programs. UTHCC was developed to study the effects of interactions among reacting chemical species, groundwater, and the host medium on the transport of chemical species through saturated and unsaturated media. The transport of toxic chemical wastes through the vadose zone and the movement of radionuclides away from a high-level-waste repository sited in the unsaturated zone are two areas of investigation in which UTHCC may be used.

DESCRIPTION OF THE THCC AND TOUGH COMPUTER PROGRAMS

The two existing programs linked to create UTHCC are THCC and TOUGH, both of which were developed at Lawrence Berkeley Laboratory. THCC was developed by C.L. Carnahan to simulate reactive chemical transport through saturated media under nonisothermal conditions. The following equilibrium reactions are included in THCC: aqueous complexation, ion exchange, precipitation-dissolution, and oxidation-reduction. THCC has been used to study the movement of uranium species under conditions of variable temperature and oxidation potential (Carnahan, 1987) and the migration of cesium and strontium through sodium bentonite that has been altered by ion exchange with groundwater cations (Jacobsen and Carnahan, 1989).

TOUGH was developed by K. Pruess to simulate the "coupled transport of water, vapor, air, and heat" through porous media (Pruess, 1987). The program keeps track of three components, water, air, and heat; the first two components may exist in two phases, gas and liquid. TOUGH has been used to study the thermal and hydrological condi-

tions in the vicinity of a high-level-waste repository in an unsaturated medium (Pruess and Wang, 1984; Pruess et al., 1985). TOUGH is applicable to multidimensional systems, whereas THCC is limited to one-dimensional linear or radial systems.

The present version of THCC assumes a constant velocity of fluid flow. TOUGH, in addition to calculating temperature, pressure, and liquid and gas saturations, also calculates time-dependent velocity fields for liquid and gas phases. Supplying the velocities calculated by TOUGH to THCC extends the capabilities of THCC to simulating reactive chemical transport in variably saturated systems in which the fluid velocities vary in space and time.

DEVELOPMENT OF UTHCC

Linking the two programs entailed the following: modifying THCC to accept spatially varying fluid velocities (to be supplied by TOUGH subroutines in the merged program), streamlining the main section of both programs to facilitate control of the execution of the merged program, modifying the input parameters for both programs to eliminate duplicate variables, and adding statements to control the sequential execution of THCC and TOUGH subroutines.

The program flow of the main program of UTHCC, after all variable initialization has taken place, is to execute the TOUGH subroutines and the THCC subroutines sequentially. The TOUGH subroutines pass the time-step size used and the pore fluid velocities calculated to the THCC subroutines. If convergence is not achieved during the THCC calculations, then the time step is reduced and the velocities are recalculated by the TOUGH subroutines.

LIMITATIONS OF THE CURRENT VERSION OF UTHCC

At this time, UTHCC may be run only in an isothermal mode, though both THCC and TOUGH simulate transport in nonisothermal systems. In future versions, the temperature distribution calculated by the TOUGH subroutines will be passed to the THCC subroutines. Another limitation is that one of the inner boundary conditions present in the current version of THCC, the advective-flux boundary condition, has been eliminated, though it will be restored in a future version. Only a constant-concentration boundary condition or a constant-diffusive-flux boundary condition may be imposed at the inner boundary at this time. Although TOUGH makes it possible to specify multiple domains, such that each domain represents a different type of medium with its own material properties, the present version of THCC is limited to a single domain. In future work, the THCC subroutines used in UTHCC will be modified to allow for multiple domains as well.

POSSIBLE IMPROVEMENTS TO UTHCC

The performance of UTHCC could be improved in two ways: by vectorizing the TOUGH subroutines and by reducing the amount of memory used. Vectorizing the TOUGH subroutines would decrease computation time, and reducing the amount of memory used would decrease memory charges. The version of THCC used in UTHCC had been previously vectorized for a Cray computer. Very little of TOUGH, on the other hand, has been vectorized. In the present version of UTHCC, arrays used by the THCC subroutines are almost entirely separate from those used by the TOUGH subroutines. Since the THCC and TOUGH subroutines are executed sequentially, it should be possible for the two sets of subroutines to share some array space.

SUMMARY

The version of UTHCC described in this report provides the capability to simulate one-dimensional reactive chemical transport through saturated and unsaturated media and is ready for testing and validation. It provides all of the equilibrium chemical reactions available in UTHCC but is not applicable to nonisothermal systems. Future versions of UTHCC will incorporate the nonisothermal capabilities

of THCC and TOUGH. In its present state, UTHCC may be used as a research tool to study how interactions among reacting chemical species found in hazardous wastes affect their transport through partially saturated media. Interactions of the reacting chemical species with the ambient groundwater and with the porous media, through which the transport is taking place, may also be included. Examples of the use of UTHCC include studying the effects of the interactions listed above on the transport of chemical wastes, leaking from a surface or buried source of contamination and passing through the vadose zone to the water table, or on the movement of radionuclides, leaking from a canister in a nuclear waste repository and passing through an engineered barrier to the host rock.

REFERENCES

- Carnahan, C.L., 1987. Simulation of uranium transport with variable temperature and oxidation potential: The computer program UTHCC. *In* J.K. Bates and W.B. Seefeldt (eds.), *Scientific Basis for Nuclear Waste Management X* (Materials Research Society Symposia Proceedings, Vol. 84). Materials Research Society, Pittsburgh, Pennsylvania, p. 713-721.
- Jacobsen, J.S., and Carnahan, C.L., 1989. Numerical simulation of cesium and strontium migration through sodium bentonite altered by cation exchange with groundwater components. *In* W. Lutze and R.C. Ewing (eds.), *Scientific Basis for Nuclear Waste Management XII* (Materials Research Society Symposia Proceedings, Vol. 127). Materials Research Society, Pittsburgh, Pennsylvania, p. 749-754.
- Pruess, K., 1987. TOUGH user's guide. Lawrence Berkeley Laboratory Report LBL-20700, 78 p.
- Pruess, K., and Wang, J.S.Y., 1984. TOUGH — A numerical model for nonisothermal unsaturated flow to study waste canister heating effects. *In* G.L. McVay (ed.), *Scientific Basis for Nuclear Waste Management VII* (Materials Research Society Symposia Proceedings, Vol. 26). North Holland, New York, p. 1031-1038.
- Pruess, K., Tsang, Y.W., and Wang, J.S.Y., 1985. Modeling of strongly heat driven flow in partially saturated fractured porous media. *Proceedings, IAH 17th International Congress on the Hydrogeology of Rocks of Low Permeability*. University of Arizona, Tucson, Arizona, p. 486-497.

Hydrothermal Mineralogy and Alteration Temperatures in the Shady Rest Drill Hole, Long Valley Caldera

S. Flexser

The Long Valley caldera, located on the eastern slope of the Sierra Nevada in east-central California, has attracted much scientific attention as a result of recent volcanism and related seismic and geothermal activity. The main cataclysmic event at Long Valley was the voluminous eruption of the Bishop Tuff 0.7 million years ago, followed closely by subsidence and the formation of the present topographic form of the caldera. Subsequent smaller eruptive episodes produced the Early Rhyolites of the resurgent dome and the later Moat Rhyolites and Moat Basalts on its margins. Eruptions have occurred in the past several hundred years along the Inyo and Mono Craters chain intersecting the western side of the caldera, and current seismic and geodetic evidence points to the presence and movement of magma at relatively shallow depths.

Core samples from six drill holes in the west moat of the caldera (Fig. 1) are being studied to characterize the hydrothermal alteration resulting from circulation of hot fluids in the caldera-filling rocks. The focus of study has been the core from the Shady Rest (SR) hole (Wollenberg et al., 1987), which has the highest downhole temperature, 202°C, of the drill holes examined (Fig. 2) and the most interesting clay alteration mineralogy. (One caldera drill hole, Unocal IDFU 44-16 near INYO-4, reaches a higher temperature than SR, 218°C, but it was not studied, as core was unavailable). This report summarizes study through 1989 of hydrothermal alteration in the SR core and shows how analysis of interstratified clay minerals can be applied in comparing present and past temperatures at depth.

Figure 1. Locations of drill holes in the west moat of the Long Valley caldera, from which core has been studied. Names correspond to those in Fig. 2. [XBL 8911-6340]

BULK MINERALOGY

The major mineral phases were identified by x-ray diffraction (XRD) analysis. Samples were crushed and ground to < 45 μm and mounted in an acetone slurry to minimize preferred orientation. (Sample preparation for clay analysis, where preferred orientation is desired, is described below.) Mineral abundances were determined by comparing ratios of diagnostic peak intensities with ratios obtained from similarly prepared mixtures of standards. This method provides a semiquantitative determination of abundance, with an error of roughly 20 wt%. (A larger error is likely for the feldspars, for which standards differ compositionally from samples, as well as for low abundances in general.) The bulk mineralogy of the main portion of the SR core is shown in Fig. 3, along with the temperature profile and lithologic features.

With regard to the clay minerals, alteration in the SR core can be divided into an upper and a lower zone. The upper zone, through the top of the Early Rhyolite (Q_{er} in Fig. 2), is dominated by kaolinite and smectite, with cristobalite also abundant. Quartz and K-feldspar are also common; they frequently occur as phenocrysts in Moat Rhyolite tuff or inclusions, however, rather than as alteration products. Unaltered glass is the major phase in tuffs above 125 m but is rare below that except in intervals of low-permeability perlite. In the lower alteration zone, kaolinite, smectite, and cristobalite are absent, and quartz, K-feldspar, and illite are the major alteration products. In a transitional zone between and partly overlapping the upper and lower zones, interstratified illite-smectite is the dominant clay phase, as will be discussed below.

The lower portion of the SR core—from the major lost-circulation zone at 328 m in Early Rhyolite to the bottom at 715 m in Bishop Tuff—has a temperature profile that is nearly isothermal, and it is pervasively cut by near-vertical fractures (Wollenberg et al., 1987). Many of the fractures are open, and they typically are lined with pyrite, quartz, calcite, and sometimes illite, in order of deposition. These minerals (along with marcasite, possibly pseudomorphous after pyrrhotite) are also deposited in secondary pores, which are common in the pumiceous Early Rhyolite tuffs below ~ 315 m. The top of the isothermal zone coincides with a marked change in mineralogy that continues for ~ 60 m below (Fig. 3): illite becomes sparse or absent, whereas albite, which is subordinate to K-feldspar in most of the core, becomes the major feldspar phase. Other secondary minerals observed in the core include chlorite, present in some brecciated intervals; zeolites, mainly clinoptilolite, occurring locally in fractures and in perlite in Moat Rhyolite; and calcite, intermittently abundant below

Figure 2. Comparative temperature profiles, maximum temperatures, and generalized lithologies of the Shady Rest and other boreholes shown in Fig. 1. Lithologic symbols depict mainly rhyolitic tuffs and breccias of the Early and Moat Rhyolites (Q_{er} and Q_{mr} , respectively), as well as basaltic rocks (e.g., top of INYO-4) and rhyolite lava (most of PLV-1); Bishop Tuff makes up the lower unit at Shady Rest. Elevation is given at left. [XBL 8911-6341]

275 m in the rock matrix, as well as in fractures and pores. Pyrite, not shown in Fig. 3, is commonly disseminated throughout the core.

CLAY MINERALOGY

Samples were prepared for clay analysis by separation of the $< 2 \mu\text{m}$ size fraction by suspension in water, followed by sedimentation onto a filter. This produces a strong preferred orientation of the crystallites, enhancing the diagnostic basal reflections. In most cases, both air-dried and ethylene glycol-saturated samples were analyzed by XRD; ethylene glycol expands the variable basal spacing in smectites from $\sim 12\text{--}15\text{\AA}$ to $17\text{\AA}$ but does not affect clays with fixed spacings, such as kaolinite ($7\text{\AA}$), illite ($10\text{\AA}$), and chlorite ($14\text{\AA}$). Glycol saturation is also essential in distinguishing the various species of interstratified illite-smectite (I/S) minerals.

In the SR core, I/S occurs mainly between 195 and 244 m; above 225 m, it coexists with smectite and kaolinite. (Between 195 and 204 m, random I/S is the phase present, and it is shown in Fig. 3 between the smectite and I/S columns.) In the I/S minerals, there is a systematic variation in the ratio of $10\text{\AA}$ -illite layers to $17\text{\AA}$ -(glycol)-smectite layers, as well as in the range of interlayer order.

The range of order is represented by R , which signifies in effect the minimum number of illite layers separating smectite layers. Thus $R = 0$ denotes a random structure; $R = 1$, a 1:1 layering (usually including excess illite layers); and $R \geq 3$, a long-range ordering of $\geq 75\%$ illite (Reynolds, 1980). These structural variations correlate with approximate ranges of crystallization temperatures; temperatures increase both with R (Table 1) and with the proportion of illite layers within each structural type. The temperature ranges are valuable as paleo-thermometers, since most evidence from hydrothermal occurrences suggests that ordered I/S structures ($R > 0$) are equilibrium phases and that their compositions are relatively independent of chemical and lithologic variability (Horton, 1985; Srodon and Eberl, 1984). (This may be less valid for diagenetic than for hydrothermal I/S.)

In SR core, the variation in I/S composition follows a fairly smooth sequence with depth, as shown in Fig. 4; below 244 m, I/S is replaced by illite. ("Illite" is meant here to include I/S with $\geq 95\%$ illite layers, as this cannot readily be distinguished from illite by XRD.) Two significant exceptions to the smooth I/S variation (both lower-temperature I/S than in surrounding samples) occur in fault zones or fractures at 231 and 289 m, and these are the only such samples noted in this core interval; the deeper one

Figure 3. Bulk mineralogy in SR core, with corresponding lithologic column and temperature profile (scale at bottom). Phases plotted are glass (gl); kaolinite (ka), smectite (sm), mixed-layer illite-smectite (i/s), and illite (ill); quartz (qz), cristobalite (cr), and feldspar (fsp); zeolite (ze), chlorite (chl), and calcite (ca). Bars indicate mineral abundance; 100% abundance corresponds to length of fine lines below column headings. Trace abundances not shown. [XBL 8911-6343]

Table 1. Structures and temperature ranges of interstratified illite-smectite minerals and illite.

Structure	Temperature range (°C)
$R = 0$ (random)	<140
$R = 1$ (allevardite)	~95 to 185
$R \geq 3$ (kalkberg)	~175 ^a to 230
Illite	>185

Source: Summarized from I/S and illite occurrences in active geothermal fields and from compilations by Horton (1985) and Srodon and Eberl (1984).

^aFrom diagenetic I/S (Hower, 1981).

coincides with a slope change in the temperature profile (Fig. 5). A small compositional discontinuity in $R = 1$ I/S at about 225 m may be related to the disappearance of smectite, kaolinite, and cristobalite near that depth.

DISCUSSION

The application of I/S and illite paleothermometry to alteration in SR core is shown in Fig. 5. The range of $R = 1$ I/S, given by the rectangle between 210 and 240 m, provides poor constraint on alteration temperatures; but it indicates that temperatures that are now at the low end of this range were probably significantly higher during alteration. A more definite indication is given by the lower boundary of illite stability at ~185°C, which shows that the alteration temperature at 244 m was at least 65°C higher than at

Figure 4. Variation of I/S structure and composition with depth in SR core. (Calculated from XRD patterns of glycolated samples, by methods of Tomita et al., 1988, and Reynolds, 1980.) The occurrence of illite to 300 m depth is also shown. [XBL 903-934]

Figure 5. Present temperature profile (dotted), along with ranges of alteration temperatures inferred from I/S and illite shown in Fig. 4. Temperature ranges of $R = 1$ and $R \geq 3$ I/S (rectangles), and upper and lower limits of $R = 0$ I/S and illite, respectively (vertical lines), are shown for core intervals in which these phases are present. See text for explanation of points A, A', B, and B'. [XBL 903-935]

present (B' versus B). Taken together with the upper boundary of $R = 0$ I/S above A', this also shows that a paleotemperature gradient of at least 1.1°C/m (A'-B') existed over the same interval where a gradient of 0.48°C/m (A-B) exists today. Whether this high gradient persisted much below 244 m cannot be determined from clay mineralogy alone, as illite is stable over a broad temperature range. But evidence from oxygen isotopes (Smith et al., 1989) and from fluid inclusions (J. Moore, personal communication, 1986) indicates that past temperatures in the lower part of the Early Rhyolite and the Bishop Tuff at SR have not been much higher than they are today.

The clay mineralogy in other cores (Figs. 1 and 2) presents a different picture than that in SR. Where I/S is present (in PLV-1, MLGRAP-1, and INYO-4), the transitions with depth in I/S composition and structure are more discontinuous and erratic than in SR core. This reflects the lithologic homogeneity (fine-grained porous tuffs) in SR core in the interval in which I/S occurs; it also reflects hydrothermal deposition and sealing in the other cores, resulting in zones of widely varying permeability. Moreover, compared with SR core, differences between present and inferred alteration temperatures are greater in the other cores, indicating that hydrothermal circulation there has cooled more than it has at SR.

REFERENCES

- Horton, D.G., 1985. Mixed-layer illite/smectite as a paleotemperature indicator in the Amethyst vein system, Creede district, Colorado, USA. *Contrib. Mineral. Petrol.*, v. 91, p. 171-179.

- Hower, J., 1981. Shale diagenesis. *In* F.J. Longstaffe (ed.), *Clays and the Resource Geologist*. Min. Assoc. Canada, Short Course Handbook (Vol. 7), p. 60–80.
- Reynolds, R.C., 1980. Interstratified clay minerals. *In* G.W. Brindley and G. Brown (eds.), *Crystal Structures of the Clay Minerals and their X-ray Identification*. Mineralogical Society Monograph (Vol. 5), p. 249–303.
- Smith, B.M., Wollenberg, H.A., and Suemnicht, G.A., 1989. O-isotope and thermal implications for past and present hydrothermal regimes beneath the Long Valley caldera (abstr.). EOS: Trans. Am. Geophys. Union, v. 70, p. 1057.
- Srodon, J., and Eberl, D.D., 1984. Illite. *In* S.W. Bailey (ed.), *Micas*. Mineralogical Society America Rev. Mineral. Short Course (Vol. 13), p. 495–544.
- Tomita, K., Takahashi, H., and Watanabe, T., 1988. Quantification curves for mica/smectite interstratifications by x-ray powder diffraction. *Clays & Clay Mineral.*, v. 36, p. 258–262.
- Wollenberg, H.A., Sorey, M.L., Farrar, C.D., White, A.F., Flexser, S., and Bartel, L.C., 1987. A core hole in the southwestern moat of the Long Valley caldera: Early results. EOS: Trans. Am. Geophys. Union, v. 68, p. 529–534.

Solubility and Speciation Studies for the Yucca Mountain Project

H. Nitsche, A. Müller, R.C. Gatti, T. Prussin, R.S. Deinhammer, and S.A. Carpenter

The purpose of the Yucca Mountain Project is to characterize Yucca Mountain in southern Nevada to determine its suitability as a potential site for a high-level nuclear waste repository. Risk-assessment studies on repository safety must consider the migration of contaminated groundwater as one principal mechanism for the transport of radionuclides from a potential nuclear waste repository to the accessible environment. The radionuclide concentrations in water that has passed through the waste package will be controlled by several mechanisms, including dissolution and colloidal formation. Colloidal formation, however, is linked to a solubility-controlled initial step that transforms the nuclear waste into a soluble form before radionuclide colloids and pseudocolloids can form. The magnitude of the contamination is controlled by the dissolution rate of the waste package, the formation of solubility-controlling solids, and the formation of soluble species. The subsequent rate of migration through the geomedium depends on the nature and charge of the soluble species. The nature of compounds and solution species depends on many parameters. They are (1) the oxidation state of the radionuclide, (2) the nature and concentration of the ions and complexing ligands present in the groundwater, (3) the pH, (4) the Eh, (5) the temperature, and (6) the nature of the geologic host.

Solubility establishes an upper limit for the dissolved components in the source term for radionuclide migration from a repository. Studies of the solubility of radionuclides in groundwaters from a repository horizon will provide limits on their potential concentrations in those waters. Such limits are important for (1) verifying the validity of an essential part of the radionuclide transport calculations and (2) providing the maximum starting concentrations for radionuclide sorption experiments. Compared with mul-

tiparameter transport models, laboratory solubility experiments are controlled by fewer variables. If geochemical codes such as EQ3/6 (Wolery, 1983, 1987) are to be included in the transport model, the model should be capable of predicting the results of solubility experiments.

We continued to study the solubilities and speciation of $^{237}\text{NpO}_2^+$, $^{239}\text{Pu}^{4+}$, and $^{241}\text{Am}/\text{Nd}$ in J-13 groundwater from the Yucca Mountain region. Each radionuclide solution was maintained at three pH values (pH 6, 7, and 8.5) and at three temperatures (25°, 60°, and 90°C). The tolerances were 0.1 pH unit and 0.5°C. Twenty-seven solubility experiments were carried out. Further details about the purification and oxidation state adjustments of the actinide stock solutions, the groundwater, the automatic pH control unit, and the method used for the determination of oxidation states of soluble species at steady state and characterization of the steady-state solids are described elsewhere (Nitsche and Edelstein, 1985; Tucker et al., 1988; Nitsche et al., 1988).

RESULTS

Figure 1 shows the results of the Pu^{4+} solubility study. The experiments ran between 60 and 150 days. No clear trend with increasing pH was observed. But the solution concentrations decreased drastically with increasing temperature. This is not surprising, considering that the solubility-controlling solids were mixtures of mainly polymeric $\text{Pu}(\text{IV})$ mixed with some plutonium carbonates. Increasing temperature peptized the $\text{Pu}(\text{IV})$ polymer, making it more stable. The distribution of plutonium oxidation states in the steady-state solutions at pH 8.5 is given in Fig. 2. Although Pu^{4+} was added initially to the groundwater,

Figure 1. Plutonium oxidation-state distributions of the supernatant at steady state for Pu^{4+} solubility experiments in J-13 groundwater at pH 8.5 and 25°, 60°, and 90°C. The solutions were filtered through 4.1-nm filters. [XBL 8911-3935]

the steady-state solutions consisted mainly of PuO_2^+ along with a lesser amount of PuO_2^{2+} . The solutions at pH 6 and 7 behaved similarly. The observed valence distributions cannot be explained by disproportionation equilibria and complex stabilization (Silver, 1972). It is possible that oxidation products formed by α -radiolysis of the water may cause the predominance of high oxidation states in the plutonium solutions.

Results of the neptunium solubility studies are shown in Fig. 3. At each temperature the neptunium solubility decreased with increasing pH. No significant temperature dependence was found within the temperature range studied. The steady-state solids in each experiment were sodium neptunium carbonate hydrates with different water content. They were identified by comparing their x-ray diffraction patterns with patterns published in the literature (Keenan and Kruse, 1964; Volkov et al., 1977; Volkov et

Figure 2. Results for Pu^{4+} solubility experiments in J-13 groundwater as a function of pH and temperature. [XBL 8911-3926]

Figure 3. Results for NpO_2^+ solubility experiments in J-13 groundwater as a function of pH and temperature. [XBL 8911-3933]

al., 1979a,b, 1981). It appears that many of the described solids are metastable and therefore difficult to reproduce. The solid formed at 90°C and pH 7 was a mixture of sodium neptunium carbonate hydrate and neptunium pentoxide. The formation of Np_2O_5 under this condition is quite surprising, because higher temperatures are normally required to produce this solid (Cohen and Walter, 1964). The solubility decrease with increasing pH is clearly connected to the increased formation of CO_3^{2-} with increasing pH. This in turn results in the formation of more insoluble sodium neptunium carbonate hydrates and in lower solubilities. The neptunium oxidation state in the steady-state solutions was unchanged and exclusively +5. The solution species present were identified by absorption spectrophotometry as NpO_2^+ , NpO_2OH (aq), and $\text{NpO}_2\text{CO}_3^-$ (Nitsche et al., 1990).

Results of the americium solubility experiments are shown in Fig. 4. Measurements at 60°C are still in progress. No clear trend of the solubility was found with increasing temperature and increasing pH. The soluble

Figure 4. Results for $^{241}\text{Am}^{3+}/\text{Nd}^{3+}$ solubility experiments in J-13 groundwater as a function of pH and temperature. [XBL 8911-3934]

americium(III) did not change its oxidation state during the experiment. The steady-state solids at pH 7 and 8.4 were orthorhombic AmOHCO_3 , whereas the solids formed at pH 5.9 and 25° and 90°C were hexagonal AmOHCO_3 . This is the first report of the existence of hexagonal AmOHCO_3 (Nitsche and Standifer, 1988), which is isomorphous with the rare-earth analogue, hexagonal NdOHCO_3 .

At the moment, we are attempting to model the laboratory solubility experiments using relevant program modules of the transport modeling code EQ3/6. Furthermore, we are currently studying the solubilities of neptunium, plutonium, and americium in a groundwater of substantially higher carbonate content and of 10 times higher ionic strength. A comparison of these results with the results of the study reported here should clarify whether the groundwater composition has a significant influence on the actinide solubilities.

REFERENCES

- Cohen, D., and Walter, A.J., 1964. Neptunium pentoxide. *J. Chem. Soc.*, p. 2696–2699.
- Keenan, T.K., and Kruse, F.H., 1964. Potassium double carbonates of pentavalent neptunium, plutonium, and americium. *Inorg. Chem.*, v. 3, 1231–1232.
- Nitsche, H., and Edelstein, N.M., 1985. Solubilities and speciation of selected transuranium. A comparison of a non-complexing solution with a groundwater from the Nevada Tuff Site. *Radiochim. Acta*, v. 39, p. 23–33.
- Nitsche, H., and Standifer, E.M., 1988. First evidence of hexagonal AmOHCO_3 . *Lanthanide and Actinide Res.*, v. 2, p. 383–384.
- Nitsche, H., Lee, S.C., and Gatti, R.C., 1988. Determination of plutonium oxidation states of trace levels pertinent to nuclear waste disposal. *J. Radioanal. Nucl. Chem.*, v. 124, no. 1, p. 171–185.
- Nitsche, H., Standifer, E.M., and Silva, R.J., 1990. Neptunium(V) complexation with carbonate. *Lanthanide and Actinide Res.*, v. 3, p. 203–211.
- Silver, G.L., 1972. Suggestion for the determination of plutonium valencies in aqueous solutions. *Radiochem. Radioanal. Lett.*, v. 9, p. 315–320.
- Tucker, D.B., Standifer, E.M., and Nitsche, H., 1988. Data acquisition and feedback control system for solubility studies of the nuclear waste elements neptunium and plutonium. *Lanthanide and Actinide Res.*, v. 2, p. 279–287.
- Volkov, Y.F., Visyashcheva, G.I., and Kapshukov, I.I., 1977. Study of carbonate compounds of pentavalent actinides with alkali metal cations. V. Production and identification of hydrate forms of sodium monocarbonatoneptunylate. *Sov. Radiochem. (Eng. transl.)*, v. 19, p. 263–266.
- Volkov, Y.F., Tomilin, S.V., Visyashcheva, G.I., and Kapshukov, I.I., 1979a. Carbonate compounds of pentavalent actinides with alkali-metal cations. VI. X-ray structure analysis of $\text{LiNpO}_2\text{CO}_3$ and $\text{NaNpO}_2\text{CO}_3$. *Sov. Radiochem. (Eng. transl.)*, v. 21, p. 579–583.
- Volkov, Y.F., Visyashcheva, G.I., Tomilin, S.V., Spiriakov, I.V., Kapshukov, I.I., and Rykov, A.G., 1979b. Carbonate compounds of pentavalent actinides with alkali-metal cations. VII. Synthesis and crystal structure of hydrate compounds with the composition $\text{Na}_{0.6}\text{NpO}_2(\text{CO}_3)_{0.8} \cdot n\text{H}_2\text{O}$. *Sov. Radiochem. (Eng. transl.)*, v. 21, p. 583–590.
- Volkov, Y.F., Visyashcheva, G.I., Tomilin, S.V., Kapshukov, I.I., and Rykov, R.G., 1981. Study of carbonate compounds of pentavalent actinides with alkali metal cations. VIII. Synthesis and x-ray diffraction investigation of several compounds of neptunium(V) with sodium and rubidium. *Sov. Radiochem. (Eng. transl.)*, v. 23, p. 191–195.
- Wolery, T.J., 1983. EQ3NR, computer program for geochemical aqueous speciation-solubility calculations: Users guide and documentation. Lawrence Livermore National Laboratory Report UCRL-53414.
- Wolery, T.J., 1987. EQ6, a computer program for reaction-path modeling of aqueous geochemical systems: Users guide and documentation. Lawrence Livermore National Laboratory Report UCRL-53788.

Synthesis and Spectroscopic Studies of Uranium Carbonate

D.L. Perry

The study of uranium carbonate systems has recently attracted much attention, primarily because of their significance in geologic and oceanographic chemistry. Uranium, for example, commonly occurs in carbonaceous materials,

such as lignite and peat; this relationship has been well established and cannot be totally fortuitous. Several investigations have been reported regarding the interaction of coal and uranium, including one addressing the uptake of the

uranium in seawater by coal. Other investigators have studied the extraction of uranium by coal from aqueous solutions under laboratory conditions.

Many of these investigations have shown that the uranium carbonate system involved in the reaction chemistry is the $\text{UO}_2(\text{CO}_3)_3^{4-}$ ion, a very stable species found in seawater. This species is considered to be the predominant one in aqueous uranium carbonate systems in which there is a large excess of the carbonate ion. Accordingly, there is an interest in a rapid atmospheric-pressure synthesis of $\text{K}_4\text{UO}_2(\text{CO}_3)_3$ that results in a large yield of a high-purity product, and this synthesis is described here. Additionally, x-ray photoelectron and x-ray induced Auger spectral data are reported.

SYNTHESIS OF $\text{K}_4\text{UO}_2(\text{CO}_3)_3$

Four grams of a mixture of uranyl hydroxides/oxides, prepared by the precipitation of an aqueous solution of $\text{UO}_2(\text{NO}_3)_2 \cdot 6\text{H}_2\text{O}$ by 1.0 M KOH, was placed in a 500-ml flask, along with 200 ml of 1.0 M K_2CO_3 . This mixture was refluxed for 6 hours; the remaining solid was allowed to settle, and the yellow solution was decanted and filtered to remove any remaining fine particulate matter. This procedure was repeated several times until almost all of the original solid had gone into solution, decanting, filtering, and adding the solution to the originally collected solution each time. The total solution was gently warmed until the final volume was 300 ml. In order to keep the solution saturated with the carbonate ion without appreciably altering the potassium concentration by the addition of more K_2CO_3 , chips of dry ice were added. The final yellow solution (pH = 11–12) was then covered with a watch glass and allowed to slowly evaporate (1–2 weeks), yielding a

crop of bright yellow crystals of $\text{K}_4\text{UO}_2(\text{CO}_3)_3$. The compound was filtered on a Buchner funnel and allowed to air-dry on the filter bed.

The method of synthesis of $\text{K}_4\text{UO}_2(\text{CO}_3)_3$ reported here, essentially an extraction of uranium oxides/hydroxides into a saturated potassium carbonate solution followed by slow crystallization, offers a major advantage over previously reported techniques of synthesis of uranium carbonates in that this synthesis can be effected quite easily at ambient pressure. Several workers prepared anhydrous uranyl carbonate; however, this involved the reaction of CO_2 with UO_3 under pressure. Again, the reaction of CO_2 under pressure with aqueous uranyl nitrate also produces an anhydrous carbonate.

X-RAY PHOTOELECTRON AND AUGER SPECTRAL DATA

Table 1 shows data measured for the model compound, $\text{K}_4\text{UO}_2(\text{CO}_3)_3$. X-ray photoelectron binding energies for the uranium $4f_{7/2,5/2}$ lines are consistent with the hexavalent state of uranium. Two other comparative model compounds— K_2CO_3 and CaCO_3 —were studied also to compare oxygen x-ray photoelectron and Auger data. This was done in order to determine which spectral parameters might be used to distinguish the $\text{UO}_2(\text{CO}_3)_3^{4-}$ ion from other carbonates. The most easily detectable difference lies in the oxygen KVV Auger lines, where there is a 1.4 eV difference in the shift. Line shape comparisons were performed on the oxygen KVV lines, but no perceptible differences exist. The oxygen $1s$ line of $\text{K}_4\text{UO}_2(\text{CO}_3)_3$ is approximately one volt lower than that of the two other model compounds; this reflects the contribution of the uranyl-related oxygen atom to the average binding energy.

Table 1. X-ray photoelectron and Auger data for $\text{K}_4\text{UO}_2(\text{CO}_3)_3$, K_2CO_3 , and CaCO_3 .^{a,b}

Compound	O $1s$	O KVV ^c	C $1s$ ^d	K $2p_{3/2}$	U $4f_{7/2}$	U $4f_{5/2}$
$\text{K}_4\text{UO}_2(\text{CO}_3)_3$	530.2(2.4)	742.7 (9.5)	288.5(1.4)	292.0(1.9)	381.4(1.9)	392.0(1.9)
K_2CO_3	530.4(2.4)	743.6(10.8)	288.4(2.4)	292.3(1.6)	—	—
CaCO_3	531.0(2.1)	744.1(10.0)	289.0(2.4)	—	—	—

^a Electron volts, eV.

^b Adventitious C $1s$ = 284.6 eV used for charge referencing.

^c Value reported is for most intense line of the triplet KVV Auger set.

^d Value reported is that of the carbonate functional group.

Thermodynamics of High-Temperature Brines

K.S. Pitzer, R.T. Pabalan, and L.M. Connaughton

Equilibrium considerations based on various types of experimental measurements interrelated and extended by thermodynamic calculations provide an important basis for understanding and prediction in a variety of geochemical systems. This article includes in its first part a new equation of state for very concentrated brines extending to pure fused salts. It is applied to NaCl-KCl-H₂O and the related binaries up to 350°C where the total Cl⁻ molality reaches 32 mol·kg⁻¹ (Pabalan and Pitzer, 1989). The second part reports results of oceanographic as well as geochemical interest, specifically equations for the volumes of mixing of any combination of the major sea salts NaCl, Na₂SO₄, MgCl₂, MgSO₄ for the range 0–95°C (Connaughton et al., 1989). The parameters determined in this research will allow the accurate calculation of the density of any Na-K-Cl-SO₄-H₂O system within the stated temperature range. From thermodynamics it also gives information on the effect of pressure on the activity coefficients of any mixture in this system.

A THERMODYNAMIC MODEL FOR IONIC SOLUTIONS VALID TO THE FUSED SALT

An equation due to Margules has been widely and successfully used for nonelectrolyte solutions over the full composition range. It is effective for systems of three or more components as well as for binaries. For ionic systems one must add a Debye-Hückel term and define the mole fractions of ionic species. Recently, this equation was tested for aqueous solutions of certain low-melting nitrates at temperatures near their melting points (or the eutectic points of mixed salts). Good agreement was obtained (Simonson and Pitzer, 1986).

This equation was applied to the data for the system KCl-NaCl-H₂O and the component binaries KCl-H₂O and NaCl-H₂O over the temperature range 25–350°C. At 350°C, the solution saturated by both salts has a Cl⁻ molality of 32 (20 molal K⁺ and 12 molal Na⁺). Most other equations for aqueous electrolytes are limited to about 6 molal or 10 molal in exceptionally favorable cases.

The details with respect to the equations, the known properties of the solids, and the evaluation of parameters for the aqueous phase are described in Pabalan and Pitzer (1989). The equations for the aqueous binaries and ternary were required to fit data for the activity of H₂O over the full range of knowledge as well as the solubilities of one or both solids. Figures 1, 2, and 3 compare the calculated curves with the measured solubilities, respectively, for the binaries of H₂O with NaCl, with KCl, and for the ternary.

Of particular interest is the behavior shown in Fig. 3 with change in temperature. At low temperature, one finds

Figure 1. Solubilities of halite (NaCl) in water to 350°C. The curve represents values calculated using the Margules-expansion model. Experimental data are taken from Keevil (1942), Linke and Seidell (1965), and Liu and Lindsay (1972). [XBL 903-722]

the expected common-ion effect in which an increase in molality of Cl⁻ leads to a decrease in solubility of either NaCl or KCl. But at 350°C the solubility of NaCl is about 12 and that of KCl is about 20, regardless of the amount of the other component in solution. The Debye-Hückel effect offers an explanation in causing a decrease in activity coefficient with increase in total ionic strength. This effect increases rapidly with temperature; it is small at 25°C but

Figure 2. Solubilities of sylvite (KCl) in water to 350°C. The curve represents values calculated using the Margules-expansion model. [XBL 903-723]

Figure 3. Solubilities of halite and/or sylvite in the NaCl-KCl-H₂O system. The squares and circles are experimental data taken from Sterner et al. (1988) and Linke and Seidell (1965), respectively (open symbols for halite, closed symbols for sylvite). The open triangles are triple-point (halite+sylvite+saturated solution) data from Linke, and the closed triangles are triple-point data from Sterner et al. The curves are calculated as in Figs. 1 and 2. [XBL 903-724]

very important at 350°C. Other effects contribute, however, so a complete explanation is more complex.

Since this thermodynamic model is based on a general equation for the Gibbs energy, other properties can be obtained from the usual thermodynamic relationships. Indeed, the volumetric properties were also treated, and the pressure derivatives are thereby available as well as the temperature derivatives.

VOLUME CHANGES IN MIXING SOLUTIONS OF THE MAJOR SEA SALTS

Accurate volumetric data for mixed aqueous electrolytes are important for many applications in oceanography, geology, steam-power engineering, oil recovery, and waste treatment, as well as being of fundamental interest in physical chemistry. Especially valuable is an equation that predicts properties for mixtures of unlimited complexity after parameters are evaluated for simple systems. In this paper we apply an equation of this type (Pitzer, 1973, 1987) to recently measured data (Millero et al., 1985; Connaughton et al., 1986, 1987) for the four major sea salts, NaCl, Na₂SO₄, MgSO₄, MgCl₂, and their common-ion mixtures. These data suffice for the evaluation of all parameters in the equations, which then predict the properties of more complex mixtures. Experimental values for non-common-ion mixtures of these salts are compared with the predictions. The experimental mixing data cover the range 5–95°C and 1–3 mol·kg⁻¹; the data base for the pure salts is even more complete.

The equations used are those based on a virial expansion together with a Debye-Hückel term. There have been many applications to activity and osmotic coefficients as well as several applications to volumetric data. Rogers and

Pitzer (1982) gave a very complete treatment of the volumetric data for NaCl-H₂O on this basis.

The volume of mixing is defined as the difference between the excess volume of the mixture and the sum of the excess volumes of the pure-electrolyte components. For mixing at constant ionic strength, the Debye-Hückel term cancels. Moreover, for symmetrical mixing (ions mixed having equal charges) the pure-electrolyte virial coefficients also cancel, and the only remaining terms are those for mixing ions of the same sign. All possible mixings of the major sea salts, however, are unsymmetrical in that Na⁺ is mixed with Mg²⁺ or Cl⁻ is mixed with SO₄²⁻. The pure electrolyte parameters do not cancel. This non-cancellation of pure-electrolyte parameters was overlooked in some published work of others. Hence the full set of equations for ΔV_m for each of the charge type situations was derived and presented.

In the calculations, previously published values for all pure-electrolyte parameters were accepted and only the terms for mixing ions of the same sign were evaluated. These are θ_{ij}^v for mixing two ions without further interaction and ψ_{ijk}^v for mixing ions *i* and *j* in the presence of an ion *k* with the opposite charge. Test calculations were made with and without the ternary terms in ψ^v , and it was found that the binary terms in θ^v sufficed to reproduce the experimental results. The resulting values of $\theta_{Na,Mg}^v$ and θ_{Cl,SO_4}^v are shown in Fig. 4, together with curves for equations giving their dependency upon temperature.

The initial calculations were made for common anion mixing (NaCl-MgCl₂ and Na₂SO₄-MgSO₄) and common cation mixing (NaCl-Na₂SO₄ and MgCl₂-MgSO₄). The resulting parameters were then tested for the additional mixing processes NaCl-MgSO₄ and Na₂SO₄-MgCl₂ and the agreement of prediction with experiment was very satisfactory. These parameters are applicable, in addition, for brines that include ions in addition to Na⁺, Mg²⁺, Cl⁻,

Figure 4. Plot of θ_{ij}^v in kg·mol⁻¹·bar⁻¹ for Na-Mg and Cl-SO₄ mixing. Symbols show values determined from common-ion mixing experiments at each temperature; curves are calculated. [XBL 903-725]

SO_4^{2-} provided the parameters for the additional ions are known or can be neglected because their concentration is small.

REFERENCES

- Connaughton, L.M., Hershey, J.P., and Millero, F.J., 1986. *PVT* properties of concentrated aqueous electrolytes: V. Densities and apparent molal volumes of the four major sea salts from dilute solution to saturation and from 0 to 100°C. *J. Soln. Chem.*, v. 15, p. 989-1002.
- Connaughton, L.M., and Millero, F.J., 1987. The *PVT* properties of concentrated aqueous electrolytes. V. The volume changes for mixing the major sea salts at an ionic strength of 3.0 from 5 to 95°C. *J. Soln. Chem.*, v. 16, p. 491-502.
- Connaughton, L.M., Millero, F.J., and Pitzer, K.S., 1989. Volume changes for mixing the major sea salts: Equations valid to ionic strength 3.0 and temperature 95°C. *J. Soln. Chem.*, v. 18, no. 1, p. 1007-1017.
- Keevil, N.B., 1942. Vapor pressure of aqueous solutions at high temperatures. *J. Am. Chem. Soc.*, v. 64, p. 841-850.
- Linke, W. F., and Seidell, A., 1965. *Solubilities of Inorganic and Metal Organic Compounds* (4th ed., Vols. 1 and 2). American Chemical Society, Washington, D.C.
- Liu, C., and Lindsay, W.T., Jr., 1972. Thermodynamics of sodium chloride solutions at high temperatures. *J. Soln. Chem.*, v. 1, p. 45-69.
- Millero, F.J., Connaughton, L.M., Vinokurova, F., and Chetirkin, P.V., 1985. *PVT* properties of concentrated aqueous electrolytes. III. Volume changes for mixing the major sea salts at $I = 1.0$ and 3.0 at 25°C. *J. Soln. Chem.*, v. 14, p. 837-851.
- Pabalan, R.T., and Pitzer, K.S., 1989. Models for aqueous electrolyte mixtures for systems extending from dilute solutions to the fused salt. Presented at the American Chemical Society Annual Meeting, Anaheim, California, September 25-30, 1988 (LBL-26468).
- Pitzer, K.S., 1973. Thermodynamics of Electrolytes. I. Theoretical Basis and General Equations. *J. Phys. Chem.*, v. 77, p. 268-277.
- Pitzer, K.S., 1987. A thermodynamic model for aqueous solutions of liquid-like density. *Rev. Mineral.*, v. 17, p. 97-142.
- Rogers, P.S.Z., and Pitzer, K.S., 1982. Volumetric properties of aqueous sodium chloride. *J. Phys. Chem. Ref. Data*, v. 11, p. 15-81.
- Simonson, J.M., and Pitzer, K.S., 1986. Thermodynamics of multicomponent, miscible, ionic systems: I. Theory and equations; II. The system $\text{LiNO}_3\text{-KNO}_3\text{-H}_2\text{O}$. *J. Phys. Chem.*, v. 90, p. 3005-3013.
- Sterner, S.M., Hall, D.L., and Bodnar, R.J., 1988. Synthetic fluid inclusions. V. Solubility relations in the system $\text{NaCl-KCl-H}_2\text{O}$ under vapor-saturated conditions. *Geochim. Cosmochim. Acta*, v. 52, p. 989-1005.

Selection and Characterization of a Radon Experimental Site

H.A. Wollenberg, S. Flexser, R.G. Sextro,* and A.R. Smith†

To study the ingress of radon into the basements of houses, small structures (i.e., "mini-basements") were designed for installation at sites of various geological, hydrological, and radiochemical character. As described by Fisk et al. (1989), these structures permit detailed examination, under controlled conditions, of the movement of radon from its sites in the soil, through the soil pore-water system, and, by way of controlled entry slots, into the basements. Important parameters monitored include the difference between the pressure in the structures, the atmosphere, and the soil pores; the soil moisture, temperature, and permeability; and the radon concentrations in the soil gases and structure interiors.

This article discusses the considerations and activities that led to the choice of an initial small-structures site, the characteristics of that site, and the considerations for selection of a second site. The essence of the installation (at the initial site) is that two nearly identical small structures were built (with one principal difference: one structure's floor slab rests directly on the soil, the other's slab rests on aggregate). The structures, nominally 2.1 by 3.4 m in plan and 2.1 m high, were emplaced in excavations ~1.8 m deep and surrounded on their sides by a ~0.6-m-wide zone of compacted backfill (Fig. 1).

CRITERIA FOR SELECTING THE INITIAL SITE

A strong consideration for the initial site was that soil conditions be as uniform as possible over the volume that

*Applied Science Division, Lawrence Berkeley Laboratory.

†Engineering Division, Lawrence Berkeley Laboratory.

Figure 1. Cross section of a small structures "mini-basement" for radon experiments. [XBL 898-6970]

encompasses both structures and that, on a centimeter scale, the soil be relatively homogeneous. Since the effect of soil moisture on the ingress of radon into a structure is an important consideration, a site with strongly contrasting rainy and dry seasons was desirable. This would permit measurements to be made under differing degrees of partial saturation. It was also desirable that the permanent water table be at least one excavation depth (~2 m) below the bottom of the structure. A soil with an appreciable but not necessarily high permeability and radium concentration and a good radon emanation was also necessary. It was considered that the initial site should be within reasonable driving distance from Lawrence Berkeley Laboratory (LBL) and should have good access to electrical power lines and telephone communications.

SCREENING AND CHARACTERIZATION

To select the initial site, geological settings and soil characteristics of coastal central California were assessed in regard to the above criteria. An idealized setting was considered where there was a deep soil with no significant lithologic or structural discontinuities within at least 3 to 4 m in any direction from the structures. Therefore, sites were sought on deep, uniform alluvial soil or on residual soil developed from deep weathering of rock. Geological reports and maps of the California Division of Mines and Geology and the U.S. Geological Survey were consulted, as were county soils reports of the U.S. Soil Conservation Service. Interpretation of the geologic reports identified

areas of appreciable radon concentration because of the presence of rocks with known moderate to high uranium concentration (Wollenberg and Revzan, 1989). The soils reports were valuable in focusing on sites in areas where climates appeared favorable and soils were well developed and of moderate to high permeability. (The permeability expressed in Soil Conservation Reports is for fluid, based on infiltration of a given amount of water into a column of soil; its rough correlation with the air permeability of soil has been discussed by Nazaroff et al., 1986.)

Six potential sites were examined in the San Francisco Bay Area (Fig. 2); their characteristics are listed in Table 1. Their radium concentrations were determined initially by field measurements of the gamma radioactivity in the energy region encompassing the 1.76-MeV photopeak of bismuth-214, a member of the uranium decay series. These measurements were followed by, and in large part confirmed by, laboratory gamma spectrometry of samples collected from the surfaces of the sites; the radon emanation (the ratio of radon emanated to radon produced) of these samples was also measured in the laboratory. At three of the sites, Ben Lomond, Las Posadas, and Oxford Tract, soil auger samples were collected at 15-cm intervals over a total depth of 1.5 m and were analyzed in the laboratory for their radium concentrations and radon emanation. These three sites were also probed to determine, in situ, their permeabilities and radon concentrations, using methods described by Nazaroff and Sextro (1988). Modifications of these methods are used for installation and instrumentation for repeated measurements of permeability

Figure 2. Location map of potential sites in the San Francisco Bay Area. BL = Ben Lomond, CP = Camp Parks, LP = Las Posadas, IG = Ink Grade, N = Napa State Hospital, OT = Oxford Tract. [XBL 898-6797]

and soil-gas radon at the small-structures site; soil moisture is measured by time-domain reflectometry.

Permeabilities at Oxford Tract and Las Posadas were relatively low compared with those at Ben Lomond, and given our field methods, these low permeabilities prohibited obtaining field measurements of radon concentrations. On the basis of results from Oxford Tract, a site within 1 km of LBL, the two other potential alluvial sites, Napa State Hospital and Camp Parks, were not examined further, nor was the Ink Grade site, which has characteristics similar to those of Las Posadas. Because of its relatively high seasonal rainfall, soil homogeneity, moderate radium concentration with relatively high radon emanation, appreciable permeability, and accommodating infrastructure (access to electricity and telephone, and a hospitable attitude of personnel of the California Division of Forestry), the site at Ben Lomond State Nursery was selected for the initial small-structures installation.

CHARACTERISTICS OF THE BEN LOMOND SITE

The site is located at an altitude of 790 m on a broad-topped oak- and Douglas-fir-studded ridge, Ben Lomond Mountain, ~12 km inland from the Pacific coast. Rainfall is high, because of the orographic effect of the ridge, and it is generally confined to the period October–April. The principal characteristics of the Ben Lomond Site are listed in Table 2. The soil is a residual sandy loam, developed from weathered quartz diorite, which is encountered at depths of 1.5 to 2 m (Leo, 1967;

Bowman and Estrada, 1980). The most prominent activity after selection and before construction was to obtain core samples to augment permeability and radon data obtained from surface measurements during the site-selection process. The array of probes and core holes in relationship to the approximate location of the structures is shown in Fig. 3, and the areal distributions of soil-gas radon concentrations and permeability are shown in Fig. 4. The cores were obtained primarily by pushing consecutive 7.6-cm-diameter by 76-cm-long Shelby tubes into the soil, using a Failing-750 drilling rig. Three of the holes reached depths of 3.6 m, one hole 4.3 m, and one 6.5 m. In this deepest hole, rotary coring was used in the bottom 3.4 m and samples recovered in a Pitcher core barrel. In all holes the depth reached was at least twice the 1.8-m depth of installation of the small structures. Permeabilities of cores from the depth interval 1.5 to 2.3 m in each of the five holes were determined in the laboratory by Tetsu Tokunaga and, as shown in Table 2, their arithmetic mean values and standard deviations agree with those determined in situ by probes from the surface. Laboratory testing by Harding Lawson Associates of two cores from depths of 0.76 to 1.5 m indicates wet densities ranging from 1.45 to 2.19 g/cm³ and moisture contents ranging from 10.4 to 19.7%. As well as indicating soil properties, these data were most valuable in designing the structures' excavations and the subsequent backfilling operations.

The backfill zone surrounding the sides of the structures ranges in width from 60 to 75 cm. Our goal was to achieve as homogeneous a backfill as possible. Soil from the structures' excavations was used; it was first blended and then emplaced in ~30 cm lifts and compacted. Compaction was monitored and controlled by use of gamma-ray and neutron measurements of density and moisture content, respectively. Based on 26 field measurements, the dry density of the backfill averages 1.41 ± 0.05 g/cm³, the moisture content $17 \pm 2.2\%$, and the relative compaction of the backfill (with respect to maximum dry density) $84 \pm 3\%$. Thus good homogeneity was attained.

Figure 5 shows the distribution with depth of radium and the radon-emanating fraction in the soil, based on auger samples at 15-cm intervals. The relatively high radium zone between 80 and 110 cm is associated with the presence of scattered rock fragments with abundant feldspar. Preliminary fission-track radiography of soil-auger and nearby rock-outcrop samples shows that uranium in unweathered outcrops is associated with accessory minerals. In weathered outcrops and soil, however, uranium is mainly associated with strongly altered mineral grains and with iron-oxide-rich coatings on grain surfaces (in concentrations of several tens of ppm U, in contrast to 1 to 3 ppm in the bulk soil). These coatings are most likely the primary loci of radon emanation in the soil.

CRITERIA FOR NEXT SITE

The small structures at Ben Lomond are encompassed by relatively homogeneous residual soil and are si-

Table 1. Possible initial installation sites.

Location	Avg. Rainfall (in.) ^a	Soil ^a	Apparent ²²⁶ Ra (pCi/g)	Soil-Gas ²²² Rn (pCi/L)	Emanation (%)	Permeability	
						Measured (m ²)	USSCS ^a (in./h)
Ben Lomond State Nursery, Santa Cruz County	50-60	Residual, Sandy Loam, (after quartz diorite) (Bowman and Estrada, 1980)	0.9 (± 0.2) ^b	1252 (± 519) ^c	32 ^b	7.5 × 10 ⁻¹³ to 4.0 × 10 ⁻¹¹	2.0-6.0
Las Posadas State Preserve, Napa County	30-50	Residual, Gravelly Loam, (Weath. Rhyolite to Clay) (Lambert and Kashiwagi, 1978)	2.1 (± 0.2) ^b	Outside air contamination due to low permeability	18 ^b	1.7 × 10 ⁻¹⁴ to 1.1 × 10 ⁻¹³	0.2-2.0
Ink Grade Site, Napa County	30-50	Residual, Gravelly Loam, (Weath. Rhyolite to Clay) (Lambert and Kashiwagi, 1978)	2.3	Not Measured	13	Not Measured	0.2-2.0
Napa State Hospital	25-30	Alluvial, Gravelly Loam (Lambert and Kashiwagi, 1978)	0.9	Not Measured	26	Not Measured	0.2-0.6
Camp Parks Reservation, Alameda County	16-20	Alluvial, Clay (Welch, et al., 1966)	0.6 ^d	Not Measured	18 ^d	Not Measured	0.05-0.2
Oxford Tract, U.C. Berkeley	20-25	Alluvial, Clay	0.45 (± 0.8) ^b	Not measurable, due to low permeability.		6.6 to 8.3 × 10 ⁻¹⁴	

^aFrom U.S. Soil Conservation Service reports.

^bMean of soil auger samples (11 at Ben Lomond, 9 at Las Posadas, 9 at Oxford Tract).

^cMean of 9 measurements at 1.5, 2, and 3 m depth.

^dSoils of Berkeley Hills, on Orinda Formation.

tuated well above the permanent water table but at a location where seasonal rainfall temporarily saturates the soil. It was desired that conditions at this initial site be relatively uniform, in some contrast to conditions at most sites of actual houses. In this regard, it is planned that the next small-structures site will be more heterogeneous. One consideration is a site that more closely simulates the conditions at housing sites in high-radon areas of the eastern U.S.:

1. Excavation in soil with quite variable permeability; a residual soil but probably with mixed soil and rock fragments,
2. Appreciable annual precipitation (76-102 cm/y) but more evenly distributed over time, so that there is less seasonal contrast in soil moisture and the depth to the saturated zone is relatively shallow.
3. A climate with prolonged cold periods when the near-surface soil is frozen.

Another consideration is a site with sharply contrasting zones of permeability: a small structure encompassed in a horizontally stratified setting of sandy and clayey beds. An alternative is a structure spanning a near-vertical discontinuity, such as a high-angle contact separating rock

Table 2. Ben Lomond site characteristics.

Residual soil (sandy loam) developed from weathered quartz diorite ^a		
Radium in soil		30–40 Bq/kg. (0.8–1.1 pCi/g)
Emanation		28–42%
Radon in soil gas		$1.6\text{--}5.5 \times 10^4$ Bq/m ³ (600–2000 pCi/l)
Permeability	(field)	$0.4\text{--}3.5 \times 10^{-11}$ m ² (mean: $1.7 \times 10^{-11} \pm 1.4 \times 10^{-11}$ m ²)
	(lab)	$0.9\text{--}6.5 \times 10^{-11}$ m ² (mean: $2.4 \times 10^{-11} \pm 2.3 \times 10^{-11}$ m ²)
		(overall mean: $1.9 \times 10^{-11} \pm 1.8 \times 10^{-11}$ m ²)
Porosity		from 29 to 33%
Degree of saturation		from 49 to 92%
Rainfall		~150 cm/y, seasonal
Depth to permanent water table		>4 m

^aGeologic setting from Leo (1967); soils description from Bowman and Estrada (1980).

(and its associated residual soil) of contrasting permeability.

Because they will be relatively heterogeneous compared with the initial site, the next sites will be more difficult to characterize. However, because they will be more typical of housing sites in areas of present concern, results of measurements in small structures there will be very germane to the understanding of the mechanisms of radon entry.

Figure 3. Layout of the Ben Lomond site, showing locations of probes used in site selection, core and auger holes, and the approximate locations of the small structures. [XBL 898-7691]

Figure 4. Areal distributions of soil-gas radon concentrations and permeability, determined by probing during site selection, Ben Lomond site. [XBL 898-7690]

Figure 5. Radium concentration and radon-emanating fraction of the soil, Ben Lomond site. [XBL 903-726]

REFERENCES

- Bowman, R.H., and Estrada, D.C., 1980. Soil survey of Santa Cruz County, California, U.S. Department of Agriculture, Soil Conservation Service.
- Fisk, W.J., Flexser, S., Gadgil, A.J., Holman, H.-Y., Modera, M.P., Narasimhan, T.N., Nuzum, T., Revzan, K.L., Sextro, R.G., Smith, A.R., Tsang, Y.W., and Wollenberg, H.A., 1989. Monitoring and modeling of radon entry into basements: A status report for the small structures project. Lawrence Berkeley Laboratory Report LBL-27692.
- Lambert, G., and Kashiwagi, J., 1978. Soil Survey of Napa County, California, U.S. Department of Agriculture, Soil Conservation Service.
- Leo, G., 1967. The plutonic and metamorphic rocks of the Ben Lomond Mountain area, Santa Cruz County, California. California Division of Mines and Geology Special Report 91, p. 27-43.
- Nazaroff, W.W., and Sextro, R.G., 1989. Analysis of a technique for measuring the indoor radon-222 source potential of soil. *Environ. Sci. & Technol.*, v. 23, p. 451-458.
- Nazaroff, W.W., Moed, B.A., Sextro, R.G., Revzan, K.L., and Nero, A.V., 1986. Factors influencing soil as a source of indoor radon: A framework for geographically assessing radon source potentials. Lawrence Berkeley Laboratory Report LBL-20645.
- Welch, L.E., Huff, R.C., Dierking, R.A., Cook, T.D., Bates, L.A., and Andrews, W.F., 1966. Soil survey of the Alameda Area, California. U.S. Dept. of Agriculture, Soil Conservation Service.
- Wollenberg, H.A., and Revzan, K. L., 1989. Radium regionalization in California. Submitted to *Geophys. Res. Letts.*

GEOPHYSICS AND GEOMECHANICS

The Geophysics and Geomechanics group conducts basic and applied research relevant to the nation's energy development programs and helps train the next generation of scientists and engineers in the geosciences. The research utilizes unique facilities at Lawrence Berkeley Laboratory and is directed toward the solution of problems related to the disposal of nuclear and toxic wastes, the exploration for and recovery of fossil fuels, the definition of fundamental properties and processes in the earth's crust, and the development of geothermal energy. The aim is to address not only today's needs, but also needs that will arise from the ever-increasing pressures placed upon the earth's resources. The group has focused, and will continue to focus, on a collaborative approach, not only between geophysical and geomechanical disciplines, but with other disciplines in government and industry as well. The thrust is for a strong theoretical foundation coupled with laboratory, numerical, and field-based studies. We are unique in that this group has a strong emphasis in all three areas. The overall philosophy is to address broad research bases rather than individual program areas. The group draws upon the unique resources within other divisions at the Laboratory and the various earth sciences departments on the U.C. Berkeley campus. Current emphasis is on the development of techniques for characterizing and monitoring processes in heterogeneous rock and soils using high-resolution geophysical imaging. Future growth will come about only through a coordinated and balanced program based on solid research principles—one that can respond to changing needs in the earth sciences and new objectives of DOE programs in a timely and efficient manner.

One-Dimensional Least-Squares Inversion of Surface-to-Borehole and Cross-Hole Electromagnetic (EM) Data

M. Deszcz-Pan, K.H. Lee, and H.F. Morrison

Borehole electromagnetics is an emerging new technique for enhanced oil recovery and for monitoring the propagation of contaminants. This kind of application demands an accurate estimate of conductivity up to several hundred meters from the well. At present, the conductivity of the medium close to the borehole is obtained from induction logs. Information about the conductivity distribution far away from the borehole is obtained either by correlating induction logs from several wells or by inverting surface data.

A new method based on low-frequency controlled-source EM measurements inside boreholes can provide better estimates of conductivities. Zhou (1989) showed that low-frequency EM tomography can be an excellent tool for detecting inhomogeneities within a conductive medium as long as the conductivity of the background medium is known quite accurately. To obtain better estimates of background conductivities for use in tomography, a cross-hole inversion program was developed. The inversion is one-dimensional (1-D), but comparison of the borehole geology from the induction logs with the conductivity structure from cross-hole inversion can suggest the presence of inhomogeneities that are not apparent by either measurement alone. This method is cheaper and easier to use in determining areas where subsequent full-scale tomography should be performed.

For example, consider the simplest possible case, presented in Fig. 1. In this highly hypothetical (but possible) situation, the induction-log results would be identical in both boreholes. If, however, the cross-hole measurements and subsequent inversion show a conductivity structure different from that obtained by the induction logs, then an inhomogeneity may be present, in which case a high-resolution electromagnetic tomography survey is justified to obtain the detailed properties of the inhomogeneity.

Figure 1. Comparison of induction logs with cross-hole EM data to detect an inhomogeneity. [XBL 903-727]

INVERSION OF CROSS-HOLE EM DATA

The nonlinear least-squares inversion program is called NLSEM1D. It is based on two algorithms. The forward problem is calculated by a modified version of program EM1D written by K.H. Lee (personal communication, 1989), and the inverse problem is handled by the subroutine NLSOL2, originally written by Dennis et al., (1979) and modified by Anderson (1982). Because of the flexibility of the forward routine, different combinations of frequency and geometrical soundings are available. The program can take any component of EM fields and invert real and imaginary parts together or either one of them separately. The same can be done with amplitude and phase.

The final results are very sensitive to the initial guess. If the initial guess is too far from the true one, then the program may converge to a local minimum. This situation is revealed by a relatively large least-squares error and the inability of the program to change the estimated parameter vector to the new value. In this case the problem has to be repeated with a new initial guess. To get a closer estimate of conductivities in the initial guess, a simple routine for calculating the apparent conductivity of the medium was added. The calculations are based on a whole-space assumption (suggested by M. Wilt). The calculated apparent conductivity was used as the initial guess, and with this initial guess the convergence to the true model was frequently obtained in the first trial. In the problems considered the parameters were constrained to their minimum and maximum possible values. For conductivities we always assumed 0.0 S/m as the minimum and 1.0 S/m for the maximum.

EXAMPLES

Two models were used to test the inversion program. The first model consists of two adjacent half-spaces of conductivity 0.01 S/m and 0.1 S/m (Fig. 2). The second model consists of a 50-m-thick layer of conductivity 0.1 S/m inside a conductive whole-space with conductivity 0.01 S/m (Fig. 3). Eleven frequency measurements were used, one per decade from 10^{-4} Hz to 10^6 Hz. The objective of the test was to see how well the program can resolve the conductivities and the location of the boundaries. The conductivities in the initial guess were always based on whole-space fields. For both models, the transmitter used was a vertical magnetic dipole.

With the initial guess of 0.05 S/m, 0.06 S/m, and boundary at $z = 0$ m, the resolution of the first model was perfect; in this case the data used were from two receiver

Figure 2. Model, initial guess, and final solution for two adjacent half-spaces. [XBL 903-728]

positions, at 50 and 100 m below the boundary. The true model, initial guess, and the final solution are given in Fig. 2. When the lower receiver was placed at the same depth (50 m below the boundary) as the upper receiver but separated by 150 m from the transmitter in the horizontal direction, the model was poorly resolved. When just one receiver position (at 50 m below boundary) was used, the program could not distinguish between the upper and lower half-spaces. These results confirm the intuitive feeling that the measurements in boreholes provide a better resolution of depth conductivity structure than expanding the array in a horizontal direction.

The resolution of the second model was poor if the same frequencies and receiver positions were used as in the first model. However, using two frequencies (10 Hz and 1000 Hz) and 10 receiver positions (spaced every 20 m from the height of 60 m above the upper layer boundary) gave a satisfactory solution. The model, initial guess, and final results are shown in Fig. 3.

Figure 3. Model, initial guess, and final solution for a layer inside a conductive whole-space. [XBL 903-729]

CONCLUSIONS

Although the program can resolve simple models, it performs poorly if the number of unknowns exceeds six or seven, which severely limits its practical application.

REFERENCES

- Anderson, W., 1982. Adaptive nonlinear least-squares solution for constrained or unconstrained minimization problems (subprogram NLSOL). USGS Open-File Report 82-68.
- Dennis, J.E., Gay, D.M., and Welsh, R.E., 1979. An adaptive nonlinear least-squares algorithm. NTIS Report AD-A079-716.
- Zhou, Q., 1989. Audio-frequency electromagnetic tomography for reservoir evaluation (Ph.D. thesis). University of California at Berkeley (LBL-28171).

Evaluating the Performance of Cross-Hole Diffusion Tomography

K.T. Nihei and Q. Zhou

The purpose of this study is to evaluate the performance of cross-hole diffusion tomography for monitoring a steam front during enhanced oil recovery. The effects of frequency, conductivity contrast, and variable background conductivity as well as the assumption of incorrect background conductivity on the quality of the diffusion-tomography reconstruction are examined.

The idealized model of a steam front used in this study is a cylindrical disk 30 m in thickness and 50 m in radius with a conductivity σ . The conductive disk is located within a homogeneous whole-space of conductivity σ_0 (see Fig. 1). The source consists of a vertical magnetic dipole

that is moved along a vertical borehole that is coaxial with the conductive disk. The data used in this study consist of measurements of the vertical magnetic field made along a vertical borehole located 100 m from the source borehole. Measurements are taken every 10 m at 32 receiver locations. The source is then moved 10 m to the next location, and measurements at the 32 receivers are repeated.

The following sections give brief descriptions of the forward- and inverse-modeling programs (Fig. 2) and the results of the numerical tests. The two programs are FORTRAN 77 codes (Zhou, 1989) with several minor modifications made to enable them to run on a SUN 4, CONVEX C-1/XP, or VAX 8650 computer.

Figure 1. Model geometry. [XBL 903-730]

THE FORWARD-MODELING CODE

Program TAHDCY (Zhou, 1989) was used to generate synthetic cross-hole data for the cylindrically symmetric model described above. TAHDCY is set up to give a Born approximation and *exact* numerical solutions for the vertical magnetic field produced by a vertical magnetic dipole source. A description of the numerical code and input variables is given in Zhou (1989; Section 4.3 and Appendix C.3, respectively).

Figure 2. Flow diagram of FORTRAN programs. [XBL 903-731]

THE DIFFUSION-TOMOGRAPHY CODE

Program TOMO2H (Zhou, 1989) is a numerical implementation of diffusion tomography for the reconstruction of cylindrically symmetric targets. TOMO2H is set up to give a Born-approximation reconstruction of the conductivity in a region between the source and receiver boreholes. Note that the dimensions of the image region should be smaller than the region over which data are collected (see Fig. 1). Selecting a smaller region for the image reconstruction ensures more complete coverage in the wavenumber domain and, hence, a higher-quality image.

The results from program TAHDCY, with a slight modification to the input, can be used as input to TOMO2H. A description of this numerical code and the input variables are given in Zhou (1989; Section 4.4 and Appendix C.4, respectively).

EFFECT OF FREQUENCY

Figure 3 shows the effect of frequency selection on the quality of the diffusion-tomography reconstruction. The target (outlined by a solid line) has a conductivity of 0.02 S/m, and the background has a conductivity of 0.01 S/m (i.e., conductivity contrast is 2). The reconstruction region is a 100 m $\times$ 160 m rectangle, shown in Fig. 1. Figure 3 demonstrates that the image quality for this particular model deteriorates at frequencies above 10 kHz. The poor image quality for a frequency of 20 kHz is most likely due to the reduced penetration of high-frequency waves into the conductive host but may also result from inaccuracies of the forward-modeling code (TAHDCY) at high frequencies.

EFFECT OF SELECTING AN INCORRECT BACKGROUND CONDUCTIVITY

Figure 4 shows the effects of using erroneous values for the background conductivity in the diffusion-tomography program (TOMO2H). The frequency used here is 10 kHz, and the host conductivity and target conductivity are 0.01 S/m and 0.02 S/m, respectively (i.e., conductivity contrast is 2). The effect of overestimating the background conductivity by 10% is to expand the image of the target. The effect of underestimating the background conductivity by 10% is to shrink the image of the target. Note that for this particular model, over- and underestimating the background conductivity does not severely distort the image. The location of the target reconstruction, despite minor distortion, remains virtually unchanged.

EFFECT OF CONDUCTIVITY CONTRAST

Figure 5 shows the effect of conductivity contrast on the diffusion-tomography image reconstruction. The synthetic data used as input into TOMO2H were generated by TAHDCY using a frequency of 10 kHz and a background conductivity of 0.01 S/m. The conductivity of the target

Figure 4. Effect of selecting an incorrect background conductivity. (a) Correct background ($\sigma_0 = 0.01$ S/m). (b) 10% too conductive ($\sigma_0 = 0.011$ S/m). (c) 10% too resistive ($\sigma_0 = 0.0091$ S/m). [XBL 903-733]

Figure 5. Effect of conductivity contrast. [XBL 903-734]

Figure 6. Effect of an inhomogeneous background. (a) Model. (b) Reconstruction. [XBL 903-735]

layers. Unfortunately, at the time this study was performed such a code was not immediately available.

To get a rough idea of the sensitivity of the diffusion-tomography method to background inhomogeneity, an alternate test using the TAHDCY was performed. The test consisted of placing a conductive disk 40 m in thickness and 80 m in lateral extent 40 m above the target (Fig. 6a) and then computing the cross-hole response using TAHDCY. Both disks are assigned conductivities of 0.02 S/m. The difference between the vertical magnetic fields obtained from this model and from the same model without the target disk was used as input into TOMO2H.

Figure 6b shows that for a frequency of 10 kHz and a conductivity contrast of 2, diffusion tomography is capable of producing an accurate reconstruction of the target. However, as the contrast between target and host conductivities increases, the electromagnetic coupling between the target and the anomalous body is expected to increase, resulting in a distorted image.

DISCUSSION

The effects of frequency, conductivity contrast, incorrect background conductivity, and inhomogeneous

background were examined for an idealized model of a steam front. Diffusion tomography appears to be a viable method for imaging conductive targets with conductivity contrasts less than 3 when a source frequency of 1–10 kHz is used and a reasonable estimate (within 10%) of the background conductivity can be made.

Although this study represents a very limited analysis of the diffusion-tomography method, it gives a rough idea when we can expect the method to work or to fail. In addition to the factors examined in this study, diffusion-tomography reconstruction quality is also dependent on the orientation and size of the target. A discussion of the effects of these geometrical factors on the quality of the diffusion-tomography reconstruction are given in Zhou (1989; Section 3.4).

REFERENCE

- Zhou, Q. (1989). Audio-frequency tomography for reservoir evaluation (Ph.D. Thesis). University of California at Berkeley. Lawrence Berkeley Laboratory Report LBL-28171.

Cross-Hole Tomographic Imaging for Fracture Characterization

E.L. Majer, J.E. Peterson Jr., L.R. Myer, K. Karasaki, T.M. Daley, and J.C.S. Long

The problem of adequate fracture detection and characterization is essential to the understanding of the hydrologic and geomechanical behavior of any underground nuclear waste repository. Fracture properties can be directly measured at the surface and underground openings, but because of the large variation in the geometry of fracture sets, it is unlikely that one can rely on the direct interpolation of structural information between boreholes for adequate fracture characterization. To address these problems one naturally turns to geophysical or remote methods for solutions, i.e., the seismic and electrical methods. The work described here concerns seismic, hydrologic, and geomechanical methods linked with the geologic description.

As applied on a large scale to a repository environment, the seismic method most likely to be applied is multi-offset/multi-source vertical seismic profiling (VSP). On smaller scales the cross-hole techniques in the underground workings could be used for detailed characterization of the rock surrounding the underground openings and canister areas. By performing a tomographic analysis of the VSP and cross-hole data from multiple offsets and azimuths, it may be possible to map the fracture characteristics between the boreholes and underground workings. This information could then be used in hydrologic or geomechanical models of fracture networks to study the behavior of the rock mass. Seismic methods would then be used to provide a method for extrapolating fracture characteristics observable at the borehole walls and underground workings to the entire repository block, thus providing a more-complete data set to characterize the overall hydrologic and geologic parameters.

SEISMIC-IMAGING EXPERIMENTS

During the past three years the USDOE, with cooperation of the Swiss cooperative for the storage of nuclear waste, NAGRA, has been carrying out experiments in The Grimsel Rock Laboratory in the Swiss alps in a granitic rock. Situated in this underground laboratory is the Fracture Research Investigation area (FRI), where these experiments have been carried out. Figure 1 is a plan view of the FRI zone, showing the two 21-m-long parallel boreholes, separated by 10 m and connecting two drifts in the laboratory, the access drift (top of Fig. 1) and the laboratory tunnel. The two drifts and boreholes form a 10 m x 21 m area that can be investigated by various geometrical cross-hole configurations. The FRI experiment area offers an excellent opportunity to perform calibrated experiments in a rock mass where the fracture locations and characteristics are relatively well known with the benefit of well-calibrated fracture sets for study. The greatest attraction, however, is the opportunity to test the fracture stiff-

Figure 1. Plan view of the FRI zone experimental area where the tomographic imaging and hydrologic tests were carried out. Shown are the two 21-m-long boreholes connecting two tunnels and the dominant geologic features. [XBL 903-736]

ness and other theories at different scales. Pyrak et al. (1989) have performed laboratory experiments that have, at small scales, confirmed the effect of fracture *stiffness*. The scaling of this phenomenon to larger distances is yet unknown. Therefore, one of the main objectives of the FRI experiments was to observe the effect of fracture density, orientation, and spacing on the propagation of the *P*- and *S*-waves. A second objective was to relate the seismic response to the hydrologic behavior of the fractures; the question to answered is whether all fractures affect the seismic wave or whether just fluid-filled or partially saturated fractures affect the seismic waves in a measurable amount. Another objective of the study was to assess the amount of seismic data necessary to provide useful information and to determine how these data should be processed to maximize information in a routine fashion. These are important questions when one progresses to the point of applying these techniques on larger scales in a systematic fashion.

The concept behind the FRI seismic experiments is relatively simple. Seismic sources were placed in the holes (boreholes 87.001, 87.002, and the shallow holes in the sides of the tunnel) and activated. The data from a three-component accelerometer package were recorded at 0.5-m

spacing in boreholes 87.001 and 87.002. The receiver package was also placed in the shallow holes to give complete four-sided coverage. The objective of the experiments was to gather high-quality *P*- and *S*-wave data across the fracture zone to determine the seismic visibility of fractures. Data from this controlled field experiment would then be compared with the laboratory results on the core and with in situ tests of the mechanical and hydrologic behavior of the rock. Three experiments were performed in the FRI zone, one each in the summers of 1987, 1988, and 1989. The data were recorded on an in-field PC-based acquisition system. Nearly 60,000 ray paths (*x*, *y*, and *z* components) were collected in the FRI zone, at distances from 1/2 m to nearly 23 m. The peak energy transmitted in the rock was 5000 to 10,000 Hz, thus yielding a wavelength of approximately 1 to 0.5 m in the 5.0 km/s velocity rock.

The travel times were inverted using an algebraic reconstruction technique (ART). A pixel array of 44×88 was chosen for the tomographic inversion. This produces a pixel size of 0.25 m, which is the size of the smallest anomaly we expect to see given the wavelength of 0.7 m and a station spacing of 0.5 m. Previous experience has shown that for this geometry a pixel size of half the station spacing gives the optimal combination of resolution and inversion stability. The result of inverting the entire data set from the 1988 survey is shown in Fig. 2. Our previous ex-

perience has shown us that the Grimsel granite is highly anisotropic ($\approx 10\%$). It is possible to obtain image improvement by removing the background anisotropy from the travel times (Johnson and Peterson, 1986). The result, after applying these travel times to the 1988 data, is a smoother image with the low-velocity zones more distinct (Fig. 3). The inversion also appears to remove some artifacts that are produced in the original inversion; among these are the smearing seen in the upper left of Fig. 2, the strong, thin low-velocity feature that extends from the middle of the laboratory tunnel to the dark zone in the middle-left of the plot, and the "secondary" fracture that parallels the main shear fracture.

The anisotropy-corrected 1988 travel times produce a good image of the velocity field at FRI. Most of the features in this image correlate well with the geology logs of boreholes 87.001, 87.002, 87.003 and the access and laboratory tunnels. These results show that the imaged velocity field and the actual velocity field can be quite different from that deduced on the basis of the geology. Unexpected zones are imaged that may be more hydrologically important than those determined from borehole and tunnel observations. At FRI it is probable that the low-velocity zones are produced primarily by lamprophyres, tension fissures, and fracture intersections.

Figure 2. A tomographic inversion of the *P*-wave velocity from a four-sided survey of the area shown in Fig. 1. The black indicates 4.9 km/s and the lightest gray is 5.4 km/s. [XBL 903-737]

Figure 3. A tomographic inversion of the *P*-wave velocity from a four-sided survey of the area shown in Fig. 1 after the data were corrected for anisotropy. The black indicates 4.9 km/s and the lightest gray is 5.4 km/s. [XBL 903-738]

HYDROLOGIC ANALYSIS OF FRI EXPERIMENTS

In addition to the seismic tests conducted by LBL, NAGRA conducted constant-pressure hydraulic tests. In a constant-pressure test, the hydraulic head in an isolated interval is kept constant and the transient flow rate is monitored. In very low permeability rocks, like the one at the Grimsel test site, constant pressure is generally easier to achieve than a constant rate. It is also easier to minimize the wellbore-storage effect in a constant-pressure case. Moreover, because the rock near the wellbore is subjected to a constant pressure throughout the test, there is less concern about the permeability changing as a function of time. However, the permeability may change in the location away from the well as the pressure front propagates into the rock.

In these tests it is important to measure early-time data as accurately as possible. Transient data reflect the change of permeability in space as a function of time. In this regard transient data are more descriptive of the rock heterogeneity than steady-state data, which are influenced by the spatial arrangement of heterogeneity in an unknown way. Especially when there is a skin zone near the well, one should be able to resolve it using a set of good transient data (i.e., flow period and shut-in period).

The hydraulic tests were planned on the basis of tomography results. Figure 4 shows the packer locations used in the tests. Each test consisted of pumping water in the zone at a constant pressure and monitoring all the other zones. The objectives of each test were (1) to find hydraulic connection with other zones, (2) to characterize the properties of zones that are hydrologically active, and (3) to try to confirm the existence of zones about which we have only inconclusive evidence. The purpose of the first test was to provide a hydrologic characterization of a feature that is clearly evidenced by the seismic results. The packers for zone A were placed so as to confine the fracture zone as tightly as possible and thereby minimize wellbore storage and isolate the hydrology of the feature. The purpose of the second test was to see if feature B is hydrologically significant. This test would have been conclusive if the result had been positive. A negative result would have meant that the zone is not connected to anyplace being monitored. A positive test result would have been very significant because geophysics was the only tool that could see this feature. The third test was designed to understand the southeastern part of the shear zone. Zone A appeared clearly in the tomogram as extending across the tomographic plane. Zone B appeared in the BOFR87.001 core and in the vicinity of the hole in the tomogram. Likewise, zone C appeared in the BOFR87.002 core and nearby in the tomogram. However, the tomogram didn't indicate that this part of the shear zone is continuous. The test was designed to see if zone B might have hydraulic continuity with some other feature.

Figure 4. Packer locations used in the hydrologic tests. [XBL 903-740]

This article briefly discusses the test in zone A; readers interested in the details of all test results are referred to Wyss (1988). Figure 5 shows the interference pressure-transient data from various observation points in the test. Note that interval 3.1 responds most markedly. The pressure observed at interval 3.1 is significantly lower than that predicted by an analytical solution. The analytical solution assumes that the fracture is infinite, isotropic, and homogeneous. Therefore, conditions must exist where one or more of the above assumptions are not appropriate. The plausible scenarios are listed below:

1. Skin: A low-permeability zone exists around the injection well, i.e., a skin that causes the effective pressure at interval 1.2 to be lower.
2. Anisotropy: The fracture is anisotropic where the maximum permeability direction is oriented vertically.
3. Leakage: There is leakage from the fracture to the adjacent rock, so that the pressure is more dispersed.
4. Boundary Effect: The boundary effect of the laboratory tunnel is keeping the pressure low at interval 3.1.

Figure 5. Interference buildup data for the first test from various observation points. Refer to Fig. 4 for the locations of the observation and injection points. [XBL 903-739]

The tests have confirmed the hydrologic significance of the fracture zone, which was previously identified by the seismic tomography. It appears that the majority of the flow occurred within the relatively thin fracture zone that connects intervals 1.2 and 3.1. A weak but definite hydrologic connection between intervals 1.2 and 2.2 was also observed. The feature that seismic tomography shows extending diagonally from the access tunnel to borehole 87.001 (large dark area in Fig. 2) may explain this hydrologic connection.

Because of the anomalous interference and flow-rate data, four different scenarios that differ from the ideal conditions were examined: (1) skin, (2) anisotropy, (3) leakage, and (4) boundary effects. In reality all four conditions

may coexist. The most significant effect, however, seems to be the leakage into the rock.

SUMMARY

The results of the field work to date indicate that the original premise of using *P*- and *S*-waves for mapping fracture content is valid. The main fracture zone in the FRI zone was detected using *P*-wave tomography. The *S*-wave was attenuated so strongly by the fractures that given a strong enough *S*-wave source, one could assume that *S*-wave data would be even more sensitive to fracture content than *P*-wave data. Other low-velocity zones in the FRI area were also detected, the most significant being the velocity anomalies associated with the stress relief at the tunnel walls. This work is rather conclusive in showing the difference in the extent of the damage zone when a tunnel is excavated with a boring machine and when a tunnel is excavated by drill and blast. Other low-velocity zones also were detected in the FRI zone, most notably the one extending along borehole 87.002 approximately 8 m in from the access tunnel (dark area in right side of Fig. 2). This may be due to small fractures, or as laboratory work suggests, a difference in the rock type. The cores do not show significant fracturing in this zone, but the core velocities are lower for this type of rock than for the rock in the lightest area of Fig. 2.

REFERENCES

- Johnson, L.R., and Peterson, J.E., 1986. Analysis of ultrasonic velocities in Kuroos, Lawrence Berkeley Laboratory Report LBID-1175.
- Pyrak-Nolte, L.J., Myer, L.R. and Cook, N.G.W., 1989. Anisotropy in seismic velocities and amplitudes from multiple parallel fractures. *J. Geophys. Res.*, in press.
- Wyss, E., 1988. Kurzbericht Zu Den Ersten Hydrogeologischen Untersuchungen Im Rahmen Des Versuches FRI. 616, NAGRA, Acoustical Astronomical benefit.

Seismic Imaging for Fracture Characterization at Yucca Mountain, Nevada

E.L. Majer, J.E. Peterson Jr., T.V. McEvilly, and M.A. Tura

The detailed resolution of subsurface properties is crucial to proving the safe disposal and storage of nuclear waste in an underground repository. The scales of interest in the application at Yucca Mountain will range from the near surface to large aquifers at great depth. Structures in the earth are complex. Those at Yucca Mountain include partially saturated volcanic rock, which has traditionally been difficult to image. As opposed to acoustic imaging in the oceans, wave propagation in rock is complicated by the

presence of the shear wave, which is produced in elastic solids but not in fluids. However, this complication also presents an opportunity, in that the images of highest resolution must be constructed using the information contained in the shear and converted waves, along with the acoustic or compressional waves.

The greatest effort by far in imaging the solid earth using seismic techniques has been exerted by the petroleum

industry. Billions of dollars have been spent in developing and applying the method of surface seismic reflection profiling and the more-recently developed techniques for vertical seismic profiling (VSP). The image resolution of these techniques is limited by the amplitude and frequency content of the seismic waves and by the level and complexity of the ambient and signal-generated noise fields. With surface sources, the heterogeneous weathered surface layer, often tens of meters thick, severely limits the high-frequency content and coherence of the input signal. VSP solves this problem in part by placing the receivers beneath the highly attenuating and variable surface layer, so that the signal is not required to pass through the surface layer twice, and also by recording the wavefield with a vertical array in the borehole, so that upgoing and downgoing waves can be identified and separated. Another limitation of the surface-based techniques is the inability to surround the target with sources and receivers, as is done in the case of medical tomographic imaging. Given these fundamental problems, enhanced resolution in surface-reflection work has come mainly from improved signal-processing techniques and data-acquisition methods. This is image enhancement, and it does not address fundamental impediments to finer-scale resolution.

An approach that does address the fundamental imaging limitations is one that incorporates properties of the secondary waves (S) and the converted waves (P to S , S to P) that are generated in the earth. This approach is particularly well suited for VSP applications, where the primary (P), secondary (S), and converted waves can be examined directly. Recent laboratory work (Pyrak-Nolte et al., 1990) and theoretical work (Schoenberg 1980, 1983) explains shear-wave anisotropy in terms of mechanical properties of the fracture discontinuity itself, i.e., a surface of finite stiffness that affects velocity as well as attenuation of a seismic wave of any wavelength. This approach may be particularly well suited to Yucca Mountain, where the anomalies of interest are fractures. In the stiffness theory the lateral extent of a target fracture is still important to seismic resolution, but with adequate fracture stiffness the thickness of the fracture can be much less than the seismic wavelength and still have a detectable frequency-dependent effect on the seismic wave. A large amount of information exists in the properties of the secondary waves, thus offering promise for substantial improvement in the resolution of seismic methods. If successful, the use of seismic methods to image fractures will be particularly well suited to the Yucca Mountain case.

Beyond VSP lies the emerging cross-hole technique. It offers the most promising approach for increasing resolution significantly. The advantages gained by placing the source in a borehole are the additional spatial coverage obtained for image construction as well as the elimination of the attenuating surface layer from the source-receiver path. Figure 1 illustrates the potential application of VSP at Yucca Mountain. Shown in Fig. 2 is one application scale within the repository for cross-hole methods. However, ei-

ther the VSP or the cross-hole seismic method can be used at many scales, assuming the availability of boreholes. For example, Fig. 2 shows planned cross-hole investigations for detailed characterization between the underground excavations.

POTENTIAL MEANS OF RESOLUTION ENHANCEMENT

Tomographic Imaging

With the advancement of medical transmission tomography, applications spread quickly to geophysics, spawning work in seismic-ray transmission tomography. Diffraction tomography in acoustic media and electromagnetic-ray tomography in electrically resistive media have followed. Our experience in VSP, microearthquake studies, and tomographic surveys has led us to conclude that a significant advance in imaging technology must combine new data-manipulation capabilities and tomographic-imaging methods, using new borehole sources and receivers that are being developed for application to toxic-waste problems and resource exploration. Diffraction and transmission-ray tomography for seismic applications each have distinct advantages, and we believe the optimal approach in a particular application will always be a combined use of these techniques. This is an important point to stress; usually only one or the other approach is used, and rarely are both done together.

Transmission Ray Tomography

Transmission tomography uses only the travel times and amplitudes of P - and S -waves, which are inverted for medium slowness and attenuation. The usual method of inversion is some form of iterative algebraic reconstruction algorithm, based on a back-projection method. The section of earth to be imaged is divided into many pixels of constant physical properties. As the waves pass through each of the pixels, amplitudes and velocities are dependent on the pixel properties, and we assume that the contribution of each pixel can be deduced by back-projecting the rays. It follows that a data set consisting of many rays crossing at all angles may be back-projected to yield an estimate of the distribution of velocities needed in each pixel to produce the observed travel times. The attenuation properties of each pixel may be determined in a similar manner, using the amplitude information.

In general, the method of processing is based on the relation between propagation velocity and the total travel time, or between attenuation characteristics and received amplitude. Algebraic reconstruction techniques (ART) developed for this problem work well only in media that have small contrasts. These techniques are iterative in nature, where one equation, i.e., one ray, is analyzed at a time and the pixel values are continually updated. A simple example of an ART algorithm is the basic back-projection

Figure 1. The anticipated geometry and scale of application for VSP work at Yucca Mountain. The cross section is from Scott and Bonk (1984). [XBL 903-741]

Figure 2. An example of the anticipated application for cross-hole seismic work at the repository horizon. [XBL 903-742]

$$x_i^{q+1} = x_i^q + \frac{\Delta y_k^q}{L_k} \quad k = 1, 2, \dots, N, \quad (1)$$

where Δy_k^q is the residual travel time (observed value minus calculated value) for the q th iteration and L_k is the length of ray k .

ART algorithms give exact solutions if the ray coverage is adequate, the ray lengths consistent, the raypaths determined exactly, and the measurements free of errors. This is never the case. Ray coverage is usually 3-sided at best, with the bounds determined by the rectangular area defined by the boreholes and the surface, and with the surface measurements often of much poorer quality than borehole data. This geometry results in incomplete coverage and ray lengths. True raypaths are curved, and they may be determined iteratively along with the pixel values, but a straight raypath is usually assumed. Measurement errors remain a source of inversion uncertainty. Increased resolution will come primarily through the elimination of inversion artifacts, such as smearing, and from the use of more-realistic 3-D raypaths. Smearing is caused by a number of problems, including inadequate angular coverage and sampling, assuming straight rays (or any improper raypaths), and errors in travel time and station location.

Our primary area of work to date has been improving the means by which the seismic energy is approximated by a raypath. We are pursuing a statistical approach for estimating the raypath from a weighted average of several raypaths. For this purpose we are investigating expectation maximization (EM), an iterative method used to compute a maximum likelihood estimate where the observations can be viewed as an incomplete data set. A second area of work in transmission tomography is in algorithm development, using the method of regularization due to Tikhonov and Arsenin (1977). Our initial focus is on developing improved penalty functions to restrain smearing in the image corners and to incorporate realistic structure into the slowness pattern. Regularization chooses the estimate $\hat{S}$, which minimizes a weighted sum of two functions:

$$L(S) + \alpha J(S) ,$$

where $L(S)$ is a likelihood function and $J(S)$ is a penalty function. In the case of seismic tomography, S is a matrix of slowness values, $L(S)$ could be a sum of error terms, and a typical $J(S)$ would be a measure of the difference between adjacent slowness pixels. Various other measures can also be used, or even a combination. For example, S -wave data could be used to constrain the solution.

Diffraction Tomography

To date the applications of full-waveform diffraction tomography are not as extensive as for ray tomography, but the potential developments may prove as valuable as ray tomography. In diffraction tomography less spatial coverage of sources and receivers is needed to obtain resolution equivalent to ray tomography, because reflected and scattered waves are used in forming the image.

To demonstrate the basic principles of full-waveform diffraction tomography, consider a simple two-dimensional case. The background medium is assumed to be a homogeneous acoustic medium, with two-dimensional velocity inhomogeneities (diffractors) embedded in it. An acoustic line pressure source, perpendicular to the plane of propagation, is harmonic in time and is operated at a fixed audio frequency. Under these conditions the acoustic field satisfies the scalar wave equation. A relation between the secondary acoustic field and the velocity to be imaged can be deduced from the integral formulation

$$U^s(\mathbf{r}_r, \mathbf{r}_s) = -\int k_0^2 O(\mathbf{r}) U(\mathbf{r}, \mathbf{r}_s) G(\mathbf{r}_r, \mathbf{r}) dx dz , \quad (2)$$

where $U^s(\mathbf{r}_r, \mathbf{r}_s)$ is the secondary acoustic field at $\mathbf{r}_r$ due to a source at $\mathbf{r}_s$; $U(\mathbf{r}, \mathbf{r}_s)$ is the total acoustic field; and $G(\mathbf{r}_r, \mathbf{r})$ is the two-dimensional Green's function. The object function $O(\mathbf{r})$ is defined as $1 - k^2(\mathbf{r})/k_0^2$. Here, $k(\mathbf{r}) = \omega/c(\mathbf{r})$ and $k_0 = \omega/c_0$ in the acoustic case, with ω denoting angular frequency and $c(\mathbf{r})$ velocity; c_0 is the background velocity and k_0 the background wavenumber, which are used as reference.

To simplify this nonlinear equation, a weak-scattering Born approximation, $U(\mathbf{r}, \mathbf{r}_s) = G(\mathbf{r}, \mathbf{r}_s)$, is em-

ployed to linearize Eq. (2):

$$U^s(\mathbf{r}_r, \mathbf{r}_s) = -\int k_0^2 O(\mathbf{r}) G(\mathbf{r}, \mathbf{r}_s) G(\mathbf{r}_r, \mathbf{r}) dx dz . \quad (3)$$

Obtaining the object function is the solution of the inverse problem, and that is our ultimate aim. It is also important to note that the model medium constructed for this theory may not be the actual medium that we want to image. For example, attenuation has not been included, and the Born approximation utilized may be inappropriate for a high-contrast medium. These problems can be overcome by the development of new data-processing schemes and the improvement of theory if necessary.

Given complete definition in the wavenumber domain, the transform of the object function can be determined exactly, and the inversion yields the unique object function. Because we do not have perfect spatial coverage, it is not possible to obtain complete wavenumber definition. In addition, sources and receivers are discrete in the transform direction, thus producing discrete samples of the object function in the transform domain. Finally, and more importantly, the maximum coverage we can obtain is determined by a circle of radius $2k_0$. This means that as the data frequency content increases, the inversion will be sharper due to the higher wavenumbers in the object function's transform. Given these limitations there is still a distinct advantage over transmission tomography, because in most real applications the access to any rock volume will be limited to no more than three sides. Although the usable frequency band is constrained by spatial aliasing considerations and by the source function, all else being equal, diffraction tomography still produces sharper images given the same spatial coverage. Moreover, inversions at different frequencies could be done and averaged in order to increase coverage in the transform domain.

A considerable amount of developmental and experimental work is necessary to modify and tune the basic (2-D acoustic) diffraction tomography method so that it works well in practical 3-D heterogeneous field situations. The extension of the basic method to the case where the source and receiver are points rather than lines (3-D versus 2-D) has just been carried out. The extension to the elastic case will be more difficult and is being addressed. One approach is to process the data in such a way as to achieve a partial separation between P - and S -waves and then apply the acoustic method to the separated data sets. The case of a strongly inhomogeneous background will also require work. In principle, there is no problem calculating the Green's functions for such a medium, but the computational time can increase dramatically and the associated expense can make the method impractical for routine application. Other approaches to this particular problem are also being investigated. The algorithms must now be tested on real data sets to determine their applicability and the improvements necessary for usefulness. Another approach is to use the available migration software to migrate the data, as is commonly done with surface reflection data, but a large amount of programming is necessary to convert these

programs for cross-well use. A recent method of initially doing a ray tomography inversion to obtain the slow variation in the medium followed by a diffraction tomography inversion to improve the resolution is being considered.

SUMMARY

The ultimate goal of this project is to provide real-time capability for high-resolution tomographic imaging. Our experience has shown us that successful seismic imaging is a result of trial and error and application of proper techniques. If it were possible to make this a real-time experience, then it may be possible to realize an order of magnitude improvement in resolution. Our approach is an integrated system that is intended to be an extension of our laboratory computational and theoretical capabilities operating in the environment of eventual application. The effort is a balanced program between theoretical and mathematical improvements in the fundamental processing algorithms and the implementation on an expert-systems-based field computer. We believe that this is the most

cost-effective and realistic approach for applying seismic imaging techniques at Yucca Mountain.

REFERENCES

- Pyrak-Nolte, L.J., Myer, L.R., and Cook, N.G.W., 1990. Transmission of seismic waves across single natural fractures. *J. Geophys. Res.*, in press (LB1-26616).
- Schoenberg, M., 1980. Elastic wave behavior across linear slip interfaces. *J. Acoust. Soc. Am.*, v. 68, no. 5, p. 1516-1521.
- Schoenberg, M., 1983. Reflection of elastic waves from periodically stratified media with interfacial slip. *Geophys. Prospect.*, v. 31, p. 265-292.
- Scott, R.B., and Bonk, J., 1984. Preliminary geologic map of Yucca Mountain, Nye County, Nevada, with geologic sections. U.S. Geol. Survey Open-File Report 84-494.
- Tikhonov, A., and Arsenin, V., 1977. *Solutions of Ill-Posed Problems*. Wiley, New York.

Anisotropic Inversion of VSP Travel-Time Data, with an Example from The Geysers

I. Pšenčík, J. Jech,* V. Cervený,* D. Gajewski,† T.M. Daley, T.V. McEvilly, and E.L. Majer*

Seismic-velocity anisotropy has been found in many geological regimes (e.g., Robertson and Corrigan, 1983; Li et al., 1988; Daley et al., 1988). In particular, zones of fracturing are often modeled as equivalent media with anisotropic propagation of seismic waves (Crampin, 1978; Hudson, 1981). Often, this effective anisotropy cannot be overlooked when interpreting data, especially if shear waves are utilized. The interpretation of data in fractured material, such as the reservoir rock in The Geysers geothermal field, would be improved by applying anisotropic inversion. However, the solution of an inverse problem is greatly complicated by assuming anisotropic media. Instead of two elastic parameters, λ and μ , for isotropic media, an anisotropic material has, in general, 21 elastic parameters, which are necessary for calculating seismic-wave velocities and directions of propagation. The study of fractured material, such as that present in The Geysers geothermal field, has recently focused on anisotropic effects. The need for inversion of data recorded in known anisotropic material

and recovery of the elastic constants controlling wave propagation is the motivation for the work summarized here.

INVERSION THEORY

In recent years different approaches have been attempted for anisotropic inversion (Crampin et al., 1980; Hirahara and Ishikawa, 1984); mostly these attempts use only P -waves and, as in our work, only travel times. Here the travel times of both P - and S -waves are used in a first-order perturbation method based on ray theory, which is valid for weakly anisotropic materials (Jech and Pšenčík, 1989). The perturbation of the total travel time for each wave type is obtained from perturbations of the elastic parameters along the raypath in the unperturbed medium. The unperturbed medium, which is the starting model for the inversion, can be isotropic or anisotropic with hexagonal symmetry, since these are the media in which the raypath can be computed. In addition, the starting model can be homogeneous or layered.

Calculating the travel-time perturbations from elastic parameters involves two separate cases, degenerate and nondegenerate. The degenerate case is when two quasi-shear waves have the same phase velocity (this is always true in isotropic material), and the nondegenerate case is when the two waves differ in phase velocity.

*Geophysical Institute, Czechoslovak Academy of Sciences, Prague, Czechoslovakia.

†Geophysical Institute, Karlsruhe University, Federal Republic of Germany.

Looking at the forward problem of calculating travel time from perturbations of elastic parameters, we find that for the nondegenerate case the correction Δt to the travel time t for a perturbation Δa_{ijkl} in the density-normalized elastic parameter a_{ijk} is given by

$$\Delta t = -\frac{1}{2} \int_0^t \Delta a_{ijkl} p_i p_l g_j^{(m)} g_k^{(m)} dt, \quad (1)$$

where p_i is the slowness vector and $g_j^{(m)}$ is the eigenvector of the matrix $a_{ijkl} p_i p_l$ (Jech and Pšenčík, 1989). The travel time is integrated along some parametrization of the ray-path. (Note that the Einstein summation convention is used in these equations.) For the degenerate case we define the quantity $B_{mn} = \Delta a_{ijkl} p_i p_l g_j^{(m)} g_k^{(n)}$; the perturbation in travel time is

$$\Delta t_I = -\frac{1}{4} \int_0^t \left[(B_{11} + B_{22}) + /- [(B_{11} - B_{22})^2 + 4 B_{12}^2]^{1/2} \right] dt \quad I = 1, 2. \quad (2)$$

The inversion, based on the forward problem, seeks perturbations of the elastic parameters, along with the angles of rotation that define the axis of symmetry of the anisotropic material, which minimize the quantity ϕ in the least-squares sense for

$$\phi = \sum_{i=1}^N (\Delta t_{io} - \Delta t_{ip})^2. \quad (3)$$

The implementation of the inversion used here allows for the solution to be constrained to be a homogenous or layered model. The elastic parameters can vary independently with depth, and any anisotropy symmetry can be considered. For a model with hexagonal anisotropy, the results of the inversion are the elastic constants a_{11} , a_{33} , a_{55} , a_{66} , a_{13} , and the orientation angle for the anisotropy axis of symmetry b .

The inversion was tested with a numerically generated data set consisting of travel-time measurements for the qP , qS_1 , and qS_2 arrivals. These data were generated from an anisotropic ray-tracing code (Gajewski and Pšenčík, 1987) derived from a model used in Shearer and Chapman (1989), which is actually more anisotropic than the assumptions of the inversion allow. Figures 1 and 2 show the results of the inversion for this theoretical model. The solution is not exact, but the resulting anisotropic solution does approach the velocities of the original model. Although other numerical examples with weak anisotropy had exactly correct solutions, this example shows that even when the initial assumption of weak anisotropy is violated, the inversion will approach the correct solution. To find a better solution to the Shearer and Chapman model, as well as other, more-anisotropic models, an iterative inversion scheme would be needed. This one-step inversion, using a first-order linearization, remains useful for weakly anisotropic materials.

Figure 1. Inversion results for theoretical model. Each graph is a plot of velocity versus depth for each of the three wave types — qP , qS_1 , and qS_2 , from top to bottom. The large dashed line is the starting model, the small dashed line is the inversion result, and the solid line is the exact solution. Each plot has the velocity at two azimuths, parallel and perpendicular to the axis of symmetry of the anisotropy. [XBL 903-743]

INVERSION OF GEYSERS VSP

A vertical seismic profile (VSP) recorded within The Geysers geothermal area provided a useful test of the inversion on field data. The 9-component VSP utilizing P - and S -wave vibrator sources and 3-component receivers was recorded such that the shear sources were parallel and perpendicular to the dominant direction of fracturing in the reservoir rock (as best determined from other geological and geophysical information). The source offset was 518 m, with receiver depths from 305 to 1555 m. Evidence of anisotropy was clearly seen as a travel-time difference between the orthogonally oriented shear sources (Majer et al., 1988). In fact, the observed travel-time difference indicated that the anisotropy may be stronger than allowed by the inversion assumptions, but we were hopeful that a solution would at least approach the correct elastic constants.

Attempts were made to invert the travel-time data using various starting models, including the following:

1. A homogeneous medium with hexagonal anisotropy and a horizontal axis of symmetry.
2. A homogeneous isotropic material.

Figure 2. Inversion result for theoretical model. Phase velocity for each wave type is plotted as a function of azimuth at one depth (700 m). E_{ij} are the exact elastic constants, and P_{ij} are the perturbed elastic constants. E_{F1} is the orientation angle, and V_p and V_s are the velocities of the starting model. The dashed line is the starting model. The exact and inverted solutions are difficult to see at this scale, but the inverted velocity is slower for qP and they are nearly identical for qS_1 and qS_2 . [XBL 903-744]

3. A 100-m layer over a half-space, with the resulting model being an isotropic layer over an anisotropic half-space with a constant vertical gradient of elastic parameters (different gradients for each parameter).

All these models used an axis of symmetry for the anisotropic material that approximately aligned with the best-known orientation for The Geysers. The best solution matches the travel times closely for all three wave types. Other solutions also matched the travel times, but they had unrealistic values for some of the elastic parameters.

A similar set of models was attempted in which anisotropy was allowed to have an axis of symmetry approximately perpendicular to the best-known orientation. Unfortunately, the best results from this test were nearly as good as the test with the "correct" orientation of the axis. Further numerical examples demonstrated that the field data from The Geysers were not sufficient for a unique inversion. More source points would be necessary for a better-constrained solution. However, data from The Geysers still give a "best" solution when constraints are placed on the orientation of the axis of symmetry. This solution is shown in Figs. 3 and 4; it used starting model number 3 above, and the inversion produced an anisotropic half-space, with the axis of symmetry having an orientation angle of 16.3° and velocities in the isotropic layer of 1.05 km/s for P and 0.7 km/s for S .

Figure 3. Inversion result for Geysers data at 305 m. A_{ij} are the inverted elastic parameters for the anisotropic half-space. The section is perpendicular to the VSP, seen in the direction from the source toward the receiver. The axis of symmetry of the resulting hexagonal medium is situated in a plane perpendicular to the profile. [XBL 903-745]

Figure 4. Inversion result for Geysers data at 500 m. A_{ij} are the inverted elastic parameters for the anisotropic half-space. The section is perpendicular to the VSP, seen in the direction from the source toward the receiver. The axis of symmetry of the resulting hexagonal medium is situated in a plane perpendicular to the profile. [XBL 903-746]

DISCUSSION

The resulting models were quite diverse; in fact, some did not correspond to the local geology, and others gave elastic constants that did not correspond with the physics of wave propagation in cracked media (i.e., these elastic constants either could not come from aligned cracks or did not correspond to physically realizable material). Despite these problems, many of these models give an excellent fit to the observed travel times. This demonstrates that although the travel-time data from The Geysers VSP clearly shows the anisotropy, it is insufficient for anisotropic inversion. One drawback is the narrow range of angles at which the rays for The Geysers VSP cross the investigated region. The numerical experiments with the Shearer and Chapman model show that for the 100- to 700-m depths recorded, source offsets of 250, 500, and 750 m would provide a consistently invertible data set (Fig. 5). A more-thorough VSP at The Geysers would have provided the opportunity for a unique anisotropic inversion.

Figure 5. Geometry of VSP source locations that should provide a unique solution for an anisotropic inversion of Geysers data. The data set used for inversion had only the 500-m offset. The rays are drawn for the P -wave using for the Shearer and Chapman model. [XBL 903-747]

REFERENCES

- Crampin, S., 1978. Seismic-wave propagation through a cracked solid: Polarization as a possible dilatancy diagnostic. *Geophys. J. R. Astron. Soc.*, v. 53, p. 467–496.
- Crampin, S., McGonigle, R., and Bamford, D., 1980. Estimating crack parameters from observations of P -wave velocity anisotropy. *Geophysics*, v. 45, no. 3, p. 345.
- Daley, T.M., McEvilly, T.V., and Majer, E.L., 1988. Analysis of P - and S -wave VSP data from the Salton Sea geothermal field. *J. Geophys. Res.*, v. 93, no. B11, p. 13025–13036.
- Gajewski, D., and Pšencik, I., 1987. Computation of high-frequency seismic wavefields in 3-D laterally inhomogeneous anisotropic media. *Geophys. J. R. Astron. Soc.*, v. 91, p. 383–411.
- Hirahara, K., and Ishikawa, Y., 1984. Travel-time inversion for three-dimensional P -wave velocity anisotropy. *J. Phys. Earth.*, v. 32.
- Hudson, J.A., 1981. Wave speeds and attenuation of elastic waves in material containing cracks. *Geophys. J. R. Astron. Soc.*, v. 64, p. 133–150.
- Jech, J., and Pšencik, I., 1989. First order perturbation method for anisotropic media. *Geophys. J. Int.*, p. 310.
- Li, Y.-G., Leary, P.C., and Henyey, T.L., 1988. Stress orientation inferred from shear wave splitting in basement rock at Cajon Pass. *Geophys. Res. Lett.*, v. 15, no. 9, p. 997–1000.
- Majer, E.L., McEvilly, T.V., Eastwood, F., and Myer, L., 1988. Fracture detection using P - and S -wave VSPs at The Geysers geothermal field. *Geophysics*, v. 53, no. 1, p. 76–84.
- Robertson, J.D., and Corrigan, D., 1983. Radiation patterns of a shear-wave vibrator in near-surface shale. *Geophysics*, v. 48, no. 1, p. 19.
- Oristaglio, M.L., 1985. A guide to the current uses of vertical seismic profiles. *Geophysics*, v. 50, no. 12, p. 2473.
- Shearer, P.M., and Chapman, C.H., 1989. Ray tracing in azimuthally anisotropic media — I. Results for models of aligned cracks in the upper crust. *Geophys. J. R. Astron. Soc.*, v. 96.

Modeling Elastic Waves in Fractured Rock with the Kirchhoff Method

K.T. Nihei, L.R. Johnson, and N.G.W. Cook

The interaction of an elastic wave with a fracture has been the subject of many experimental and theoretical studies. The insight gained from these studies may aid in the development of seismic methods for locating and characterizing fractures. This article presents a numerical approach for modeling elastic-wave transmission and reflection from single and multiple fractures. The approach, which is based on the elastic Kirchhoff method, provides a high-frequency solution for reflected and transmitted waves from fractures with arbitrary shapes and stiffness distributions.

THEORY

Integral Representation Theorem

The integral representation theorem for an elastic medium specifies the manner in which the displacement at an observation point is constructed from a surface integral over surface traction and displacement (Aki and Richards, 1980)

$$\mathbf{u}(\mathbf{r}, \omega) = \int_S [\mathbf{G}(\mathbf{r} | \mathbf{r}', \omega) - \hat{n} \cdot \boldsymbol{\Sigma}(\mathbf{r} | \mathbf{r}', \omega) \cdot \mathbf{u}(\mathbf{r}', \omega)] dS, \quad (1)$$

where $\mathbf{u}$ is the displacement, $\boldsymbol{\tau}$ is the stress, $\mathbf{G}$ is the Green's function, $\boldsymbol{\Sigma}$ is the third-rank Green's stress tensor, ω is the frequency, dS is an element of the surface S , $\hat{n}$ is the unit normal to dS , and $\mathbf{r}$ and $\mathbf{r}'$ are the position vectors shown in Fig. 1.

Numerical evaluation of Eq. (1) for the displacement at a point in the medium requires a knowledge of the terms appearing in the integral. When the medium is homogeneous and isotropic, the free-space expressions for $\mathbf{G}$ and $\boldsymbol{\Sigma}$ can be used. The displacement and stress on S can be obtained by the boundary integral equation method (BIEM), which consists of placing the receiver on S , discretizing S into surface elements ΔS , applying the boundary conditions on displacement and traction across S , and solving the resulting system of linear equations. Once the values of stress and displacement are known along S for a particular source, the displacement can be evaluated for a receiver located anywhere in the medium.

Kirchhoff Approximation

A problem with the BIEM approach is that for high-frequency, three-dimensional elastic problems typically encountered in fracture studies, it requires large matrix inversions that are computationally intensive. A more-feasible approach is to approximate the surface displacements and tractions using ray theory and plane-wave reflection and transmission coefficients. This approximation, which is

Figure 1. Problem geometry used in the numerical evaluation of the integral representation theorem. [XBL 903-748]

called the Kirchhoff or tangent-plane approximation, is valid when the incident wave is of sufficiently high frequency (i.e., the wavelength is much smaller than the correlation distance of any variation in material properties) that locally its amplitude decay is described by geometric ray theory and plane-wave reflection and transmission coefficients (Scott, 1985). The Kirchhoff approximation has the following implications: (1) every point on the surface of material discontinuity reflects the incident wave as though there were an infinite plane tangent to the surface at that point, and (2) the values of displacement and traction at a point are independent of the boundary values at other points. This independence of displacement and traction between neighboring elements suggests that interface waves and multiply scattered waves will not be included in the Kirchhoff solution.

The Kirchhoff method has several advantages over geometric ray theory: it includes diffractions from surface irregularities and does not break down when the receiver is located on a caustic. Application of the Kirchhoff approximation to the integral representation theorem given in Eq. (1) results in the following integral for elastic-wave transmission across a three-dimensional surface.

$$\begin{aligned}
u_n(\mathbf{r}, \omega) = \int_S \{ & T^{pp} [\hat{n}_l \tau_{lm}^p G_{mn}^\alpha - u_m^p(\hat{n}_l \Sigma_{lmn}^\alpha)] G_{mn}^\beta \\
& - u_m^{sv}(\hat{n}_l \Sigma_{lmn}^\beta) + T^{ps} [\hat{n}_l \tau_{lm}^p G_{mn}^\beta - u_m^p(\hat{n}_l \Sigma_{lmn}^\beta)] G_{mn}^\alpha \\
& - u_m^{sv}(\hat{n}_l \Sigma_{lmn}^\alpha) + T^{sh} [\hat{n}_l \tau_{lm}^{sh} G_{mn}^\beta - u_m^{sh}(\hat{n}_l \Sigma_{lmn}^\beta)] \} dS.
\end{aligned} \quad (2)$$

Equation (2) is the Kirchhoff integral. It is obtained by separating Eq. (1) into terms propagating as P - P , SV - SV , P - SV , SV - P , and SH - SH waves. The superscripts α and β denote the parts of $\mathbf{G}$ and Σ associated with the P - and S -wave velocities. T^{pp} and T^{ps} are the plane-wave transmission coefficients for an incident P -wave, T^{ss} and T^{sp} are the transmission coefficients for an incident SV -wave, and T^{sh} is the transmission coefficient for an incident SH -wave. The reflected wave field can be computed from the same equation by replacing the transmission coefficients with reflection coefficients.

The displacement at the receiver location is obtained by substituting expressions for the displacement and stress obtained from geometric ray theory, the free-space Green's displacement dyadic and Green's stress tensor, and the plane-wave transmission coefficients into Eq. (2) and evaluating the integral numerically. This procedure can be viewed as a four-step process: (1) trace ray from source to surface, (2) calculate the surface tractions assuming a plane wave, (3) propagate the wave field across the surface using plane-wave transmission and reflection coefficients, and (4) propagate the wave field from surface to receiver using the free-space Green's function.

Displacement-Discontinuity Fracture Model

The numerical evaluation of Eq. (2) requires the specification of the plane-wave transmission (or reflection) coefficients. Shoenberg (1980) presents expressions for the plane-wave reflection and transmission coefficients of a nonwelded interface. Recently, Pyrak (1988) has verified experimentally the appropriateness of this model for describing the transmission of ultrasonic waves across natural fractures in crystalline rock.

In Shoenberg's model for wave propagation across a nonwelded interface, the boundary conditions are (1) continuity of stress and (2) discontinuity of displacement proportional to the stress divided by the stiffness of the interface:

$$\tau_{lm}^1 = \tau_{lm}^2, \quad (3)$$

$$u_l^1 - u_l^2, \quad (4)$$

where $\mathbf{K}$ is the specific stiffness of the nonwelded interface and the superscripts 1 and 2 refer to the material above and below the interface, respectively.

Plane-wave reflection and transmission coefficients are calculated by substituting the expressions for the plane-wave displacement into the isotropic stress tensor, applying the boundary conditions given by Eqs. (3) and (4), and solving the resulting systems of linear equations.

The plane-wave reflection and transmission coefficients obtained from the displacement-discontinuity model are frequency dependent. Thus the effect of a nonwelded interface on an incident elastic wave is to attenuate the wave and filter out its high-frequency content by an amount that depends on stiffness of the interface. For these expressions and details of the displacement-discontinuity model, the reader is referred to Shoenberg (1980) and Pyrak (1988).

NUMERICAL EXAMPLE: FRACTURE WITH RANDOM-STIFFNESS DISTRIBUTION

The numerical example presented here is for a point source and a planar fracture with a stiffness that varies randomly along the surface of a two-dimensional fracture (i.e., 2.5-D problem geometry). For the Kirchhoff method to be applicable, the correlation length of the stiffness variations along the fracture surface must be large compared with the seismic wavelength and the amplitude of the stiffness variations should be small.

The fracture surface is first discretized and assigned a random-stiffness value taken from a uniform distribution. The FFT (Fast Fourier Transform) of this random-stiffness surface is filtered with a Gaussian correlation function. The inverse FFT produces a random-stiffness surface with a correlation length a .

Random-stiffness surfaces for two correlation lengths, $a = 0.5$ m and $a = 0.2$ m, and for a surface with a constant stiffness ($a = \infty$) are displayed in Fig. 2. The random-stiffness surfaces range in value from 1×10^{10} Pa/m to 1×10^{11} Pa/m. The constant-stiffness surface has a stiffness of 5×10^{10} Pa/m. The Kirchhoff transmission synthetics generated by the FORTRAN code KIRCH25D (Nihei, 1989) for $\rho = 2600$ kg/m³, $\alpha = 5200$ m/s, and $\beta = 4000$ m/s are shown in Fig. 3. The effects of the random-stiffness surfaces are to attenuate the transmitted wave and remove a portion of its high-frequency content. In addition, the random-stiffness surfaces excite scattered waves that appear on the y component of displacement. These scattered waves are not present for the constant-stiffness surface. Because the peak amplitude of the y component is over 150 times smaller than that of the z component (y - and z -component traces are not scaled to each other), the scattered waves are not visible on the z component, since they are many times smaller than the direct P - P wave. The amplitudes of the scattered waves increase as the correlation length decreases. The latest arrival appearing on the z component is the S - S diffraction from the edges of the fracture.

Figure 2. Random stiffness distributions along a 2.5D surface for Gaussian correlation lengths of $a = 0.5$ m and $a = 0.2$ m and stiffness values ranging from 1×10^{10} Pa/m to 1×10^{11} Pa/m. [XBL 903-749]

DISCUSSION

The Kirchhoff method is an asymptotic method that can be used to model high-frequency wave propagation across three-dimensional fractures. The method includes diffracted waves from the edges of fractures and scattered waves from irregularities on the fracture surface (e.g., variations in topography and stiffness). The numerical example presented for a single fracture with a random-stiffness distribution demonstrates the utility of the method for modeling diffracted and scattered waves. The method can also be used to model elastic-wave reflection and transmission from multiple fractures, provided the fracture spacing is larger than the seismic wavelength. This is accomplished by performing additional surface integrations over each additional fracture. The next phase of this work will consist of the validation the Kirchhoff method approach for modeling elastic-wave propagation across fractures with field observations.

Figure 3. Kirchhoff transmission synthetic seismograms for the random stiffness models shown in Fig. 2. [XBL 903-750]

REFERENCES

- Aki, K., and Richards, P.G., 1980. Quantitative Seismology (Vol. I). W.H. Freeman and Co., New York.
- Nihei, K.T., 1989. Modeling elastic waves in fractured rock with the Kirchhoff method (M.S. thesis). University of California at Berkeley.
- Pyrak, L.J., 1988. Seismic visibility of fractures (Ph.D. thesis). University of California at Berkeley.
- Scott, P., 1985. Application of the Kirchhoff-Helmholtz integral to problems in body wave seismology (Ph.D. thesis). California Institute of Technology.
- Shoenberg, M., 1980. Elastic wave behavior across linear slip interfaces. *J. Acoust. Soc. Am.*, v. 68, p. 1516-1521.

Compaction of Porous Rock under an Indenter

R. Suárez-Rivera, N.G.W. Cook, G. Cooper, and Z. Zheng

The present goal to reach yet deeper regions of potential hydrocarbon entrapment in the earth's crust and the need to accomplish such objectives at competitive costs has provoked a review of all aspects of the drilling operation to maximize its efficiency. This article summarizes our work on rock compaction. Compaction is one of the main sources of energy losses during the drilling of porous rocks, for energy otherwise available for brittle fracture propagation is used for grain crushing and pore collapse. In addition, compaction provides the means to accommodate the material displaced by the indenter within the rock matrix and consequently suppresses the production of chips. Using results from experiments on porous rocks, it will be shown that the size of the compaction zone is a function of the material porosity and its resistance to compaction, that its growth is controlled not only by the penetration of the indenter but also by the amount of the total deformation that is accommodated elastically, and that the shape of the indenter influences only the initial stages of the indentation, after which the process is controlled solely by the size and shape of the compaction zone itself. The last effect was pointed out earlier by Yoffe (1982) and confirmed in our observations.

EXPERIMENTAL OBSERVATIONS

We present results obtained on Indiana limestone and Berea sandstone using cylindrical indenters with hemispherical ends. The characteristic properties of these rocks are given in Table 1. The specimens were confined laterally to simulate their condition in an infinite medium. Wood's metal porosimetry was used to preserve the fractures and compaction patterns as they exist under load. By solidifying the Wood's metal at the end of the experiment, while maintaining the final load constant, we were able to exclude the fractures that originate during the unloading stage of the indentation. Our observations thus correspond solely to the failure that developed during the loading stage. After testing, we sectioned the specimens and observed the region of compaction with the aid of an optical microscope.

Table 1. Rock properties.

Specimen	σ_c (MPa)	ϕ (%)	E (GPa)	ν
Indiana limestone	69	10.3	27	0.16
Berea sandstone	71.7	21	19.3	0.38
Refractory brick	—	65	—	—

We also performed experiments using weak, highly porous refractory brick specimens with axisymmetrical indenters of equal cross-sectional area but having conical, spherical, or flat ends. These specimens were unconfined and saturated in a low-viscosity, long-setting-time epoxy resin, which was allowed to set once the indentation had taken place. Sectioning of the samples, after the resin had cured, allowed us to observe the compacted zones and to compare their growth, size, and shape. Porous refractory brick specimens were used because their failure came about almost exclusively by compaction and consequently allowed us to visualize the development of the compacted zone isolated from influences of other modes of failure. The porosity of the refractory bricks is given in Table 1; no information was available on elastic properties.

Figures 1 and 2 show the compacted zones for Indiana limestone and Berea sandstone specimens under spherical indenters. The region of compaction in both cases is seen to be very clearly differentiated from the surrounding material. Within the compaction zone in the limestone specimen, the pore structure is no longer recognizable and instead a homogeneous region of compacted material exists; individual calcite grains most probably were subjected to large amounts of dislocation; future scanning electron microscope observations should help to validate this supposition. Along its boundaries, the material under compaction contains a very high density of tensile cracks; split and severely broken grains are observed in this region. This process can be seen in Fig. 3, which depicts a detail of the compaction zone of a limestone specimen at its upper boundary, in contact with the indenter cavity. From this image it can be inferred that a further increase in loading would extend the area of contact, increase the density of cracks in the compacting material until the grains are fully crushed, and at the same time displace the zone of high

Figure 1. Compacted zone in Indiana limestone under a 12.7-mm hemispherical indenter. [XBB 890-10755]

Figure 2. Compacted zone in Berea sandstone under a 10-m hemispherical indenter. [XBB 890-10758]

crack density to the immediately adjacent region. The compaction zone in the sandstone specimen is formed by extensively broken quartz grains, which gradually increase in size away from the area of contact, with debris from the broken grains filling the pore spaces. Its boundary is more abrupt than for the limestone specimen, and no zone of high density of microcracks is observed. For both specimens the compaction zone along the free surface falls within the perimeter of the contact area. From this boundary they are seen to extend downwards, with an initial dip angle of 55–60 degrees for limestone and 75–80 degrees for sandstone, enclosing the indenter surface completely, like bubbles hanging from the area of contact. At certain locations around the compaction zone, macroscopic tensile cracks are observed, and in the limestone specimens they

Figure 3. Detail of the region of compaction in Indiana limestone bounded by the upper free surface and the indenter cavity. [XBB 890-10756]

seem to originate from the coalescing of microcracks. Their origin is no doubt a result of the extensile stresses produced by the expansion of the compacted zone. The macroscopic cracks propagate into the elastic region in a direction that must coincide with the direction of the local maximum principal stress; thus, according to their location, they propagate parallel to the free surface if they originate in the region laterally adjacent to the indenter or down at a certain angle with the vertical stress if they originate in the region below the indenter. This type of macroscopic crack is seen at the bottom of Fig. 2. The load-displacement curves that result from the indentation represent the combination of failure processes, such as elastic deformation, localized rock compaction, localized dilatation, and extensile cracking, all taking place concurrently in the rock. Because the load-displacement curves for both specimens were surprisingly linear and because different forms of macroscopic failures in several specimens of Indiana limestone resulted in equally linear load-displacement curves, we are led to believe that the linear character of these curves is a result of the compaction process, which overshadows the other modes of deformation.

Results of the indentation experiments performed in the porous brick material are shown in Figs. 4 to 6. The region of compaction under each indenter is very clear and distinct. The pore structure within this region has disappeared, and instead a uniformly compacted region exists; however, near its external boundary the porosity increases gradually back to its original value. The compacting region is devoid of microcracks and devoid of nearby macrocracks. (The macroscopic cracks seen around and within the compaction zone formed after the indentation as a result of contraction of the epoxy resin during curing.) Their absence is an indication of the weakness of the elastic field outside the compacted region. In neither case did the material adjacent to the vertical surfaces of the indenter suffer any compaction. The load-displacement curves for all three indenters were initially different from each other. However, once the compaction zone was fully developed

Figure 4. Indentation in weak, highly porous refractory brick using a hemispherical indenter. [XBB 890-10917]

Figure 5. Indentation in weak, highly porous refractory brick using a flat indenter. [XBB 890-10916]

below the indenters, the curves became almost identical; at this point, the shape of the indenter was no longer relevant to the indentation process, which was in fact totally controlled by the size of the compaction zone.

CONCLUSIONS

Indentation of porous materials differs fundamentally from that of nonporous materials in that the most important

Figure 6. Indentation in weak, highly porous refractory brick using a conical indenter. [XBB 890-10918]

mode of failure beneath an indenter is one of compaction due to pore collapse. Within the compacted zone the stresses increase up to a point when an irreducible porosity is reached, after which the material no longer compacts. Thereafter, it moves as a unit ahead of the indenter providing the means to transfer the load from the indenter face to the uncompacted material. In this way, the effective area of contact is the boundary between the compacted material and the uncompacted rock. At that point the stress field that is generated, as well as the new modes of failure that originate, is independent of the geometry differences between indenters.

Macroscopic fractures originating near the periphery of the compacted zone may develop and propagate into the elastic region of the porous material, provided that they are located in regions of low confinement where the dilation process overcomes compaction.

During oil-well drilling of porous rocks, brittle fracture occurs once compaction and, to a certain extent, plastic flow have taken place. In addition to the parameters related to the loading conditions, the relative contribution of these combined effects to the overall failure of the rock depends on rock characteristics such as compaction strength, itself a function of the pore structure and the strength of the grains, and the deformation properties of the matrix, which vary with saturation, permeability, and the characteristics of the saturating fluid. The energy that is absorbed within the compacted zone is energy that has to be provided in excess of the amount required to create brittle failure of the rock, rendering the efficiency of the process of drilling by indentation a function of the compactability of the rock.

In our experiments, chip production was not observed. It is possible, however, that chip production nevertheless occurs during the unloading stage of the indentation or occurs as a result of the interacting effects caused by "indexing" of the consecutive indentations by the roller bit. Such effects were not investigated during our experiments.

REFERENCE

- Yoffe, E.H., 1982. Elastic stress fields caused by indenting brittle materials. *Phil. Mag. A.*, v. 46, no. 4, p. 617-628.

The Effects of Tortuosity on Flow through a Natural Fracture

A.M. Cook, L.R. Myer, N.G.W. Cook, and F.M. Doyle

Fractures can play a dominant role in the movement of fluid through rock media. As a result, much work has been done, both theoretical and experimental, on laminar fluid flow through open fractures consisting of parallel plates of varying degrees of surface roughness. In many cases the behavior of the fluid can be described using the expression developed by Lomize (1951) and used by others such as Witherspoon et al. (1980):

$$Q = \frac{1}{f} \frac{b^3}{12\mu} \frac{dp}{dx} \quad (1)$$

where Q is the flow rate per unit width of fracture normal to the flow direction, x ; b is the aperture between the plates; μ is the viscosity of the fluid; dp/dx is the pressure gradient in the direction of flow; and $1/f$ is an empirical factor that accounts for the effects of surface roughness.

This equation has become generally known as the "cubic law equation" because flow rate is proportional to the cube of the aperture. Although the relation of fracture aperture to flow is obvious, tortuosity of the flow paths in a fracture may also have a significant effect on flow.

LABORATORY PROCEDURES

The siltstone sample was a rectangular parallelepiped about 25 mm thick whose top surface measured 25 mm in width by 75 mm in length. A single natural fracture lay in a plane at mid-height approximately parallel to the top surface. Each half of the sample was embedded into a steel casing using a low-melting-temperature metal alloy called Cerrosafe®. The casings were machined in such a way that the separation between the fracture surfaces of the sample could be controlled by shims over a range of apertures, from conditions where the two surfaces of the fracture were mechanically held apart by shims up to 0.25 mm thick to conditions where the two surfaces were in contact and under moderate stress up to 11 MPa. Except for the inlet and outlet ports, the sides and ends of the fracture were sealed to prevent leakage. Measurements over a range of heads indicated that laminar flow had been maintained.

By "aperture" is meant fracture displacement relative to a reference state, which was taken as the highest stress level used in the experiments. Linear variable differential transformers (LVDT's) were used to measure fracture displacement between zero load on the fracture and the highest stress level. The LVDT measurements were corrected for effects of sample cycling and intact rock deformation. For the tests in which the fracture was held apart by shims, a micrometer was used to measure the distance between the surfaces of the steel casings. These measurements were used to determine the fracture displacement relative to the zero load condition. It should be noted that, according to this convention, shim thickness and

aperture are not synonymous; rather, the aperture used in the "cubic law" calculations was equal to the shim thickness plus the fracture displacement, which resulted from loading the fracture up to 11 MPa.

EXPERIMENTAL RESULTS

Experimental results are shown in Fig. 1; the broken line represents the flow calculated for each aperture based on the cubic law, assuming f in Eq. (1) equals 1. In plotting the experimental data it was assumed that the aperture at the highest stress level was 5 μm . The figure shows that the flow rate was about proportional to the cube of the aperture when the fracture surfaces were not in contact, though the curve for these data is displaced above the cubic law curve by a nearly constant amount. A very good fit was obtained at the large apertures by assuming (unrealistically, since flow was nonzero) a zero aperture at the highest stress level. Even so the experimental data points were slower by 5–20% than those predicted by the cubic law.

At the lower apertures, where the fracture surfaces were in contact and under moderate stress, the flow rate was not proportional to the cube of the aperture, but instead to some higher and variable power. In other words, the experimental flow rates decreased at a higher power than those predicted from the cubic law relationship. At higher stresses flow rate approached a constant value, which did not change even with further decreases in aperture. This irreducibility of flow (Raven and Gale, 1985; Pyrak-Nolte et al., 1987) indicates that a residual aperture exists even at very high stresses. Although the values of fracture aperture depend upon the value assumed for the residual aperture, the shape of the curve formed by the experimental data points does not. Thus the generally observed discrepancies

Figure 1. Comparison of experimental data with those predicted assuming smooth parallel plates. Residual aperture is assumed to be 5.0 μm . [XBL 901-107]

between the experimental data and those predicted from the cubic law relationship will not be affected by the absolute value chosen for the residual aperture.

AN IDEALIZED MODEL FOR TORTUOSITY

An explanation for the departure from the cubic law equation is motivated by observations that the rough surfaces of many natural fractures have rugged topographies made up of a rich spectrum of wavelengths and amplitudes (e.g., Brown, 1987). At the longer wavelengths the topographies of the two surfaces of a fracture are correlated. However, at the shorter wavelengths they are uncorrelated, and it is these shorter wavelengths and amplitudes that produce asperities of contact between the fracture surfaces. These long wavelengths introduce out-of-plane tortuosity, which accounts for both the increase in flow path length and the variation in cross-sectional area of flow due to surface roughness. In-plane tortuosity arises when areas of surface are in contact. Fluid can flow only through connecting void spaces around the areas of contact and therefore encounters increases in path length.

To quantitatively evaluate the effects of these factors on flow, an idealized model was created to represent the rough surface topography of a natural fracture. To model out-of-plane tortuosity, a cosine wave of amplitude A and frequency ω (equal to $2\pi/L$ where L is the wavelength) is used to describe the longer wavelengths at which the two fracture surfaces are correlated. Figure 2 shows two cosine curves, greatly exaggerated with respect to scale for the purpose of clarity, each separated from an imaginary mid-line curve by a distance equal to $a/2$. The length of the flow path is denoted by l . Assuming unit width for the aperture, the total flow rate between the surfaces can be given as

$$Q = \frac{b^3}{12\mu} \frac{dp}{dl} \quad (2)$$

Figure 2. Two cosine waves that represent the surfaces of a fracture. [XBL 901-4506]

To account for the change in flow-path length, Eq. (2) becomes

$$\frac{P}{Q} = 12\mu \int_0^1 \frac{(1 + A^2 \omega^2 (\sin \omega x)^2)^{1/2} dx}{b^3} \quad (3)$$

The effect of variations in cross-sectional aperture for flow between two cosine surfaces (Fig. 2) is found using the relationship between the vertical separation, a , and the separation, b , locally perpendicular to the direction of flow, and is given by

$$\frac{P}{Q} = \frac{12\mu}{a^3} \int_0^1 \frac{(1 + A^2 \omega^2 (\sin \omega x)^2)^{1/2} dx}{(\cos(\arctan(-A \omega \sin \omega x)))^3} \quad (4)$$

or, by denoting the integral as f ,

$$\frac{P}{Q} = \frac{12\mu}{a^3} f \quad (5)$$

This expression incorporates both the effects of increased flow-path length and the variation in cross-sectional area of flow due to surface roughness. Examination of the above equation shows these effects to be independent of aperture.

In-plane tortuosity effects arise because the flow path is obstructed by areas of contact between the fracture surfaces. For a given separation distance, h , between the fracture surfaces with no areas of contact, assume that flow can be approximated by equivalent parallel plates, so that

$$Q = k_o \frac{dp}{dx} \cdot \frac{1}{f} \quad (6)$$

where k_o is equal to $h^3/12\mu$. For the case where areas of contact exist between the fracture surfaces it can be postulated that the flow can be approximated by

$$Q = k_e \frac{dp}{dx} \cdot \frac{1}{f} \quad (7)$$

where k_e is the effective flow conductance. Using the analogy of two-dimensional laminar flow of an incompressible fluid and heat conduction, Walsh (1981) developed an expression for effective flow conductance to account for the effect of areas of contact across the plane of the fracture on flow conductivity. The effective flow conductance, k_e , can be given as

$$k_e = \frac{1-d}{1+d} k_o \quad (8)$$

where k_o is the conductance of the fracture with no asperities, and d is the ratio of the contact area of the asperities to the total area of the fracture.

To model in-plane tortuosity when the fracture surfaces are in contact, a "carpet" of very small, equally sized cones, whose bases form a hexagonal close-packed arrangement, is laid on top of the longer-wavelength cosine wave forming the lower surface of the fracture in the out-of-plane tortuosity model. These cones represent the asperities of contact formed by the shorter uncorrelated wavelengths. Calculations determining the effects of the

asperities of contact on tortuosity are based on the assumption that the volume of rock is conserved during interpenetration of the asperities into the fracture surface (Pyrak-Nolte et al., 1988). Figure 3a shows the upper fracture surface in point contact with the cones used to represent asperities. The aperture under this condition is a_o . Now assume that a far field stress is applied. Figure 3b shows the change in displacement, D , that would be measured between two reference points external to the fracture and on either side of it, a typical practice in laboratory measurements of fracture deformations. With the assumption of conservation of volume, the volume displaced by the penetration of the cones is redistributed over the remaining portion of the upper fracture surface. This yields a thickness, z , shown in Figure 3c. As a result, the change in fracture aperture is equal to D plus z ; i.e., the change in fracture aperture is greater than the measured fracture displacement. The aperture of the fracture, h , can now be given as

$$h = a_o - D - z \quad (9)$$

After transforming the volume of the deformed cores to equivalent cylindrical volumes, the contact area for the equivalent cylindrical asperities per unit area can then be given as

$$d = \frac{\pi/6}{2 \sin 60^\circ} \left[\frac{(a_o - h)^2}{a_o^2} \right], \quad (10)$$

where h is given in Eq. (12).

The equation for flow through the idealized model can now be given as

$$\frac{Q}{dp/dx} = \frac{h^3}{12\mu} \cdot \frac{1-d}{1+d} \cdot \frac{1}{f} \quad (11)$$

Finally, to account for an irreducible flow (Q_∞) at high stress levels, Eq. (14) becomes

Figure 3. (a) Point contact between fracture surface and cones. (b) Measured displacement, D , due to far field stress. (c) Volume of the interpenetrating cones is redistributed over the remaining fracture surface area between the cones, resulting in a thickness, z . [XBL 901-103]

$$\frac{Q}{dp/dx} = \frac{h^3}{12\mu} \cdot \frac{1-d}{1+d} \cdot \frac{1}{f} + \frac{Q_\infty}{dp/dx} \quad (12)$$

COMPARISON BETWEEN THEORETICAL AND EXPERIMENTAL RESULTS

Using Eqs. (12) and (4), developed for the idealized model, a set of theoretical data points was generated and compared with those obtained experimentally. Figure 4 shows the theoretical and experimental data points as well as the predicted cubic law relationship. To generate the theoretical data points, values of aperture were chosen that fell in the same range as those used in the flow experiments, i.e., from 2.5 μm to 500 μm . The value of a_o was estimated to be 50 μm . Values of D were chosen to correspond with the values of displacement measured during the flow experiments and ranged from 15 to 35 μm . The value of $Q_\infty/(dp/dx)$ was taken to be $1.26 \times 10^{-13} \text{ m}^4/\text{Pa}\cdot\text{s}$ for a residual aperture of 2.5 μm . Calculations to determine f in Eq. (5) were based on an estimate of the geometry of the fracture surface used in the flow experiments and resulted in a factor whose value equaled 1.12. The figure shows very good agreement between the theoretical and experimental data, particularly in the regions of the smaller apertures and irreducible flow. When the two surfaces of the fracture are not in contact, the ratio of asperity contact area to fracture surface area is zero and the factor involving the contact area in Eq. (8) is 1. Thus only out-of-plane tortuosity affects flow when the fracture surfaces are not touching. Evidence of these effects is shown by the constant ratio between both the experimental and theoretical data points and those predicted by the cubic law, confirming that the effects of out-of-plane tortuosity are aperture independent.

The theoretical data points generated for flow through the idealized model of a fracture under conditions where the surfaces are in contact reflect the effects of both in-plane and out-of-plane tortuosity. Conservation of volume during the interpenetration of the asperities into the

Figure 4. Comparison between data generated using theoretical equations and experimental data, showing the effect of taking the irreducible flow into account. [XBL 901-109]

fracture surface, and the resulting effect on aperture closure, causes the effects of in-plane tortuosity to outweigh those of out-of-plane tortuosity. It is evident that the effect of contact area increases with decreasing aperture.

CONCLUSIONS

By generating equations for a simple theoretical model, the effects of tortuosity on fluid flow through a fracture have been evaluated. The significance of these effects is such that they must be included in flow-rate calculations. The effects of out-of-plane tortuosity have been found to be independent of aperture and result in a constant ratio between observed flow rates and those predicted from the cubic law relationship. In-plane tortuosity effects, which arise when the fracture surfaces are in contact, outweigh the effects of out-of-plane tortuosity. Because the volume of the asperities is conserved, the area of contact between the asperities and the fracture surface increases very quickly with decreasing aperture. As a result flow rate decreases rapidly with aperture closure to an irreducible, aperture-independent value.

ACKNOWLEDGMENTS

In addition to the support from the Department of Energy, we acknowledge Mobil Research and Development Corporation for providing the test sample and, in particular, Dr. Alvis McDonald for his thoughtful suggestions and comments.

The Effects of a Clay Coating on Fluid Flow through Simulated Rock Fractures

J.J. Carter, L.R. Myer, and N.G.W. Cook

Research concerning fluid flow through fractures has typically focused on the flow characteristics of rock fractures subject to different states of stress (Witherspoon, 1980). It is also important to consider the coupling between hydraulic flow and geochemical effects. In crystalline rocks, fractures are often partially or completely filled by deposits of calcite, silica, or clay (de Marsily, 1986). The fracture walls may simply be coated with clays that have chemically altered from the wall rock or deposited by percolating fluid. Within a fracture, chemical interactions between the groundwater and the clay may result in clay swelling. Depending on the chemical composition of the groundwater, the type of clay, and the fracture aperture, clay swell within a fracture can significantly affect the permeability of the fracture.

This experimental work investigates the effects of a thin clay coating on fluid flow through a simulated rock

REFERENCES

- Brown, S.R., 1987. Fluid flow through rock joints: The effect of surface roughness. *J. Geophys. Res.*, v. 92, p. 1337–1347.
- Lomize, G.M., 1951. *Water Flow through Jointed Rock* (in Russian). Moscow, Gosenergoizdat.
- Pyrak-Nolte, L.J., Myer, L.R., Cook, N.G.W., and Witherspoon, P.A., 1987. Hydraulic and mechanical properties of natural fractures in low permeability rock. *In* G. Herget, and S. Vongpaisal (eds.), *Proceedings of the Sixth International Congress on Rock Mechanics*. A. A. Balkema, Rotterdam, The Netherlands.
- Pyrak-Nolte, L.J., Cook, N.G.W., and Witherspoon, P.A., 1988. Fluid percolation through single fractures. *Geophys. Res. Lett.*, v. 15, p. 1247–1250.
- Raven, K.G., and Gale, J.E., 1985. Water flow in a natural rock fracture as a function of stress and sample size. *Int. J. Rock Mech. Min. Sci. & Geomech. Abstr.*, v. 22, p. 251–261.
- Walsh, J.B., 1981. Effect of pore pressure and confining pressure on fracture permeability. *Int. J. Rock Mech. Min. Sci. & Geomech. Abstr.*, v. 18, p. 429–435.
- Witherspoon, P.A., Wang, J.S.Y., Iwai, K., and Gale, J.E., 1980. Validity of cubic law for fluid flow in a deformable rock fracture. *Water Resour. Res.*, v. 16, p. 1016–1024.

fracture. Various concentrations of electrolytes were flowed through clay-coated (sodium montmorillonite) fractures of various apertures. Effective hydraulic apertures were inferred from measured flow rates assuming laminar flow between parallel plates. Reductions in the flow rates in response to electrolyte concentration were attributed to decreases in the effective hydraulic aperture due to clay swelling. Gravimetric water-content values, determined for each fracture upon completion of the experiment, provided additional evidence for clay swell.

EXPERIMENTAL PROCEDURE

Idealized rock fractures with clay coatings were simulated by sedimenting and air-drying a fine layer of sodium montmorillonite onto two glass plates. Clay coatings were determined to be 13 μm thick. Coatings used in

the flow experiments were assumed to be slightly thicker because of the potential for Na-montmorillonite to adsorb water vapor. Fracture apertures were simulated using mylar shims of various thicknesses. The mylar shims were placed lengthwise along the outside edges of the plates (Fig. 1). Mylar shims used in these experiments were 124, 186, and 258 μm thick. A constant-head apparatus was used to maintain a constant-head drop across the fracture. Flow rates were measured using a fraction collector (Fig. 1).

RESULTS

The Effect of Changing NaCl Concentration

The effect of changing NaCl concentration on measured flow rates can be seen in Fig. 2. A 0.75 M NaCl solution was flowed through a simulated fracture with an aperture of 124 μm . Flow rates are plotted against hydraulic head in Fig. 2a and inferred effective hydraulic apertures are plotted against time in Fig. 2b. In plots of flow rate as a function of hydraulic head, the points plotted are the last flow rates recorded at each hydraulic head prior to raising the head. The data points are numbered in chronological order. Inferred hydraulic aperture is then plotted against time to illustrate the dynamics of the system. It can be seen from Fig. 2b that the aperture reduction, and therefore the clay swell, is time dependent as well as dependent on electrolyte concentration. The marked change in flow rate with the introduction of a 0.5 M NaCl solution is surprising but consistent with results from further experiments.

Figure 1. Experiments were performed by flowing various electrolyte solutions through clay-coated, simulated rock fractures. The flow rates were measured as a function of time using a fraction collector. A constant-head value was maintained by a constant-head apparatus. [XBL 8911-4740]

Figure 2. The effect of changing NaCl concentration on measured flow rates and inferred hydraulic apertures, assuming laminar flow between parallel plates. A 0.75 M NaCl solution was flowed through the fracture followed by a 0.5 M NaCl solution. Reductions in measured flow rates in response to decreased electrolyte concentration were attributed to decreases in the effective hydraulic aperture due to clay swelling. [Part a, XCG 8911-4741; part b, XCG 8911-4742]

A similar test was performed on fractures with apertures of 186 μm and 258 μm (Fig. 3). The results are in excellent agreement with those in Fig. 2. There is a substantial reduction in the effective hydraulic aperture as calculated from measured flow rates. It is inferred that this is due to the swelling of the Na-montmorillonite in response to decreased electrolyte concentration. According to double-layer theory, as the electrolyte concentration is decreased,

Figure 3. The same test as in Fig. 2 was performed at a fracture aperture of 258 μm . The measured flow rates are greater than those at the smaller apertures, but the response of the clay to a more dilute electrolyte solution is consistent with the previous tests. [Part a, XCG 8911-4745; part b, XCG 8911-4746]

the thickness of the double layer is expected to increase. As the thickness of the double layer increases, the double-layer repulsive forces around each clay plate will cause the clay plates to repel one another and the clay will swell. Interestingly, according to the double-layer theory, at the range of electrolyte concentration used here (0.75–0.5 M NaCl), there should be very little clay swell. It appears from the test results that the clay swells upon hydration with the 0.75 M NaCl and then continues to swell slowly over time. There is then substantial swelling upon the introduction of a 0.5 M NaCl solution. The effective hy-

draulic aperture is significantly reduced, and there is a marked decrease in measured flow rate.

The approximate linearity in flow as a function of hydraulic head in all tests indicates that flow was not affected by particle migration. In addition, significant particle migration can be observed through the glass plates of the simulated fracture, and no particle migration was observed in these tests. This suggests that the reduction of effective hydraulic aperture is due to the stationary swell of the Na-montmorillonite upon the introduction of a more-dilute electrolyte concentration.

The low flow rate (or high swell values of the Na-montmorillonite) measured for 0.5 M NaCl in the experiments discussed above were confirmed by a series of tests that used only 0.5 M NaCl as the flowing fluid. A 0.5 M NaCl solution was flowed through three fractures with apertures of 124 μm , 186 μm , and 258 μm . The flow rates recorded for these apertures are slower than the flow rates recorded for 0.5 M NaCl in Figs. 2 and 3, indicating that the degree of swelling is higher when 0.5 M NaCl solution is flowed through the clay-coated fracture first rather than following a 0.75 M NaCl solution.

The Schulze-Hardy rule states that the critical coagulation concentration of a clay, or the concentration at which the clay will flocculate, will vary with cation valence as $(1/n^6)$, where n is equal to the cation valence in the electrolyte solution. This was interpreted by the author as suggesting that perhaps clay behavior may also vary with cation valence in this manner. The response of the clay to a 0.5 M NaCl solution should then be similar to the response to a 7.8×10^{-3} M CaCl_2 solution. A 7.8×10^{-3} M CaCl_2 solution was flowed through a fracture with an aperture of 124 μm . The clay apparently swelled to essentially seal the fracture aperture in accordance with the Schulze-Hardy Rule and the results for 0.5 M NaCl.

Ion Exchange with a 0.05 M CaCl_2 Solution

A strong solution of calcium chloride (0.05 M) was flowed through a simulated fracture coated with Na-montmorillonite in an attempt to convert the clay to a Ca-montmorillonite. The mylar thickness used was 258 μm , and the hydraulic head raised in six stages to 23.9 cm. There was no evident erosion or particle migration. The solution was then changed to D.I. water and the hydraulic head was raised in six steps to 23.9 cm. The fact that there was no swelling or erosion upon introduction of the D.I. water into the fracture was remarkable in comparison with a previous test run with a 0.75 M NaCl solution followed by D.I. water. In this test the clay had apparently instantly dispersed in distilled water. The results indicate that the 0.5 M calcium chloride solution stabilized the clay. The apparent lack of swelling suggests that the ion exchange—that is, the substitution of the Ca^{2+} for the Na^+ ions in the clay—was sufficient to convert the clay to more stable Ca-montmorillonite.

Interparticle Spacing

In the range of NaCl concentration used in the experiments reported here (0.5 M to 0.75 M), the degree of clay swell far exceeds the degree of swell predicted by double-layer theory. The double-layer repulsive forces are expected to decrease with increasing electrolyte concentration in the bulk solution. In Fig. 4, one-half the interparticle spacing ($d/2$) is calculated from double-layer theory for various NaCl concentrations.

The upper curve in Fig. 4 is calculated from the measured gravimetric water-content values. If clay plates are assumed to be flat and in parallel alignment, the interparticle spacing can be found by simply dividing the water content by the surface area of the clay and the solution density, assuming that there is no quasicrystal formation. The results are far greater than the interparticle spacings predicted by double-layer repulsive forces and are much more consistent with the degree of swelling observed. It is apparent that the range of the double-layer repulsive forces is much too small to be responsible for clay swelling at these electrolyte concentrations.

Rowell (1963) and Rowell et al. (1969) also found measured values of swell for a sedimented Wyoming Na-montmorillonite to be much greater than calculated values. To explain the disparity between the measured and calculated water-content values, Rowell (1965) suggested the presence of "crystals" or groups of parallel plates that retain their identity upon swelling.

Figure 4. Interparticle spacings as calculated from double-layer theory and from gravimetric water-content values. At the electrolyte concentrations used in these experiments, the range of the double-layer repulsive forces are clearly too small to account for observed clay swell. The nonlinearity of the interparticle spacing as calculated from measured water-content values additionally indicates that the observed clay behavior is due to particle association and not simply to surface effects. [XCG 8911-4749]

Clay Structure

Clay structure was investigated using freeze-fracture in combination with transmission electron microscopy (TEM). This technique was used to study samples of clay after 0.75 M and 0.5 M NaCl had been flowed through two different fractures.

In the past there has been concern that freezing the clay slurry may cause the formation of ice crystals, which could alter the structure of the clay. In the sample studied here, this was not a serious concern because the high salt

(a)

(b)

Figure 5. TEM pictures of (a) 0.5 M and (b) 0.75 M NaCl samples prepared by the freeze-fracture techniques, magnified 24,900 times. [Part a, XBB 902-1591; part b, XBB 902-1592]

concentration acts as a cryoprotectant and inhibits ice-crystal formation. The TEM pictures in Fig. 5 show a definite structural difference at 0.5 M and 0.75 M NaCl. In both cases the clay is flocculated, but the aggregates are substantially larger in 0.75 M solution than in 0.5 M NaCl solution. The relationship between these structural differences and apparent swell in clay is currently being investigated.

SUMMARY

It is apparent from this study that the effect of electrolyte concentration on flow through Na-montmorillonite coated fractures is significant. The clay swells to approximately five times the original thickness within the six hour experiments. The results from all tests are consistent and indicate that clay swell is time dependent and also strongly depends on electrolyte concentration in the 0.5 M NaCl range. The results from this work are surprising and do not agree with the degree of clay swelling predicted by double-layer theory. It appears that clay swell in the 0.5 M NaCl range is due to particle association that is strongly dependent on electrolyte concentration and not simply due to surface effects. This is significant in that similar observations have been made by others (Rowell 1963, 1965,

1969), but no working model has been established for the mechanism of clay swell at high salt concentrations. The freeze-fracture TEM results shown in Fig. 5 are a first attempt to study possible structural changes that may occur between 0.75 M and 0.5 M NaCl.

REFERENCES

- de Marsily, G., 1986. Quantitative Hydrogeology. Academic Press, San Diego, California.
- Rowell, D.L., 1963. Effect of electrolyte concentration on the swelling of oriented aggregates of montmorillonite. *Soil Sci.*, v. 96, p. 368-374.
- Rowell, D.L., 1965. Influence of positive charge on the inter- and intra-crystalline swelling of oriented aggregates of Na-montmorillonite in NaCl solutions. *Soil Sci.*, v. 100, no. 6, p. 340-347.
- Rowell, D.L., D. Payne, and N. Ahmad, 1969. The effect of the concentration and movement of solutions on the swelling, dispersion, and movement of clay in saline and alkali soils. *J. Soil Sci.*, v. 20, no. 1, p. 176-188.
- Witherspoon, P.A., et al., 1980. Validity of cubic law for fluid flow in a deformable rock fracture. *Water Resour. Res.*, v. 16, p. 1016-1024.

APPENDIXES

APPENDIX A: ABSTRACTS OF JOURNAL ARTICLES

Ahn, J., Chambré, P.L., and Pigford, T.H., 1989. Transient diffusion from a cylindrical waste solid into fractured porous rock. *Radioactive Waste Manage. & Nucl. Fuel Cycle*, v. 13, no. 1-4, p. 263-279 (LBL-25284).

Numerical illustrations for transient mass transfer from an infinitely long cylinder intersected by a planar fracture are shown based on an exact analytical solution. The concentration at the cylinder surface is maintained at the solubility. In the fracture contaminant diffuses in the radial direction. In the rock matrix three-dimensional diffusion is assumed in the cylindrical coordinate. No advection is assumed. Radioactive decay and sorption equilibrium are included. Comparison between the cylinder model and the previous plane model is given. Radioactive decay enhances the mass transfer from the cylinder. Even though the fracture is assumed to be a faster diffusion path than the rock matrix, the larger waste surface exposed to the matrix and the greater assumed matrix sorption result in greater release rate to the matrix than to the fracture. The cylinder model gives more conservative results than the plane model with respect to the mass transfer from the source and the far-field transport for the diffusion-dominant field.

Asch, T., and Morrison, H.F., 1989. Mapping and monitoring electrical resistivity with surface and subsurface electrode arrays. *Geophysics*, v. 54, no. 2, p. 235-244 (LBL-24168).

Electrical resistivity measurements using combinations of subsurface and surface electrodes are more sensitive to subsurface inhomogeneities than arrays confined to the surface. A further advantage of the subsurface configuration is that the strong influence of near-surface inhomogeneities can be reduced by differencing the measured apparent resistivities with a reference set of values obtained with the subsurface electrode(s) at a particular depth. This process accentuates the response of features near the downhole electrode while canceling the response of the near-surface features.

An idealized two-dimensional model of a nuclear waste repository has been used to demonstrate the effectiveness of this differencing scheme. It is shown that resistivity measurements using borehole electrodes well away from the repository and on the surface are sensitive to changes in the repository that could not be practically observed from surface measurements. This sensitivity is preserved in the presence of a conducting and inhomogeneous surface layer and, most importantly, it is preserved even if the resistivities of the near-surface features also change.

Augustin, A.M., Kennedy, W.D., Morrison, H.F., and Lee, K.H., 1989. A theoretical study of surface-to-borehole electromagnetic logging in cased holes. *Geophysics*, v. 54, no. 1, p. 90-99 (LBL-25052).

A new electromagnetic logging method, in which the source is a horizontal loop coaxial with a cased drill hole and the secondary axial fields are measured at depth within the casing, has been analyzed. The analysis, which is for an idealized model of an infinite pipe in a conductive whole space, has shown that the casing and formation are uncoupled at the low frequencies that would be used in field studies. The field inside the casing may be found by first finding the field in the formation and then using this

field as an incident field for the pipe alone. This result permits the formation response to be recovered from the measured field in the borehole by applying a correction for the known properties of the casing. If the casing response cannot be accurately predicted, a separate logging tool employing a higher frequency transmitter could be used to determine the required casing parameters in the vicinity of the receiver.

This logging technique shows excellent sensitivity to changes in formation conductivity, but it is not yet known how well horizontal stratification can be resolved. One of its most promising applications will be in monitoring, through repeated measurements, changes in formation conductivity during production or enhanced recovery operations.

Billiaux, D., Chiles, J. P., Hestir, K., and Long, J., 1989. Three-dimensional statistical modelling of a fractured rock mass—An example from the Fanay-Augères mine. *Int. J. Rock Mech. Min. Sci. & Geomech. Abstr.*, v. 26, no. 3/4, p. 281-299 (LBL-27030).

This paper describes a new technique for stochastic modelling of 3-D fracture networks. We use geostatistical simulation methods to reproduce features of the spatial structure of the rock, such as the variation of fracture density and fracture orientation in space. For an example of the method, we use mapped fracture data from the Fanay-Augères mine, in Limousin, France. Two different sections of a drift wall, S1 and S2, were mapped. The S1 section is wet, and the S2 section is dry. For each case, the fractures are divided into five different sets and each set is modelled separately. The fractures in each set are represented as discs placed randomly in space. The diameter of each disc is chosen independently from a fixed probability distribution determined from the trace length distribution. A point process, called the parent-daughter process, is used for locating discs. This process gives a clumping or swarming of fractures not found in the usual Poisson model.

The orientation of the discs is characterized as a fluctuation about the mean orientation for the set. This fluctuation has a spatial structure that is simulated with geostatistics. Geostatistical simulations of the two fracture systems are made in a 68 m cube which contains over 5 million fractures. The connectivities of the simulations are assessed to see if there is any correlation with the hydrologic observations. The connectivity of S1 appears to be larger than the connectivity of S2. The S1 simulation has a smaller overall density of fractures but a larger density of big fractures. These larger fractures result in more connectivity which is consistent with the field observation that the S1 section of drift is wet and the S2 section is dry. The reason for this difference is apparently related to the presence of a fault in the rock surrounding S1, thus indicating the need to understand the role of faults or fracture zones in characterizing the hydrology of fractured rock.

Billiaux, D., and Fuller, P., 1989. An algorithm for mesh simplification applied to fracture hydrology. *Math. Geol.*, v. 21, no. 2, p. 221-232 (LBL-24717).

Numerically generated discrete fracture networks are used to simulate the flow of water through rock fractures. The fractures are modeled as random assemblages of conductive elements in a nonconductive matrix. Because large numbers of fractures often are needed to represent fractured

rock adequately, minimizing the required computer time and memory is crucial. For steady-state flow, any portion of the mesh that is linked to the rest of the mesh by only one point is a dead end and does not contribute to water flow. The removal of such dead-end clusters simplifies the mesh and therefore speeds up computation, without changing its response. An algorithm for removing these dead ends is described in detail. Its effectiveness is discussed with regard to the connectivity of a network.

Bischoff, J.L., and Pitzer, K.S., 1989. Liquid-vapor relations for the system NaCl-H₂O: Summary of the P-T-x surface from 300° to 500°C. Am. J. Sci., v. 289, p. 217-248 (LBL-25108).

Experimental data on the vapor-liquid equilibrium relations for the system NaCl-H₂O were compiled and compared in order to provide an improved estimate of the P-T-x surface between 300° to 500° C, a range for which the system changes from subcritical to critical behavior. Data for the three-phase curve (halite + liquid + vapor) and the NaCl-H₂O critical curve were evaluated, and the best fits for these extrema then were used to guide selection of best fit for isothermal plots for the vapor-liquid region in-between. Smoothing was carried out in an iterative procedure by replotting the best-fit data as isobars and then as isopleths, until an internally consistent set of data was obtained. The results are presented in table form that will have application to theoretical modelling and to understanding of two-phase behavior in saline geothermal systems.

Bodvarsson, G.S., Cox, B.L., and Ripperda, M.A., 1989. Effects of steam-liquid counterflow on pressure transient data from two-phase geothermal reservoirs. SPE Res. Eng., v. 4, no. 2, p. 187-193 (LBL-26964).

Numerical studies were performed to investigate the effects of localized feed zones on the pressure transients in the densities of liquid water and vapor. Production from such systems enhances steam/liquid-water counterflow and expands the vapor-dominated zone at the top of the reservoir. Subcooled liquid regions develop in the center of the reservoir as a result of gravity drainage of cooler liquid water. The vapor zone acts as a constant-pressure boundary and helps to stabilize the pressure decline in the system. The pressure transients at observation wells were shown to depend greatly on the location (depth) of the major feed zone; if this is not accounted for, large errors in deduced reservoir properties will result. At shallow observation points, pressures may actually increase as a result of enhanced steam upflow caused by production at a deep feed zone.

Bodvarsson, G.S., and Stefansson, V., 1989. Some theoretical and field aspects of reinjection in geothermal reservoirs. Water Resour. Res., v. 25, no. 6, p. 1235-1248 (LBL-24101).

Theoretical and field aspects of reinjection into geothermal reservoirs is discussed using examples from various geothermal fields. Reinjection effects can be observed in terms of pressure maintenance, changes in chemical concentrations, and temperature decline. Pressure support due to injection is observed in many liquid-dominated fields, and in two-phase field pressure, effects are often felt through mobility changes. In most geothermal fields where injection is employed, changes in chemical concentrations of the produced fluids have been observed, due to the higher salinity of the injected fluids. In some cases the returns of the injected fluids observed through chemical changes have results in temperature declines at the producing wells. In those cases the fluid flow is probably concentrated through a few fractures or faults with insufficient surface area for heat exchange with the host rock.

Bodvarsson, G.S., and Witherspoon, P.A., 1989. Geothermal reservoir engineering. Part I. Geotherm. Sci. & Tech., v. 2, no. 1, p. 1-68 (LBL-26881).

Geothermal reservoir engineering has been rapidly developing over the past ten years as a new field of engineering. Although similar in many respects to its counterpart in the field of petroleum, the differences between petroleum and geothermal reservoirs are significant and cannot be ignored in developing methods of characterizing and exploiting geothermal systems. Various aspects of geothermal reservoir engineering are presented on such topics as: the governing physical processes, rock and fluid properties, well testing methods, resource assessment and the importance of reinjection. Most geothermal systems are found in fractured rocks where the permeability of the matrix is quite small. Conventional well testing methods have been found useful in dealing with many single-phase reservoirs but are less reliable in high temperature, two-phase systems. Resource assessment must consider the dynamic nature and complex physical processes that occur in geothermal systems. Numerical modeling of the reservoir under different exploitation schemes is necessary and models that use the well-by-well approach yield the most reliable results. This approach will generally yield the most complete resource evaluation in terms of the overall generating capacity of the field as well as the predicted performance of individual wells. During the early stages of field development, simpler methods of assessment such as stored heat calculations, decline curve analysis, or lumped-parameter models are useful. It is important to realize that because the vast majority of the heat in a geothermal reservoir is stored in the rock matrix, a program of reinjecting water is necessary to maximize the energy recovery. To be successful, the program must be designed to minimize the effects of injectivity decline and thermal interference. A number of examples from field experience are used throughout this discussion to illustrate the specialized problems that confront the geothermal reservoir engineer.

Connaughton, L.M., Millero, F.J., and Pitzer, K.S., 1989. Volume changes for mixing the major sea salts: Equations valid to ionic strength 3.0 and temperature 95°C. J. Soln. Chem., v. 18, no. 11, p. 1007-1017 (LBL-27304).

Equations in the ion-interaction (Pitzer) system are derived for the volume change on mixing any combination of the sea salts NaCl, Na₂SO₄, MgSO₄, MgCl₂ at constant ionic strength. For these mixings of different charge types, the equations include complex differences of pure electrolyte terms. Recently measured data for each of the pure electrolytes provide these pure electrolyte terms. Other recent measurements on the volume change on mixing are compared with values calculated from the equations. At 25°C there is no need to introduce the mixing terms based on differences in the interactions of ions of the same sign. At other temperatures, the agreement without the mixing term is good, but significant improvement is obtained by inclusion of the binary mixing terms $\Theta_{\text{Cl}_2\text{SO}_4}^X$ and $\Theta_{\text{Na}_2\text{Mg}}^X$. The equations and parameters can then predict the volumetric properties of any mixed solution of these salts over the range 0-100°C and to at least 3 mol·kg⁻¹ ionic strength.

Falta, R.W., Javandel, I., Pruess, K., and Witherspoon, P.A., 1989. Density-driven flow of gas in the unsaturated zone due to the evaporation of volatile organic compounds. Water Resour. Res., v. 25, no. 10, p. 2159-2169 (LBL-26373).

A theoretical investigation of factors affecting the gas phase transport of evaporating organic liquids in the unsaturated zone is presented. Estimates of density-driven advective gas flow using a simple analytic expres-

sion indicate that significant advective gas flow will result from the evaporation of volatile liquids in soils having a high permeability. Numerical simulations using a two-dimensional cylindrical geometry and including the effects of phase partitioning between the solid, gas, water, and organic liquid phases show that mass transfer due to density-driven flow may dominate the gas phase transport of some organic chemical vapors in the unsaturated zone.

Flueh, E.R., Mooney, W.D., Fuls, G.S., and Ambros, E.L., 1989. Crustal structure of the Chugach Mountains, southern Alaska: A study of peg-leg multiples from a low-velocity zone. *J. Geophys. Res.*, v. 94, no. B11, p. 16023-16035 (LBL-24699).

A seismic refraction profile recorded along the geologic strike of the Chugach Mountains in southern Alaska shows three upper crustal high-velocity layers (6.9, 7.2, and 7.6 km/s) and a unique pattern of strongly focussed echelon arrivals to a distance of 225 km. The group velocity of the ensemble of echelon pattern is due to peg-leg multiples generated from within a low-velocity zone between the second and third upper crustal high-velocity layers. The third high-velocity layer (7.6 km/s) is underlain at 18 km depth by a pronounced low-velocity zone that produces a seismic shadow zone wherein peg-leg multiples are seen as echelon arrivals. The interpretation of these echelon arrivals as multiples supersedes an earlier interpretation which attributed them to successive primary reflections arising from alternating high- and low-velocity layers. Synthetic seismogram modeling indicates that a low-velocity zone with transitional upper and lower boundaries generates peg-leg multiples as effectively as one with sharp boundaries. No *PmP* or *Pn* arrivals from the subducting oceanic Moho at 30 km depth beneath the western part of the line are observed on the long-offset (90-225 km) data. This may be due to a lower crustal waveguide whose top is the high-velocity (7.6 km/s) layer and whose base is the Moho. A deep (-54 km) reflector is not affected by the waveguide and has been identified in the data. Although peg-leg multiples have been interpreted on some long-range refraction profiles that sound to upper mantle depths, the Chugach Mountains profile is one of the few crustal refraction profiles where peg-leg multiples are clearly observed. This study indicates that multiples and converted phases may be more important in seismic refraction/wide-angle reflection profiles than previously recognized.

Flueh, E.R., and Okaya, D.A., 1989. Comparison of near-vertical and intermediate offset seismic reflection data from west of the Whipple Mountains, SE California. *J. Geophys. Res.*, v. 94, no. B1, p. 625-636 (LBL-24641).

During a seismic reflection survey conducted by the California Consortium for Crustal Studies in the Basin and Range Province west of the Whipple Mountains, SE California, a piggyback experiment was carried out to collect intermediate offset data (12-31 km). These data were obtained by recording the Vibroseis energy with a second, passive recording array, deployed twice at fixed positions at opposite ends of the reflection lines. The reflection midpoints fall into a 3-km-wide and 15-km-long region in Vidal Valley, roughly parallel to a segment of one of the near-vertical reflection profiles. This data set makes three unique contributions to the geophysical study of this region. (1) From forward modeling of the observed travel times using ray-tracing techniques, a shallow layer with velocities ranging from 6.0 to 6.5 km/s was found. This layer dips to the south from 2-km depth near the Whipple Mountains to a depth of 5 km in Rice Valley. These depths correspond closely to the westward projection of the Whipple detachment fault, which is exposed 1 km east of the near-vertical profiles in the Whipple Mountains. (2) On the near-vertical profile, the reflections from the mylonitically deformed lower plate at upper crustal and mid-crustal depths are seen to cease underneath a sedimentary basin in Vidal Valley. However, the piggyback data, which undershoot this basin, show that these reflections are continuous beneath the basin. Thus near-surface energy transmission problems were responsible for the apparent lateral termination of the reflections on the near-vertical reflection profile. (3) The areal distribution of the midpoints allows us to construct a quasi-three-dimensional image on perpendicular profiles; at the

cross points we determined the true strike and dip of reflecting horizons. This analysis shows that the reflections from the mylonitically deformed lower plate dip to the southwest westward of the Whipple Mountains and dip to the south southward of the Turtle Mountains. The results of this study support the interpretation of crustal reflectivity in the near-vertical reflection profiles to be related to the mid-Tertiary episode of extension which produced the Whipple metamorphic core complex. This association geometrically suggests a more regionally distributed mechanism from crustal thinning as compared with single detachment fault models.

Gauglitz, P.A., and Radke, C.J., 1989. Dynamics of Haines jumps for compressible bubbles in constricted capillaries. *AIChE J.*, v. 35, no. 2, p. 230-240 (LBL-27140).

The unsteady, impulsive motion of a compressible bubble expanding out of a constricted capillary is quantified with a macroscopic momentum balance. Numerical solution demonstrates the importance of the Ohnesorge number, the geometry of the constriction, the length of the initial gas bubble, and the surface tension, density, and unconstricted capillary radius, which combine to form a characteristic scaling time. Experimental data for the position of the bubble front as a function of time confirm the theoretical result when the time scale for the bubble jump is longer than that required to achieve fully developed parabolic flow. Theory also predicts the capillary number of the bubble jump which, in conjunction with previous theoretical results, determines the time to snap-off of gas bubbles moving through constricted capillaries. Excellent agreement is found with existing experimental data for Ohnesorge numbers ranging from 5×10^{-3} to 0.3.

Jahnke, F.M., and Radke, C.J., 1989. A radially perfused cell for measuring diffusion in compacted, highly sorbing media. *Ind. & Eng. Chem. Res.*, v. 28, p. 347-355 (LBL-27021).

The unique radially perfused cell designed specifically to measure the transient diffusion of species in compacted, highly adsorbing and swelling porous media is described in this paper. The perfused cell exhibits extremely high mass-transfer coefficients while resisting large swelling pressures. It also allows a simultaneous determination of the effective diffusion and sorption retardation coefficients of species from a single experiment. The concentration boundary layer resulting from the radial flow configuration is sufficiently uniform that one-dimensional, axial diffusion is studied in the sample medium. Over the range of Peclet numbers studied, from 10^3 to 3×10^5 , overall Nusselt numbers range from 70 to 550, in excellent agreement with a theoretical convective dispersion prediction containing no adjustable parameters. Use of the cell is illustrated by an experiment in which cesium chloride diffuses into a moderately compacted sodium montmorillonite clay gel. We find that surface diffusion controls the migration of cesium in these clays.

Lee, K.H., Liu, G., and Morrison, H.F., 1989. A new approach to modelling the electromagnetic response of conductive media. *Geophysics*, v. 54, no. 9, p. 1180-1192 (LBL-26033).

We introduce a new and potentially useful method for computing electromagnetic (EM) responses of arbitrary conductivity distributions in the earth. The diffusive EM field is known to have a unique integral representation in terms of a fictitious wave field that satisfies a wave equation. We show that this integral transform can be extended to include vector fields. Our algorithm takes advantage of this relationship between the wave field and the actual EM field. Specifically, numerical computation is carried out for the wave field, and the result is transformed back to the EM field in the time domain.

The proposed approach has been successfully demonstrated using two-dimensional (2-D) models. The appropriate TE-mode diffusion equation in the time domain for the electric field is initially transformed into a scalar wave equation in an imaginary q domain where q is a time-like variable. The corresponding scalar wave field is computed numerically

using an explicit q -stepping technique. Standard finite-difference methods are used to approximate the fields, and absorbing boundary conditions are implemented. The computed wave field is then transformed back to the time domain. The result agrees fairly well with the solution computed directly in the time domain.

We also present an approach for general three-dimensional (3-D) EM problems for future studies. In this approach, Maxwell's equations in the time domain are first transformed into a system of coupled first-order wave equations in the q domain. These coupled equations are slightly modified and then cast into a "symmetric" and "divergence-free" form. We show that it is to this particular form of equations that numerical schemes developed for solving wave equations can be applied efficiently.

Majer, E.L., 1989. The application of high frequency seismic monitoring methods for the mapping of grout injections. *Int. J. Rock Mech. Min. Sci. & Geomech. Abstr.*, v. 26, no. 3/4, p. 249-256 (LBL-25088).

Several different field experiments have been carried out at two different field sites to develop high-frequency seismological methods for the mapping of grout injections in real time. Both sites were in fractured crystalline rock with permeabilities of the fractured rocks ranging from 10^{-5} to 10^{-8} m/sec. The injection rates varied from 1 to 200 l/min. The viscosity was also varied. The injection pressures varied from 0.1 to 2 MPa over hydrostatic. Deviatoric *in situ* stress ranged from near zero (one site was at the surface) to 15 MPa for the deepest injections. The results of these field tests indicate that there is usable seismic energy between 1000 and 10,000 Hz. There are basically two different types of energy: discrete seismic events (acoustic emission), and in some cases an increase in continuous seismic energy that appears to be associated with the grout sheet when very viscous fluids are used. A field system has been built, that using the results of these experiments, will be used in future experiments for mapping the grout location.

Martel, S.J., and Pollard, D.D., 1989. Mechanics of slip and fracture along small faults and simple strike-slip fault zones in granitic rock. *J. Geophys. Res.*, v. 94, no. B7, p. 9417-9428 (LBL-26983).

We exploit quasi-static fracture mechanics models for slip along pre-existing faults to account for the fracture structure observed along small exhumed faults and small segmented fault zones in the Mount Abbot quadrangle of California and to estimate stress drop and shear fracture energy from geological field measurements. Along small strike-slip faults, cracks that splay from the faults are common only near fault ends. In contrast, many cracks splay from the boundary faults at the edges of a simple fault zone. Except near segment ends, the cracks preferentially splay into a zone. We infer that shear displacement discontinuities (slip patches) along a small fault propagated to near the fault ends and caused fracturing there. Based on elastic stress analyses, we suggest that slip on one boundary fault triggered slip on the adjacent boundary fault, and that the subsequent interaction of the slip patches preferentially led to the generation of fractures that splayed into the zones away from segment ends and out of the zones near segment ends. We estimate the average stress drops for slip events along the fault zones as ~ 1 MPa and the shear fracture energy release rate during slip as $5 \times 10^2 - 2 \times 10^4$ J/m². This estimate is similar to those obtained from shear fracture of laboratory samples, but orders of magnitude less than those for large fault zones. These results suggest that the shear fracture energy release rate increases as the structural complexity of fault zones increases.

McKibbin, R., and Pruess, K., 1989. Some effects of non-condensable gas in geothermal reservoirs with steam-water counterflow. *Geothermics*, v. 18, no. 3, p. 367-379 (LBL-28028).

A mathematical model is developed for one-dimensional fluid and heat flow in two-phase geothermal reservoirs containing non-condensable gas (CO₂). Vertical profiles of temperature, pressures and phase saturations in steady-state conditions are obtained by numerically integrating the coupled

ordinary differential equations describing conservation of water, CO₂ and energy. Solutions, including binary diffusion effects in the gas phase, are generated for cases with net mass throughflow as well as for balanced liquid-vapor counterflow. Calculated examples illustrate some fundamental characteristics of two-phase heat transmission systems with non-condensable gas.

Nitsche, H., Standifer, E.M., and Silva, R.J., 1989. Americium(III) carbonate complexation in aqueous perchlorate solution. *Radiochimica Acta*, v. 46, p. 185-189 (LBL-25118).

The formation constant for the reaction $\text{Am}^{3+} + \text{CO}_3^{2-} = \text{AmCO}_3^+$ was determined in 0.1 M NaClO₄ solutions by absorption spectrophotometry. The absorption band at 502.8 nm shifted to longer wavelength when increasing amounts of carbonate were added to americium perchlorate solutions. The absorption bands were fitted with a non-linear least-squares method. The resulting $\log \beta(0.1 \text{ M}) = 6.69 \pm 0.15$ was extrapolated to infinite dilution. Taking lanthanum as a model substance and using available activity coefficients at 0.1 M gave $\log \beta_1^0 = 8.36 \pm 0.15$. Using the specific ion interaction theory (S.I.T.) with literature data, the weighted $(1/\sigma^2)$ linear least-squares regression resulted in $\log \beta_1^0 = 8.16 \pm 0.10$ (2 σ) and the interaction coefficient $\epsilon(\text{AmCO}_3^+, \text{ClO}_4^-) = 0.31 \pm 0.08 \text{ kg} \cdot \text{mol}^{-1}$ (2 σ). No evidence was found for the existence of americium bicarbonate complexes.

Nolte, D.D., Pyrak-Nolte, L.J., and Cook, N.G.W., 1989. The fractal geometry of the flow paths in natural fractures in rock and the approach to percolation. *Pure & Appl. Geophys.*, v. 131, no. 1/2, p. 111-138 (LBL-23320).

The distributions of contact areas in single, natural fractures in quartz-monzonite (Stripa granite) are found to have fractal dimensions which decrease from $D = 2.00$ to values near $D = 1.96$ as stress on the fractures is increased from 6 MPa up to 85 MPa. The effect of the changing contact area on fluid flow is considered, and a general flow law is presented which decouples the effects of fracture aperture and contact area on fluid flow through the fracture. A fractal model of correlated continuum percolation is presented which adequately describes the flow path geometries. The fractal dimension can be used as a fittable parameter to determine how far the flow system is from the percolation threshold.

Noorishad, J., Carnahan, C.L., and Benson, L.V., 1989. Simulation of fractionation of ¹³C during nonequilibrium reactive solute transport in geologic systems: Formulation and example calculation. *Water Resour. Res.*, v. 25, no. 4, p. 754-756 (LBL-25011).

Equations of transport for the fractionating stable carbon isotope ¹³C have been formulated and implemented in a nonequilibrium reactive chemical transport code. Application is demonstrated by solution of a generic problem. The new modeling capability adds a new dimension to investigation of groundwater evolution.

Pigford, T.H., Chambre, P.L., and Lee, W.W.-L., 1989. Mass transfer and transport in geologic repositories: Analytic studies and applications. *Radioactive Waste Manage. & Nucl. Fuel Cycle*, v. 13, no. 1-4, p. 241-262 (LBL-25285).

Assessing the long-term performance of geologic repositories for radioactive waste requires reliable quantitative predictions of rates of release of radionuclides from the waste into the rock, transport through the geologic media, cumulative release to the accessible environment, and maximum concentrations in ground water and surface water. Analytic mass transfer and transport analyses have apparent usefulness in making such predictions. In this paper we present three examples of mass transfer analyses, transport of long radioactive chains in semi-infinite media, migration of readily soluble species into rock and radionuclide migration

from multiple patch sources into a planar fracture. These examples include the assumptions, governing equations, solutions and numerical illustrations using parameter values typical of geologic repositories. Through these examples the advantage of using analytic solutions as well as limitations and directions for future work are discussed.

Tanger, J.C. IV, and Pitzer, K.S., 1989. Calculation of the thermodynamic properties of aqueous electrolytes to 1000°C and 5000 bar from a semicontinuum model for ion hydration. *J. Phys. Chem.*, v. 93, p. 4941–4951 (LBL-26251).

A semicontinuum approach for prediction of standard-state Gibbs free energies of ionic hydration, $\Delta_h G$, at high temperature steam conditions has been revised to permit predictions at temperatures from 0 to 1000°C and any pressure up to 5 kbar. The revised semicontinuum model provides for a more realistic identification of inner-shell and outer-shell contributions. The inner-shell term accounts for contributions to $\Delta_h G$ from the first six H_2O molecules of hydration. Inner-shell contributions are calculated by using available experimental equilibrium constants for successive ionic hydration reactions and an empirical parameter that represents the effective volume increment per H_2O of hydration. The outer-shell term accounts for contributions to $\Delta_h G$ from H_2O molecules outside the inner-shell region. Outer-shell contributions are obtained from the Born equation using the bulk solvent dielectric constant and an empirical parameter that represents the effective Born radius. The empirical parameters in the revised model are characterized in a manner that ensures reasonable consistency with experimental standard-state volumes and heat capacities for aqueous electrolytes. Calculations on alkali-metal halide and alkali-metal hydroxide electrolytes are considered, and the results for NaCl are used to illustrate the pressure and temperature behavior of standard-state properties. Evaluation of uncertainties in predicted values for $\Delta_h G$ supports application of the revised model for rough quantitative estimation of standard-state properties at supercritical conditions. The validity of the revised model at supercritical conditions is also supported by a comparison of calculated and experimental apparent molal heat capacities for NaCl.

Tsang, C.-F., 1989. Tracer travel time and model validation. *Radioactive Waste Manage. & Nucl. Fuel Cycle*, v. 13, no. 1–4, p. 311–323 (LBL-26518).

The performance assessment of a geologic nuclear waste repository involves the estimation of radionuclide transport extrapolated thousands of years into the future. Mathematical models used to make these estimates need to be validated. In model validation it is important to consider the performance measures. Once the proper performance measures are decided we have to consider the model structure and processes that are appropriate for the repository site. These can be validated by a number of existing methods. As an example of the choice of performance measure, tracer transport in highly heterogeneous media is considered. Here, point measurements of tracer transport are subject to large variability. However, point predictions are perhaps not necessary, but averaged line or areal predictions are more feasible and may be the more appropriate performance measure. This conclusion, although very tentative, may have significant impacts on the design of experiments for model validation.

Tsang, Y.W., and Tsang, C.F., 1989. Flow channeling in a single fracture as a two-dimensional strongly heterogeneous permeable medium. *Water Resour. Res.*, v. 25, no. 9, p. 2076–2080 (LBL-26596).

The void space of a rock fracture is conceptualized as a two-dimensional heterogeneous system with variable permeabilities as a function of position in the fracture plane. The apertures are generated using geostatistical methods. Fluid flow is simulated with constant head boundary conditions on two opposite sides of the two-dimensional flow region, with

closed boundaries on the remaining two sides. The results show that the majority of flow tends to coalesce into certain preferred flow paths (channels) which offer the least resistance. Tracer transport is then simulated using a particle tracking method. The apertures along the paths taken by the tracer particles are found to obey a distribution different from that of all the apertures in the fracture. They obey a distribution with a larger mean and a smaller standard deviation. The shift in the distribution parameters increases with increasing values of variance for the apertures in the two-dimensional fracture. Provided that the correlation length is no greater than one fifth of the scale of measurement, the aperture density distributions of tracer particle paths remain similar for flow in two orthogonal directions, even with anisotropy ratio of spatial correlation up to 5. These results may be applicable in general to flow and transport through a two-dimensional strongly heterogeneous porous medium with a broad permeability distribution, where the dispersion of the system may be related to the parameters of the permeability distribution along preferred flow channels.

Weres, O., Jun, C.H., and Tsao, L., 1989. Production of liquid hydrocarbons from a geopressured gas well: Migration of dispersed hydrocarbons induced by brine flow. *J. Pet. Sci. & Eng.*, v. 2, p. 269–279 (LBL-23658).

Several geopressured gas wells have produced small amounts of liquid hydrocarbons. They all produced an unusual gas condensate which differs dramatically from oil, containing predominantly light aromatic hydrocarbons. Two of the wells have also produced paraffinic oil. A series of hydrocarbon liquids produced from the Gladys-McCall No. 1 well (Cameron Parish, La.) is described here.

The phase relations of brine, oil and gas in the producing formation and wellbore of this well were calculated using a three-phase, many-component computer program. A single gas-rich, dispersed hydrocarbon phase was present downhole, initially at some distance from the wellbore. The aromatic condensate represents the relatively water soluble hydrocarbons which dissolved in the brine. Prolonged production of brine from the well caused the hydrocarbon phase to move toward the well, ultimately leading to production of oil. Movement of less volatile hydrocarbons was retarded by adsorption, producing chromatographic separation.

These data and conclusions were used to test several theories of primary migration of petroleum in nature. Whereas the aromatic condensate is derived from hydrocarbons dissolved in brine, it is very different from common petroleum, indicating a completely different origin for the latter. Expulsion of a dispersed hydrocarbon fluid from shale together with water is indicated, as in the "water flushing" theories of petroleum migration.

Weres, O., and Tsao, L., 1988. The activity of NaOH buffered by silicate solids in molten sodium acetate-water at 317°C. *J. Soln. Chem.*, v. 17, no. 8, p. 777–790 (LBL-23934).

Silica and sodium acetate are present in the steam generator tube sheet crevices of many nuclear power plants. Trace solutes in the condensate are tremendously concentrated in the crevices by boiling. Sparingly soluble sodium silicates and other solids precipitate from the crevice liquid leaving an extremely concentrated molten mixture of water, sodium acetate and other salts. The precipitates buffer the activity of sodium hydroxide in the superheated liquid that remains. The activity of NaOH corresponding to the buffers quartz/sodium disilicate and sodium disilicate/sodium metasilicate at 317°C has been determined experimentally. The sodium hydroxide content of a sodium acetate-water melt buffered by these reactions was determined by chemical analysis, and the corresponding activity of NaOH at temperature was calculated using the recently published Pitzer-Simonson Model of molten salt-water mixtures. The molten mixture of sodium acetate and water plays the role of solvent in these experiments and calculations. The free energies of formation of solid sodium silicates at 317°C were also determined. The activity of NaOH corresponding to other silicate and phosphate buffers was calculated using published thermodynamic data and estimated from phase diagrams.

Wilt, M.J., Morrison, H.F., Lee, K.H., and Goldstein, N.E., 1989. Electromagnetic sounding in the Columbia Basin, Yakima, Washington. *Geophysics*, v. 54, no. 8, p. 952-961 (LBL-25293).

A controlled-source electromagnetic (CSEM) survey was conducted near Yakima, Washington, to map the thickness and resistivity of a thick volcanic sequence overlying a sedimentary section and to infer structure in the sediments. The survey was conducted with a frequency-domain system employing loop transmitters 400-500 m on a side and three-component SQUID magnetometer receivers separated from the loop by 1 to 5 km. Data collected along a 30 km profile orthogonal to regional strike were interpreted initially with 1-D layered models, which were then pieced together to make a geoelectric section. Induction logs in a 5000 m exploration hole at one end of the profile agree very well with the CSEM soundings made around the hole. The geoelectric section reveals a smoothly varying thickness of volcanics with a pronounced anticlinal structure approximately concordant with a surface topographic ridge. To assess the validity of inferring lateral structure from 1-D interpretations, we made scale models of an anticlinal structure and of a surface inhomogeneity and conducted CSEM measurements over the scale models. Layered-model inversions of these data show that the anticlinal structure and its location are very well determined by 1-D inversion, but its height and width are not accurately determined. CSEM sounding over the surface inhomogeneity model shows that this feature does not significantly degrade the interpretation of a deep target layer. In this setting, a geoelectric section made up from 1-D interpretations provides good qualitative measures of subsurface structure and also provides excellent starting models for detailed 2-D or 3-D modeling.

Wollenberg, H., Elchelberger, J., Elders, W., Goff, F., and Younker, L., 1989. DOE thermal regimes drilling program through 1988. *EOS Trans. Am. Geophys. Union*, v. 70, no. 28, p. 697, 706-707 (LBL-27443).

In response to strong endorsement from the scientific community, in the form of a report by the Continental Scientific Drilling Committee of the National Academy of Sciences [CSDC, 1984], the Department of Energy undertook a program of investigations of young magmatic intrusions and their associated thermal systems. To date, the effort has encompassed the first phases of a program to investigate the roots of active hydrothermal systems and has also investigated the intrusions beneath geologically recent (less than 600 years) volcanos. Shallow- to intermediate-depth holes have been drilled and cored into hydrothermal systems in the silicic Valles and Long Valley calderas and at the crustal spreading center of the Salton Trough (Figure 1).

Zheng, Z., Kemeny, J., and Cook, N.G.W., 1989. Analysis of borehole breakouts. *J. Geophys. Res.*, v. 94, no. B6, p. 7171-7182 (LBL-23941).

Boreholes drilled into rock, which is subjected to stresses that amount to a significant fraction of the strength of the rock, may cause the rock to fail adjacent to the borehole surface. Often this results in the elongation of the cross section of the borehole in the direction of the minimum principal (compressive) stress orthogonal to the borehole axis. Such breakouts are valuable indicators of the direction of the minimum compressive stress orthogonal to the axis of the borehole. Their shapes may provide information about the magnitudes of both the maximum and minimum stresses relative to the strength of the rock. Borehole breakouts also may be impediments to drilling and to in situ measurement techniques, such as hydraulic fracturing. Observations and analyses of borehole breakouts raise three important questions. First, how does the shape of the borehole breakout evolve? Second, why are breakout shapes stable despite the very high compressive stress concentrations that they produce? Third, how is the shape of the breakout related to the magnitudes of the stresses in the rock? In this paper, extensile splitting of rock in unconfined, plane strain

compression is assumed to be the process of rock failure adjacent to the circumference of the borehole, by which a breakout forms. To simulate the evolution of a borehole breakout, this process is combined with a numerical boundary element analysis of the stresses around a borehole as its cross section evolves from the originally circular shape to that of a stable breakout. The tangential stresses around a stable breakout cross section are found to be everywhere less than the unconfined, plane strain tensile or compressive strength of the rock. The stresses outside the stable breakout are found to be everywhere less than the limiting values of shear strength given by a Mohr-Coulomb criterion. In the regions of great stress concentrations at the ends of a breakout cross section, which have a pointed shape, the state of stress concentrations at the ends of a breakout cross section, which have a pointed shape, the state of stress approaches that of equal biaxial compression in plane strain, as it does ahead of a mathematical crack or notch. The fact that the stresses around a breakout are less than the relevant strength establishes both the stability of the final breakout cross section and the appropriateness of an elastic analysis of the stresses. According to this model, the cross-sectional shapes of stable breakouts are not related uniquely to the state of stress and the strength of the rock. For example, stable breakouts created instantly in rock already subjected to stress are much larger than stable breakouts created in the same rock with a preexisting borehole by subsequently increasing the stresses to the same values. The results of drilling into an actual rock probably lie between these extremes. Modest changes in borehole cross section as a result of breakout do not alter significantly the minimum tangential (tensile) stress around a borehole with internal pressure from that given by the Kirsch solution for a circular hole subjected to the same stresses. Therefore hydraulic fracturing interpretations based on the Kirsch solution give the correct values for the far-field stresses.

Zimmerman, R.W., 1989. Thermal conductivity of fluid-saturated rocks. *J. Pet. Sci. & Eng.*, v. 3, p. 219-227 (LBL-25197).

A theoretical model is presented for the prediction of the thermal conductivity of fluid-saturated rocks. Rock is idealized as being composed of a connected mineral phase permeated with non-intersecting oblate spheroidal pores. The pores are assumed to be completely saturated with a single-phase fluid. An effective medium theory is used to predict the overall conductivity in terms of the conductivities of the solid and fluid phases, the porosity, and an average aspect ratio of the spheroidal pores. In the limiting case where the pores are thin cracks, the predicted conductivity coincides with the known (Hashin-Shtrikman) lower bound, while the limiting case of spherical pores reproduces the upper bound. The theory is tested against experimental data from various sedimentary and crystalline rocks, and it is shown to allow the prediction of liquid-saturated conductivities based on gas-saturated measurements, without the need for any arbitrary parameters. The model also provides a link to other petrophysical properties that depend on pore structure, such as compressibility.

Zimmerman, R.W., and Bodvarsson, G.S., 1989. An approximate solution for one-dimensional absorption in unsaturated porous media. *Water Resour. Res.*, v. 25, no. 6, p. 1422-1428 (LBL-25629).

The "boundary layer" or "integral" method is used to derive a closed-form approximate solution for one-dimensional absorption of water in an unsaturated porous medium whose characteristic curves are of the van Genuchten type. In this approach, an assumed saturation profile is substituted into the governing equation, and integrated from the boundary out to the wetting front. This yields closed-form solutions for the front location and the instantaneous liquid flux at the boundary. The accuracy of this solution in predicting the flux, as determined by comparison with numerical solutions utilizing a Boltzmann-type transformation, is always within 15%, for any value of the initial saturation. As an example of the use of this approximate solution, saturation profiles are calculated for absorption into the Topopah Spring volcanic tuff at Yucca Mountain, Nevada, the site of the proposed nuclear waste repository.

Zimmerman, R.W., and Bodvarsson, G.S., 1989. Integral method solution for diffusion into a spherical block. J. Hydrol., v. 111, p. 213-224 (LBL-26020).

An approximate analytical solution is derived for the problem of a Newtonian fluid infiltrating into a porous spherical block. The fluid in the block is initially at a constant pressure p_i , and the pressure at the outer

boundary is held at a constant value p_o . Using the simple assumption of linear pressure profiles, the instantaneous and cumulative fluxes into the sphere are predicted with surprisingly high accuracy. The solution applies to all other physical processes governed by the same equation, such as heat conduction and chemical diffusion. The solution should be very useful for incorporation into double-porosity models for fractured reservoirs and aquifers.

APPENDIX B: OTHER PUBLICATIONS

TOPICAL REPORTS

- LBL-20778
Pruess, K., Wang, J.S.Y., and Tsang, Y.W., 1988. Effective continuum approximation for modeling fluid and heat flow in fractured porous tuff.
- LBL-23546
Bjornsson, G., 1988. A multi-feedzone geothermal wellbore simulator (M.S. thesis).
- LBL-24758
Earth Sciences Division, 1988. Geotechnical support and topical studies for nuclear waste geologic repositories.
- LBL-24967
Billaux, D., Uszyski, M., and Benson, S.M., 1988. The applicability of expert systems to risk analysis for waste disposal problems.
- LBL-25073
Bodvarsson, G.S., Niemi, A., Spencer, A., and Attanayake, M.P., 1988. Preliminary calculations of the effects of air and liquid-water drilling on moisture conditions in unsaturated rocks.
- LBL-25486
Wollenberg, H., Eichelberger, J., Elders, W., Goff, F., and Younker, L., 1988. The DOE Thermal Regimes Drilling Program through 1987.
- LBL-25505
Morrison, H.F., Majer, E.L., and Tsang, C.-F., 1988. Critical parameters and measurement methods for post closure monitoring: A review of state-of-the-art and recommendation for further studies.
- LBL-25586
Flexser, S., 1988. Lithologic composition and variability of the sediments underlying Kesterson Reservoir as interpreted from shallow cores.
- LBL-25767
Hwang, Y., Lee, W.W.-L., Chambré, P.L., and Pigford, T.H., 1988. Release rates in a salt repository by diffusion.
- LBL-25768
Hwang, Y., Chambré, P.L., Pigford, T.H., and Lee, W.W.-L., 1989. Pressure-driven brine migration in a salt repository.
- LBL-25769
Light, W.B., Chambré, P.L., Pigford, T.H., and Lee, W.W.-L., 1988. The effect of precipitation on contaminant dissolution and transport: Analytical solutions.
- LBL 26362
Earth Sciences Division, 1989. Earth Sciences Division Annual Report 1988.
- LBL-26438
Earth Sciences Division, 1988. Hydrological, geochemical, and ecological characterization of Kesterson Reservoir.
- LBL-26557
Goldstein, N.E., Pillsbury, S.L., Daggett, J.S., and Benson, S.M., 1988. Contaminant plume monitoring adjacent to the Kesterson Reservoir, California.
- LBL-26672
Lee, W.W.-L., 1989. UCB-NE-107, User's manual.
- LBL-26679
Stark, C.L., and Majer, E.L., 1989. Seismicity of the southeastern Geysers.
- LBL-26700
Lee, W.W.-L., 1989. UCB-NE-102, User's manual.
- LBL-26703
Hwang, Y., Lee, W.W.-L., Chambré, P.L., and Pigford, T.H., 1989. Mass transport in salt repositories: Transient diffusion into interbeds.
- LBL-26704
Hwang, Y., Lee, W.W.-L., Chambré, P.L., and Pigford, T.H., 1989. Mass transport in salt repositories: Steady-state transport through interbeds.
- LBL-26780
Earth Sciences Division, 1989. Geotechnical support and topical studies for nuclear waste geologic repositories: Annual report, fiscal year 1988.
- LBL-27044
Kang, C.-H., and Lee, W.W.-L., 1989. UCB-NE-108 user's manual.
- LBL-27156
Nitsche, H., 1989. Progress report on solubility measurements.
- LBL-27157
Nitsche, H., Standifer, E.M., Lee, S.C., Gatti, R.C., and Tucker, D.B., 1987. Solubility and speciation studies of waste radionuclides pertinent to geologic disposal at Yucca Mountain: Results on neptunium, plutonium and americium in J-13 groundwater (Letter Report R707, October 1, 1985–September 30, 1987).
- LBL-27179
Coakley, K.J., 1989. Spatial statistics for predicting flow through a rock fracture (Ph.D. thesis).
- LBL-27226
Earth Sciences Division, 1989. Soil water and vegetation management for cleanup of selenium contaminated soils.

BOOK CONTRIBUTIONS

- Ginley, G.M., and Radke, C.J., 1989. Influence of soluble surfactants on the flow of long bubbles through a cylindrical capillary. In J.K. Bechard and T.F. Yen (eds.), *Oil Field Chemistry: Enhanced Recovery and Production Stimulation*. ACS Symposium Series No. 396. American Chemical Society, Washington, D.C., p. 480–501 (LBL-24370).

- Jiménez, A.I., and Radke, C.J., 1989. Dynamic stability of foam lamellae flowing through a periodically constricted pore. *In* J.K. Borchardt and T.F. Yen (eds.), *Oil Field Chemistry: Enhanced Recovery and Production Stimulation*. ACS Symposium Series No. 396. American Chemistry Society, Washington, D.C., p. 460-479 (LBL-24369).
- Narasimhan, T.N., 1989. Numerical simulation of Richards equation: Current approaches and an alternative perspective. *In* H.J. Morel-Seytoux (ed.), *Unsaturated Flow in Hydrologic Modeling*. Kluwer Academic Publishers, Dordrecht, The Netherlands, p. 325-341 (LBL-26897).

CONFERENCE PAPERS

- Aunzo, Z., Steingrímsson, B., Bodvarsson, G.S., Escobar, C., and Quintanilla, A., 1989. Modeling studies of the Ahuachapán geothermal field, El Salvador. Presented at the Fourteenth Workshop on Geothermal Reservoir Engineering, Stanford, California, January 21-24, 1989 (LBL-26872).
- Benson, S.M., Daggett, J., Ortíz, J., and Iglesias, E., 1989. Permeability enhancement due to cold water injection: A case study at the Los Azufres geothermal field, Mexico. Presented at the Final Symposium—Agreement between U.S. Department of Energy and Comisión Federal de Electricidad de México in the Field of Geothermal Energy, San Diego, California, April 4-5, 1989 (LBL-27350).
- Carnahan, C.L., 1989. Theory and calculation of water distribution in bentonite in a thermal field. *In* W. Lutze and R.C. Ewing (eds.), *Scientific Basis for Nuclear Waste Management XII* (Berlin, FRG, October 10-13, 1988). Materials Research Society Symposium Proceedings (Vol. 127). Materials Research Society, Pittsburgh, Pennsylvania, p. 729-734 (LBL-26058).
- Carnahan, C.L., 1988. Modeling of coupled chemistry and chemical transport in ground water systems. Presented at the Workshop on Modeling of Dispersion Processes in the Ground, Lejondals Slott, Bro, Sweden, November 29-30, 1988 (LBL-26393).
- Chen, D.W., Zimmerman, R.W., and Cook, N.G.W., 1989. The effect of contact area on the permeability of fractures. *In* A.W. Khair (ed.), *Rock Mechanics as a Guide for Efficient Utilization of Natural Resources: Proceedings, 30th U.S. Symposium on Rock Mechanics*, Morgantown, West Virginia, June 19-21, 1989. A.A. Balkema, Rotterdam The Netherlands, p. 81-88 (LBL-27357).
- Goldstein, N.E., and Alvarez R., J., 1989. Self-potential anomaly changes at the Cerro Prieto geothermal field. Presented at the Final Symposium—Agreement between U.S. Department of Energy and Comisión Federal de Electricidad de México in the Field of Geothermal Energy, San Diego, California, April 4-5, 1989 (LBL-26948).
- Halfman-Dooley, S.E., Lippmann, M.J., and Bodvarsson, G.S., 1989. Progress report on LBL's numerical modeling studies on Cerro Prieto. Presented at the Final Symposium—Agreement between U.S. Department of Energy and Comisión Federal de Electricidad de México in the Field of Geothermal Energy, San Diego, California, April 4-5, 1989 (LBL-27159).
- Jacobsen, J.S., and Carnahan, C.L., 1989. Numerical simulation of cesium and strontium migration through sodium bentonite altered by cation exchange with groundwater components. *In* W. Lutze and R.C. Ewing (eds.), *Scientific Basis for Nuclear Waste Management XII* (Berlin, FRG, October 10-13, 1988). Materials Research Society Symposium Proceedings (Vol. 127). Materials Research Society, Pittsburgh, Pennsylvania, p. 749-754 (LBL-26395).
- Javandel, I., 1989. On the field determination of effective porosity. *In* Proceedings, National Conference on New Field Techniques for Quantifying the Physical and Chemical Properties of Heterogeneous Aquifers, Dallas, Texas, March 20-23, 1989. National Water Well Association, p. 155-172 (LBL-27525).
- Laky, C., Lippmann, M.J., Bodvarsson, G.S., Retana, M., and Cuellar, G., 1989. Hydrological model of the Ahuachapán geothermal field, El Salvador. Presented at the Fourteenth Workshop on Geothermal Reservoir Engineering, Stanford, California, January 24-26, 1989 (LBL-26869).
- Lee, W.W.-L., Pigford, T.H., and Chambré, P.L., 1989. Release rates of soluble species at Yucca Mountain. Presented at the American Nuclear Society meeting "FOCUS '89, Nuclear Waste Isolation in the Unsaturated Zone," Las Vegas, Nevada, September 19-21, 1989 (LBL-26828).
- Light, W.B., Pigford, T.H., Chambré, P.L., and Lee, W.W.-L., 1989. Analytical models for ^{14}C transport in a partially saturated, fractured, porous media. Presented at the American Nuclear Society meeting "FOCUS '89, Nuclear Waste Isolation in the Unsaturated Zone," Las Vegas, Nevada, January 19-21, 1989 (LBL-26827).
- Lippmann, M.J., 1989. Geothermal field case studies that document the usefulness of models in predicting reservoir and well behavior. Presented at the DOE Geothermal Program Review VII, San Francisco, California, March 21-23, 1989 (LBL-26898).
- Lippmann, M.J., Truesdell, A.H., Manón M., A., and Halfman, S.E., 1989. The hydrogeologic-geochemical model of Cerro Prieto revisited. Presented at the Fourteenth Workshop on Geothermal Reservoir Engineering, Stanford, California, January 24-26, 1989 (LBL-26819).
- Long, J.C.S., Hestir, K., Karasaki, K., Davey, A., Peterson, J., Kemeny, J., and Landsfeld, M., 1989. Fluid flow in fractured rock: Theory and application. Presented at the NATO Advanced Study Institute on Transport Processes in Porous Media, Pullman, Washington, July 9-18, 1989. *In* J. Bear and M.Y. Corapciog'u (eds.), *Transport Processes in Porous Media*. Kluwer Academic Publishers, The Netherlands (LBL-27879).
- Majer, E.L., 1989. GTO-DOE/industry cost shared research: Microseismic characterization and monitoring in geothermal systems. Presented at the DOE Geothermal Program Review VII, San Francisco, California, March 21-23, 1989 (LBL-26899).
- Majer, E.L., Peterson, J.E., Myer, L.R., Karasaki, K., Daley, T.M., and Long, J.C.S., 1989. VSP and cross hole tomographic imaging for fracture characterization. Presented at the American Nuclear Society meeting "FOCUS '89, Nuclear Waste Isolation in the Unsaturated Zone," Las Vegas, Nevada, September 18-21, 1989 (LBL-27778).

- Mensch, A., and Benson, S.M., 1988. WES, a robust expert system for well test analysis. Presented at the 1988 American Geophysical Union Fall Meeting, San Francisco, California, December 5-9, 1988 (LBL-27846).
- Narasimhan, T.N., 1988. Theis' contribution and parallel developments in the earth sciences. *In* Recent Advances in Ground-Water Hydrology, Proceedings of the International Conference on Advances in Ground-water Hydrology, Tampa, Florida, November 16-18, 1988 (LBL-26136).
- Persoff, P., Radke, C.J., Pruess, K., Benson, S.M., and Witherspoon, P.A., 1989. A laboratory investigation of foam flow in sandstone at elevated pressure. Presented at the 1989 California Regional Meeting of the Society for Petroleum Engineers, Bakersfield, California, April 5-7, 1989 (LBL-26639).
- Pigford, T.H., and Lee, W.W.-L., 1989. Waste package performance in unsaturated rock. Presented at the American Nuclear Society meeting "FOCUS '89, Nuclear Waste Isolation in the Unsaturated Zone," Las Vegas, Nevada, September 18-21, 1989 (LBL-26934).
- Pruess, K., 1989. Modeling studies of multiphase fluid and heat flow processes in nuclear waste isolation. *In* W. Lutze and R.C. Ewing (eds.), Scientific Basis for Nuclear Waste Management XII (Berlin, FRG, October 10-13, 1988). Materials Research Society Symposium Proceedings (Vol. 127). Materials Research Society, Pittsburgh, Pennsylvania, p. 793-803 (LBL-25688).
- Pruess, K., 1988. Modeling of geothermal reservoirs: Fundamental processes, computer simulation, and field applications. Presented at the Tenth New Zealand Geothermal Workshop, Auckland, New Zealand, November 2-4, 1988 (LBL-25135).
- Pruess, K., 1988. Modeling of fluid and heat flow in fractured geothermal reservoirs. Presented at the International Symposium on Geothermal Energy, Kumamoto and Beppu, Japan, November 10-14, 1988 (LBL-25710).
- Pruess, K., and Tsang, Y.W., 1989. On relative permeability of rough-walled fractures. Presented at the Fourteenth Workshop on Geothermal Reservoir Engineering, Stanford, California, January 24-26, 1989 (LBL-26509).
- Pruess, K., and Wu, Y.S., 1989. A new semianalytical method for numerical simulation of fluid and heat flow in fractured reservoirs. Presented at the Tenth SPE Symposium on Reservoir Simulation, Houston, Texas, February 6-8, 1989 (LBL-26121).
- Ripperda, M., and Bodvarsson, G.S., 1988. A database for the Geysers geothermal field. Presented at the Geothermal Resources Council 1988 Annual Meeting, San Diego, California, October 9-12, 1988 (LBL-26918).
- Steingrimsson, B., Bodvarsson, G.S., Cuellar, G., and Escobar, C., 1989. Changes in thermodynamic conditions of the Ahuachapan reservoir due to production and injection. Presented at the Fourteenth Workshop on Geothermal Reservoir Engineering, Stanford, California, January 21-24, 1989 (LBL-26871).
- Truesdell, A.H., Aunzo, Z., Bodvarsson, G.S., Alonso, J., and Campos, A., 1989. The use of Ahuachapan fluid chemistry to indicate natural state conditions and reservoir processes during exploitation. Presented at the Fourteenth Workshop on Geothermal Reservoir Engineering, Stanford, California, January 21-24, 1989 (LBL 26870).
- Tsang, C.-F., 1989. A new approach to tracer transport analysis: From fracture systems to strongly heterogeneous porous media. Presented at the International Workshop on "Appropriate Methodologies for Development and Management of Groundwater Resources in Developing Countries," Hyderabad, India, February 28-March 4, 1989 (LBL-27031).
- Tsang, C.F., and Hale, F., 1989. A direct integral method for the analysis of borehole fluid conductivity logs to determine fracture inflow parameters. Presented at the National Water Well Conference on New Field Techniques for Quantifying the Physical and Chemical Properties of Heterogeneous Aquifers, Dallas, Texas, March 20-23, 1989 (LBL-27930).
- Yang, G., Cook, N.G.W., and Myer, L.R., 1989. Network modeling of flow in natural fractures. Presented at the 30th U.S. Symposium on Rock Mechanics, Morgantown, West Virginia, June 19-22, 1989 (LBL-26594).
- Zheng, Z., Myer, L.R., and Cook, N.G.W., 1989. Stress induced microcrack geometry at failure in unconfined and confined axial compressive tests. Presented at the 30th U.S. Symposium on Rock Mechanics, Morgantown, West Virginia, June 19-22, 1989 (LBL-26595).

END

DATE FILMED

12 / 27 / 90