NUREG/CP-0040

Proceedings of Workshop V: Flow and Transport Through Unsaturated Fractured Rock—Related to High-Level Radioactive Waste Disposal

Held at
Radisson Suite Hotel
Tucson, Arizona
January 7–10, 1991

Edited by D. D. Evans/UAZ
T. J. Nicholson/NRC

Sponsored by
U.S. Nuclear Regulatory Commission
Center for Nuclear Waste Regulatory Analyses
University of Arizona

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Edited by
D. D. Evans, University of Arizona
T. J. Nicholson, U.S. Nuclear Regulatory Commission

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Center for Nuclear Waste Regulatory Analyses
6220 Culebra Road
San Antonio, TX 78228–0510

Department of Hydrology & Water Resources
University of Arizona
Tucson, AZ 85721

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ABSTRACT

The "Workshop on Flow and Transport Through Unsaturated Fractured Rock Related to High-Level Radioactive Waste Disposal" was cosponsored by the NRC, the Center for Nuclear Waste Regulatory Analyses, and the University of Arizona (UAZ) and was held in Tucson, Arizona, on January 7 - 10, 1991. The focus of this workshop, similar to the earlier four (the first being in 1982), related to hydrogeologic technical issues associated with possible disposal of commercial high-level nuclear waste (HLW) in a geologic repository within an unsaturated fractured rock system which coincides with the UAZ field studies on HLW disposal. The presentations and discussions centered on flow and transport processes and conditions, relevant parameters, as well as state-of-the-art measurement techniques, and modeling capabilities. The workshop consisted of: four half-day technical meetings, a one day field visit to the Apache Leap test site to review ongoing field studies that are examining site characterization techniques and developing data sets for model validation studies, and a final half-day session devoted to examining research needs related to modeling groundwater flow and radionuclide transport in unsaturated, fractured rock. These proceedings provide extended abstracts of the technical presentations and short summaries of the research group reports.

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EXECUTIVE SUMMARY

Proceedings of Workshop V: Flow and Transport Through Unsaturated Fractured Rock — Related to High-Level Radioactive Waste Disposal

D.D. Evans and T.J. Nicholson
University of Arizona and
U.S. Nuclear Regulatory Commission, respectively

A workshop was held in Tucson, Arizona, on January 7 - 10, 1991, to consider various aspects of the hydrogeologic assessment of partially saturated fractured rock for the containment of commercially generated high-level radioactive waste. The impetus for the technical discussions was the possibility of a nuclear waste repository being placed at depth within such a geologic environment. The workshop was sponsored by the U.S. Nuclear Regulatory Commission, both the Division of Engineering in the Office of Nuclear Regulatory Research and the Division of High-Level Waste Management in the Office of Nuclear Materials Safety and Safeguards, the Center for Nuclear Waste Regulatory Analyses, and the University of Arizona. The 60-plus invited participants had extensive research experience in the subject area and several were requested to present up-to-date papers on their recent results and innovative methods to stimulate and direct discussions. Based on these discussions, the final session was devoted to arriving at critical research questions for which answers are needed to improve estimates of travel times and radionuclide release rates within an unsaturated fractured rock setting.

These proceedings are a compilation of extended abstracts (or short papers) for most of the papers presented and the reports of subgroups on their conclusions from the research needs discussions. A list of participants with addresses and phone numbers is included as Appendix A.

Tucson was selected for the workshop in order to observe and discuss ongoing field and laboratory experiments being performed by the University of Arizona under sponsorship of the Nuclear Regulatory Commission (NRC), as well as nearby studies by the Department of Energy (DOE) contractors. The University of Arizona has been under contract with the NRC since 1980 to provide an improved understanding of flow and transport through unsaturated fractured rock and to assess site characterization methods and computer models. This workshop was the fifth in a series on the topic, with the first held in 1982.

The morning before the workshop began, participants were invited to visit the unsaturated rock laboratories at the University of Arizona for demonstrations of several experimental techniques used to characterize the properties of rock matrices, to study nonisothermal flow within a rock matrix, and to examine fracture flow in relation to matrix flow within a fractured block of rock. In addition, laboratory geochemistry techniques were demonstrated.

One full day of the workshop was spent in the field at the Apache Leap Tuff Site where the group was divided into six subgroups to rotate independently among six experimental sites. The activities presented at the sites were: (1) *in situ* fracture characterization using air injection into packed off sections of boreholes and geophysical techniques (Guzman et al.); (2) site characterization for a proposed heater experiment (Rasmussen); (3) rainfall/runoff relationships for two instrumented watersheds (Anderson); (4) geochemical studies relating water chemistry of local surface waters to groundwater discharging to a haulage tunnel after passage through several meters of tuff (Lyons and Bassett); (5) assessment of prototype dry core drilling by DOE at the site (Long, no abstract included); and, (6) an evaluation of gas tracer injection and recovery for the dry-drilled boreholes (Peters et al.). These discussions were of great benefit to the researchers involved at the site and also they set the stage for more meaningful discussions during the remainder of the workshop.

Two of the experiments viewed in the laboratory and two of the field experiments were test cases for Phase I of the international INTRAVAL project and are continuing as test cases in Phase II. Data from the experiments are to be made available to INTRAVAL participants for model calibration and validation. The status of the INTRAVAL project was discussed by Tom Nicholson and Charlie Voss during the workshop. Also, one evening was spent on revising a Phase 1 draft final report for the unsaturated test cases. Another evening was devoted to a discussion of regulatory questions on travel times and release rates, while a third evening session was devoted to a discussion of the general design of the proposed heater experiment at the Apache Leap Tuff Site.

During the four half-day workshop sessions, discussion papers covered a range of subtopics, all focused on the hydrogeologic aspects of performance assessment for a repository in an unsaturated fractured rock setting. To provide background for further discussions, the first presentation of the workshop, by Budhi Sagar, specifically dealt with performance assessment with emphasis on hydrogeologic considerations and questions. Although the discussions were to be generic in nature, a major research effort on the topic is centered on Yucca Mountain at the Nevada Test Site, where the geologic medium is unsaturated welded tuff to a great depth. Allan Freeze had recently chaired a DOE sponsored peer review committee to evaluate the overall hydrologic study program there and he reported on the committee's conclusions as further background for discussions. During the course of the workshop, several other presentations related to specific projects at Yucca Mountain being conducted by DOE contractors which aided in the generic understanding of the processes and characterization techniques related to the workshop topic.

The basic interacting flow and transport processes with the long temporal and spatial scales of interest are unique to the high-level waste repository program and were points of discussion by several participants, especially by Shlomo Neuman. He gave a proposed theoretical framework for the treatment of travel time and radionuclide release rates as two important criteria for site performance assessment. Tom Buscheck and John Nitao presented an assessment of interacting fracture and matrix flow during and following episodic infiltration events.

Research on saturated fractured rock has preceded research on unsaturated rock. The results from research on saturated rock provide insight to unsaturated conditions and methodology development. As an example, a study presented by Yvonne Tsang performed at the Stripa mine in Sweden showed that under near saturated conditions only a few of the many fractures present were significant water conductors. As was stressed, those highly conductive fractures under saturated conditions may be major barriers to flow under unsaturated conditions since they are likely to be drained and air filled. The saturated case is an important limiting case for the study of unsaturated conditions and from which hydraulic properties deviate as the water potential becomes negative.

During an earlier workshop, a possible radionuclide transport mechanism was brought to the attention of the group. Under certain topographic conditions natural air flow through a rock mass may be significant in altering hydrologic conditions and providing a vapor transport role. Since then, this mechanism has been examined and E.P. Weeks gave a report on its magnitude at Yucca Mountain. He concluded that this phenomenon must be considered as a viable mechanism for vapor transport.

Since the liquid in unsaturated fractured rock generally occurs as thin surface films, the physical-chemical properties of the films in relation to the bulk liquid are important considerations to the understanding of flow and transport at larger scales. John Cushman and Martin Schoen evaluated several properties, such as diffusion, density and activation energies, and found the differences to be dramatic when the films are less than 10 fluid molecular diameters.

Rock matrix characterization using cores in the laboratory may be useful estimates of similar parameters in the field. Several techniques and relationships developed primarily in soil physics are being assessed for application to rock core analyses. Alan Flint discussed the approach of model simulation of imbibition experiments to test the adequacy of laboratory determined moisture retention and relative permeability curves and also soil physics generated equations to represent the experimental

data. Lorraine and Alan Flint described a new technique using an automated submersible pressure outflow cell for determining moisture release curves for rock cores. E.M. Kwicklis presented numerical and laboratory results showing flow characteristics of a fractured core in relation to fracture aperture. They also presented innovative techniques being used at their laboratory.

Modeling of hydrologic processes was given considerable consideration during the workshop. Bill Ford presented a summary of unsaturated fractured rock modeling methods in relation to scientific investigations to generate more confidence in numerical modeling results. He pointed out the dire need for verification and calibration at all scales. Rachid Ababou emphasized the complex, three-dimensional nature of the repository large scale problem, with the inherent geologic heterogeneities encountered. His discussion centered on the complexity on modeling flow only, without the added complexities associated with including transport. He proposed the extensive use of submodels as a means of alleviating the problems of a global model. Roger Eaton emphasized through modeling the effects of material heterogeneities on the flow of water through rock.

Several presentations related to the nonisothermal conditions expected around a radioactive source within a repository. Chin-Fu Tsang discussed the coupled processes (i.e., hydrologic, chemical, mechanical and thermal) that will occur in the geologic environment surrounding buried high-level radioactive materials. As an example, he pointed out that the water permeability of a fracture can be increased several orders of magnitude by applying shear stress, or it can be reduced orders of magnitude by the application of normal stress. Approaching the problem from the view of coupled processes leads to a more complete analyses of the relative importance of various processes.

Tom Buscheck and John Nitao, in another paper, discussed their efforts in modeling hydrothermal flow in a variably saturated, fractured rock. They were simulating a nonisothermal experimental case at the Yucca Mountain site. An important outcome of the simulation was a sensitivity analysis of the numerous parameters involved. They compared a fracture-matrix model with an equivalent continuum model using different codes.

Rex Wescott presented a survey of hydrothermal modeling as related to Yucca Mountain. He considered the waste package scale as well as the repository scale. He presented four areas that need further investigation to accomplish a comprehensive model of a repository hydrothermal system. They are: (1) accurate data on fracture and matrix properties as well as initial conditions; (2) a better understanding of fracture transport characteristics; (3) a better understanding of flow and transport characteristics below Yucca Mountain; and, (4) improved thermomechanical and thermochemical models that include changes with time from coupled processes. Karsten Pruess reviewed the present state-of-the-art for modeling two-phase nonisothermal flow.

Data sets for validating nonisothermal models of unsaturated fractured rock are extremely limited. Ron Green presented some preliminary data from nonisothermal laboratory-scale experiments. Injected dye gave a visual demonstration of the general behavior of water in relation to the thermal gradient and a simulated fracture. Further refinements of the experimental arrangement were deemed necessary before a reliable and complete data set can be obtained for model evaluation. As mentioned earlier, some of the experiments discussed during the laboratory and field visits were focused on data sets for nonisothermal flow systems.

Several papers dealt with solute transport. R.S. Bowman evaluated the previous use of tracers for hydrologic studies at Yucca Mountain. The results showed that tracers such as bromide and iodide are subject to anion exclusion, while a tracer like borate is influenced by sorption. By using a suite of tracers simultaneously, several geochemical properties of the rock can be evaluated. Fred Phillips discussed the use of isotopic tracers to study water flow and solute transport in desert soils. He stressed the use of "bomb" tracers because of the slow movement of water under desert conditions and concluded that isotopic tracers are very useful for understanding hydrologic conditions in desert soils and also near surface conditions at a proposed desert repository site. J.T. McCord discussed the

use of environmental tracers for examining flow and transport processes and the characterization of unsaturated rock.

John Stuckless continued the discussion on isotopes by presenting his results for vein deposits in the vicinity of Yucca Mountain and discussed four depositional models for interpretation of the results and the implications for performance assessments. Don Thorstenson reported on gas analysis results for samples extracted at different depths in the unsaturated tuff members at Yucca Mountain as they relate to flow and transport.

The presented papers and the ensuing discussions as well as the laboratory and field trips provided an excellent background for the consideration of technical areas where further research in needed to better predict flow and transport through unsaturated fractured rock. To further set the stage, a paper was provided on research needs by Don Chery and another one by Tom Nicholson. The conclusions of the subgroups were orally reported to the entire group at the end of the last session and are included in these proceedings as prepared by the reporters.

WORKSHOP V

ORGANIZATION AND PROGRAM

Workshop V -	Flow and Transport Through Unsaturated Fractured Rock -- Related to High-Level Radioactive Waste Disposal
Sponsored by -	Nuclear Regulatory Commission Center for Nuclear Waste Regulatory Analyses University of Arizona
Date and Place -	January 7-10, 1991 Radisson Suite Hotel 6555 E. Speedway Tucson, AZ 85710 (602) 721-7100 (800) 333-3333
Organizing - Committee	Thomas J. Nicholson, NRC-RES/WMB Donald L. Chery, NRC-NMSS/TR John L. Russell, CNWRA Al Yang, USGS/Denver Daniel D. Evans, Coordinator Dept. of Hydrology and Water Resources University of Arizona, Tucson, AZ 85721 Tel: (602) 621-7118 Fax: (602) 621-1422
General Scope -	Physical, chemical and coupled processes and relevant parameters, experimental methods and results, modeling -- as related to water flow and transport of contaminants through unsaturated fractured rock

Schedule -	Jan 7	Monday a.m. - Open House, Dept. of Hydrology and Water Resources, University of Arizona Monday p.m. - Technical Session, Radisson Suite Hotel
	Jan 8	Tuesday - Field Trip, Apache Leap Tuff Site
	Jan 9	Wednesday - Technical Sessions, Radisson Suite Hotel
	Jan 10	Thursday a.m. - Technical Session, Radisson Suite Hotel Thursday p.m. - Future Research Session, Radisson Suite Hotel
Registration Fee -	$125.00	

Tentative Program

Workshop V

(Some Titles are Tentative)

Monday Morning - 01/07/91

8:30 to noon	Open House at the Department of Hydrology and Water Resources, University of Arizona.

Monday Afternoon

12:30	Registration in Radisson Suite Hotel Foyer
General	Chairperson: Tom Nicholson, RES/NRC, Salon B
1:00	Introductory remarks -- Dan Evans, U of AZ.
1:15	Performance assessment/hydrogeologic research -- Budhi Sagar, CNWRA
1:45	Hydrogeologic issues at Yucca Mountain: Findings of a DOE peer review team -- Allan Freeze, UBC
2:15	On the relationship between information content and model structure: Advective travel (time) versus dispersion - Shlomo Neuman, U of AZ.
2:45	Break
3:00	Tracer transport in fracture systems -- Yvonne Tsang, LBL
3:30	Nonequilibrium fracture - matrix flow during episodic infiltration events in Yucca Mountain -- Tom Buscheck and John Nitao, LLNL
4:00	Update on INTRAVAL/Phase II Cases -- Thomas Nicholson, NRC and Charlie Voss, Golder and Associates
4:30	Does the wind blow through Yucca Mountain? -- Ed Weeks, USGS, Denver
4:40	Discussion
5:00	Adjourn
5:30	Reception

Monday Evening

7:00-11:00	INTRAVAL Phase I Working Group. Charlie Voss, Leader, Rm 101
8:00-10:00	Travel times and release rates - Discussion: Ron Green, Leader, Salon B

Tuesday Morning and Afternoon - 01/08/91

Field discussions - Apache Leap Tuff Site -- Leaders: Todd Rasmussen and Mike Sully

8:00	Leave hotel with box lunch
10:30	Arrive at field stations -- subgroups rotate among sites
	1. Cross borehole testing/geophysics site -- Mike Sully, U of AZ.
	2. Geochemical site -- Randy Bassett, U of AZ.
	3. Watershed site -- Ingrid Anderson, U of AZ.
	4. Heater experiment site -- Todd Rasmussen, U of AZ.
	5. Gas sampling site -- Al Yang, USGS
	6. Prototype drilling at Apache Leap -- Roy C. Long, DOE
3:00	Leave field sites
5:15	Arrive at hotel

Tuesday Evening

7:00 Group Dinner, Hidden Valley Inn

Wednesday Morning - 01/09/91

Flow and Transport, Chairperson: John Russell, CNWRA, Salon B

8:00	Physical-chemical properties of thin water films -- John Cushman, Purdue Univ.
8:30	Characterization of hydraulic rock properties and verification through modeling -- Alan Flint, USGS/Las Vegas
9:00	Geophysical methods for hydrogeologic characterizations -- Gary Olhoeft, USGS Denver
9:30	Numerical and laboratory investigations of transient and steady - state flow in a fractured core -- E.M. Kwicklis, F. Thamir, R.W. Healy, Carol Boughton, USGS Denver
10:00	Break
10:20	Issues related to modeling -- Bill Ford, NRC/NMSS
10:50	Unsaturated flow and transport modeling -- Rachid Ababou, CNWRA
11:20	Hysteresis Measurement -- Lorraine Flint, Fenix & Scisson
11:50	Discussion
12:00	Group Lunch

Wednesday Afternoon

Nonisothermal multiphase flow and transport. Chairperson: Karsten Pruess, LBL, Salon B

1:15	Coupled processes -- Chin Fu Tsang, LBL
1:45	Field heater test, G-tunnel -- Tom Buscheck, LLNL
2:45	Break
3:00	Status of nonisothermal modeling at Yucca Mountain -- Rex Wescott, NRC/NMSS
3:30	Nonisothermal laboratory experimental results -- Ron Green, CNWRA
4:00	Modeling 2-phase nonisothermal flow -- Karsten Pruess, LBL
4:30	Material heterogeneities and flow -- Roger Eaton, Sandia
4:40	Discussion
5:00	Adjourn

Wednesday Evening

7:30 Proposed field heater experiment: Discussion -- Dan Evans, U of AZ, Discussion Leader, Salon B

Thursday Morning - 01/10/91

Gas and aqueous tracers. Chairperson: Al Yang, USGS/Denver, Salon B

8:00 Evaluation of tracers for hydrologic studies at Yucca Mountain -- Robert Bowman, New Mex. Tech.
8:30 The carbon dioxide and carbon isotopes of gases from borehole UZ-6 at Yucca Mountain -- Donald C. Thorstenson, USGS/Reston
9:00 Flow and transport through unsaturated rock at Yucca mountain: Preliminary stable- and radioactive-isotope analyses - Al Yang, USGS/Denver
9:30 Stable and tracer isotopic studies of hydrogenic deposits exposed at Trench 14, Nevada Test Site, Nevada -- John S. Stuckless, USGS/Denver
10:00 Break
10:20 Isotopic tracer for water and solute movements in desert soils -- Fred Phillips, New Mex. Tech.
10:50 Discussion
12:00 Group Lunch

Thursday Afternoon

1:15 Future Research Session
Co-Chairpersons: Don Chery, Jr., NRC; Dan Evans, U of AZ, Salon B

Objective: To arrive at lists of prioritized technical questions which could be answered through reasonable research endeavors to yield improved estimates of travel times and radionuclide releases for a high-level nuclear waste repository in unsaturated fractured rock.

Procedure:

1. Participants are divided into subgroups with a designated group leader and reporter for each subgroup
2. Each participant independently prepares a list of 10 technical questions considered of highest priority (should be completed prior to the session)
3. Questions are presented to the subgroup, one list at a time with no discussion or elaboration
4. The lists of 10 questions are combined and edited for duplications to form a single list
5. Each participant selects the 20 most important questions and ranks them from 1 to 20, with 1 being of highest priority
6. The rankings are tallied and the 20 with the lowest scores are arranged in ascending order
7. Each of the 20 questions is written at the top of a separate pad of paper. Participants write brief statements of justification and research approaches on pad for each question in turn
8. Group leader leads discussion of products generated. The group summarizes its efforts for reporting to the complete group
9. Each subgroup gives a brief presentation to the entire group and each reporter prepares a written report for inclusion in the final workshop report.

Thursday Evening

7:30 INTRAVAL Working Group I meeting. (All participants are invited)
Group Chairman: Tom Nicholson, NRC/RES, Room 101

FOREWORD

This technical proceedings report was prepared by the University of Arizona as a subcontractor to the Center for Nuclear Waste Regulatory Analyses (CNWRA) under the CNWRA's overall research project (FIN L1810) with the Waste Management Branch in the Office of Nuclear Regulatory Research. The purpose of the workshop was to provide a forum for exchange of technical information related to unsaturated flow and transport in fractured rock related to high-level radioactive waste disposal. While the workshop focused primarily on accomplishments and opportunities at the Apache Leap Tuff field site, scientists working on DOE-sponsored research also made presentations on field, laboratory and computer simulation studies relevant to the Yucca Mountain site. Information and ideas presented at the workshop greatly assisted the University of Arizona and the CNWRA in their research planning. The workshop discussions contributed information to the NRC staff in their evaluation of flow and radionuclide transport in heterogeneous unsaturated fractured rock related to the Yucca Mountain site. This documentation of the proceedings does not constitute the full record of the workshop but only those papers submitted by the speakers and approved by their funding sponsors. The greatest value this proceedings offers the reader is an overview of the scientific arguments, theories, assumptions, and reported field and laboratory data in this newly emerging topical area of unsaturated flow and transport in fractured rock.

NUREG/CP-0040 is not a substitute for NRC regulations, and compliance is not required. The approaches and/or methods described in this NUREG/CP are provided for information only. Publication of this report does not necessarily constitute NRC approval or agreement with the information contained herein.

Hydrologic Research For Performance Assessment

B. Sagar, Center for Nuclear Waste Regulatory Analyses[1]
Southwest Research Institute

INTRODUCTION

Radioisotopes in either the spent fuel or processed waste (such as glass) stored in an underground geologic repository would eventually, after the engineered barriers fail, find their way into the ground water. The times at which such releases would occur, rates of these releases in either the aqueous or the gas phase, rates of transport to the biosphere of the isotopes as dissolved species or colloidal particles in the liquid phase and as volatized particles in the gas phase are germane to assessing the safety of the disposal system. It is, therefore, obvious that the sciences dealing with flow and transport of fluids in geologic materials are central to the successful development and licensing of the geologic repository.

Geologic repositories are supposed to provide permanent disposal of the nuclear waste. Principally, this means that after closure, there will be no long-term (>100 yrs) plans for monitoring of the repository and more importantly there will be no plans for retrieval of the waste. Thus, no long-term (> 100 years) active human management and control of the repository is expected after permanent closure.

The above points to one of the main problems inherent in the concept of the geologic repository. The problem is that the future performance of the repository has to be established with some reasonable confidence, preferably at the time that construction begins, but certainly before decision for permanent closure is made (which may be as much as 100 yrs after construction begins). Of course, performance assessment is required of most engineering entities. However, in the case of the geologic repository this problem is particularly difficult because the time frames are exceedingly long (tens of thousands of years); the geologic materials under consideration vary in space (and in time especially when long time periods are considered) and are therefore difficult to characterize; space scales are large (tens of kilometers); predictive models for estimating future performance are very difficult to verify and validate; and there is little recourse for corrective action after closure.

It is in the context of such a performance assessment that hydrogeologic research needs are to be defined. As explained in the following, what is expected to be calculated during assessment of the performance is defined in the regulations.

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[1] A Federally Funded Research & Development Center supported by the U.S. Nuclear Regulatory Commission. The views expressed in this paper are those of the author and are not intended to represent the positions of either the NRC or the CNWRA.

REGULATORY PERFORMANCE REQUIREMENTS

As stated in the Nuclear Waste Policy Act as Amended (NWPAA 1987), "the disposal system must provide a reasonable assurance that the public and the environment will be adequately protected from the hazards posed by high-level radioactive waste and such spent nuclear fuel as may be disposed of in a repository". The standards for adequate protection of public and environment are encoded as regulations. The primary regulation applicable to high-level waste repositories is contained in 10 CFR Part 60. It incorporates, by reference, applicable parts of another regulation (40 CFR Part 191) in which the U.S. Environmental Protection Agency (EPA) has defined its generally applicable environmental standards vis-a-vis high level and transuranic wastes. The 40 CFR Part 191 is currently under review after being remanded by a federal court.

While one may question the extent to which the regulations of 10 CFR Part 60 are synonymous with 'adequate protection of public and environment' (arguments that these regulations are too strict or not strict enough are advanced in public debates), they never-the-less provide a concrete goal that may focus site investigations and direct repository design and operations. While some of the performance standards of 10 CFR Part 60 are qualitative in nature, others are quantitative. We are primarily interested in the quantitative standards in this paper which may provide pointers towards future research to be done. Rather than verbatim quotations, we paraphrase these requirements. Containment standard of 40 CFR Part 191 require that the cumulative release over 10,000 years of radionuclides at the (arbitrarily defined) accessible environment boundary be less than certain specified limits (known in general parlance as EPA limits) at a specified probability level. Two probability levels are specified. With a probability of at least 99% the cumulative release is to be no more than one EPA limit. At a probability level of 99.99% or greater, the cumulative release is to be no more than 10 EPA limits. In calculating the cumulative release, all possible (credible) future states of the system that may evolve over the 10,000 year period must be considered. There are other numerical standards in 10 CFR Part 60 that apply to parts of the system. These include a requirement on the minimum life time of the waste package (300 to 1,000) years; a maximum annual release rate of no greater than 10^{-5} of the inventory; and a minimum pre-waste emplacement ground water travel time of 1,000 years. All of these numerical standards require modeling involving hydrogeology.

The point we want to emphasize in this section is that the abstract phrase "adequate protection of public and environment" in the NWPAA has been translated in the form of regulations into concrete numerical performance requirements. These regulatory performance standards may or may not help in determining research needs in hydrogeology but should be given due consideration.

HYDROGEOLOGY FOR PERFORMANCE ASSESSMENT

The broad research objective of hydrogeology is to develop methods (field testing, laboratory research, and mathematical modeling) that would lead one to predict the space-time distribution of pressures, temperatures, concentrations, and other such variables of interest. In parallel, the ultimate research objective of other geo-disciplines is to determine the

initial conditions (existing geologic setting), boundary conditions and future states (evolution of geologic setting including volcanism, seismicity and climate). If and when both these research objectives are fulfilled, then the future performance of the system can be determined (we are excluding the more difficult problem of evolution of humans and their diet in the 10,000 years since these are not directly a part of the regulatory performance requirements) provided that the needed parameters that occur in the theoretical models can be measured. In a purely research context, and in the long term, those are the hydrogeologic research objectives that should be pursued.

In practice, within the constraints of schedule and resource availability, these research objectives are unlikely to be met. The question then becomes: Is it possible to formulate research objectives that may be somewhat more limited than the scientific objective stated above, yet sufficient (in the regulatory sense) for "assessing performance with reasonable assurance?"

An attractive resolution to the above question is to stipulate that all currently known fundamental questions in hydrogeology are equally important and must be resolved before undertaking any performance assessment. Another resolution will be pragmatic and set research priorities based on performance assessments that are based on existing knowledge and what is determined to be important from these assessments. The second resolution is fraught with the possibility that some phenomena not considered in current performance assessments may be found to be important later. On the other hand, the first resolution may focus on certain questions that are later found to be not important to the performance of the repository. Perhaps, an acceptable answer to the question lies between these two resolutions. This is slated to be the topic of discussion on Thursday afternoon of this workshop and we assume that some collective conclusions will be drawn at that time.

SOME SPECIFIC HYDROGEOLOGIC ISSUES IN PERFORMANCE ASSESSMENT

Hydrogeology at the Near-Field Scale

At least two spatial scales are easily identifiable for hydrogeology as it is expected to be used in performance assessment. The smallest of these, the near-field scale, has spatial dimensions of the order of the waste package (few meters) or at most a group of waste packages (tens of meters). At this scale, water either as liquid or as vapor transports degradation agents (e.g., oxidants) to the surface of the waste packages that eventually result in their failure. The volatile materials are released from the waste packages at this time and are ready to be transported to the accessible environment. Subsequently, as the water comes into contact with the waste form, waste leaches into the water. This provides the source term for the far-field transport. From the regulatory performance point of view, unless the engineered barriers are predicted to last for over 10,000 yrs or the geologic setting is predicted to not transport any material for the same period, the source term is extremely important.

In general, the hydrogeologic environment in the near-field can be characterized as non-isothermal, multi-phase (liquid and gas), multi-species (radionuclides dissolved in water, volatiles as part of the gas phase) fluids

moving in fractured heterogeneous media. The degradation of waste packages is a complex process that is dependent upon waste package material type, temperature, flow rate, and chemical conditions.

O'Neal et al. (1984), for the reference design of the proposed Yucca Mountain repository, estimated the maximum temperatures at the bore hole wall to be 236° C at about 20 years. In contrast, taking mobile water in fractures into consideration and hence considering formation of heat pipe, Pruess et al. (1990a) estimated the maximum temperature to be close to 100° C. Obviously, consideration of water flow in fractures is extremely important for thermal and hence geochemical analysis in the near field. It would be interesting to investigate the relation between the highest temperature achievable and heat loading or other design parameters. If the heat pipe is proven to be as efficient a heat carrier as Pruess et al. (1990a,b) show in their calculations, then first the recent discussions about cooling of the waste outside of the repository appears to be moot and secondly, if it is indeed a design objective to keep the waste packages dry for a certain time period, then an increase in the heat loading may be possible resulting in economy of design. Interestingly, Pruess et al. (1990b) also show that the equivalent continuum approach (Klavetter and Peters, 1986) produces results very similar to the discrete fracture approach. This may simplify the analyses somewhat provided that some acceptable method of estimating the equivalent conductivities can be found. However, it is to be noted that Buscheck in his recent work (unpublished) disputes this conclusion as it may be applied to radionuclide transport. He finds that the equivalent continuum approach tends to predict a delayed breakthrough. Ultimately, we must conduct well-designed tests to decide upon which of these approaches would be acceptable for performance assessment. We believe that similitude principles thought to be applicable to this problem need to be developed as a first priority for hydrogeologic research at this scale.

Speciation and solubility of waste elements is another important but highly uncertain feature of determining the source term. Calculations based on partial equilibrium and reaction kinetics (Ogard and Kerrisk, 1984, Arthur and Murphy, 1989) have shown that the aqueous silica concentration and CO_2 pressure exert important controls on the chemistry of the solid and liquid phases at the Yucca Mountain site. Current models, however, are limited by the lack of thermodynamic and kinetic data. Precise site-specific space-time evolution of geochemistry, like hydrogeology, is a research aim to be strived for. However, from a regulatory performance assessment point of view, it appears that research ought to be focused on establishing upper bounds on elemental solubilities.

Hydrogeology at the Far-Field Scale

The far-field scale extends from the repository to the accessible environment boundary (few kilometers) and beyond. Assuming that the engineered barriers would last for some minimum period of time in which the heat will be dissipated (probably efficiently due to the heat pipe effect), it may be possible to consider the far-field hydrogeologic problem to be isothermal.

Percolation from precipitation at the surface is considered to be the main force driving water flow in the unsaturated zone at the Yucca Mountain

site and its estimates remain highly uncertain. Current models assume an average uniform recharge rate of anywhere from 0.01 mm/yr to 5 mm/yr. From the precipitation distribution in space and time at the Yucca Mountain, it can be easily inferred that percolation is non-uniform both in space and time. Obviously, a flow field produced by average percolation may be very different from the one produced by episodic percolation events. Based on the current understanding of flow in fractures, larger percolation events (in contrast to a small average yearly rate) can be expected to produce more frequent fracture flow events and may transport radionuclides to greater depths. Measured ^{36}Cl concentrations at depths of over 150 meters from underground bomb tests support such conclusions. In addition to variable recharge, due to the draining capabilities of faults intersecting proposed repository and due to the presence of intersecting fractures at the site, the partially saturated flow system is in transient conditions at most times. Due to the varying boundary conditions on the mountain and due to layered hydrostratigraphy, the flow is also multi-dimensional.

Recent (unpublished DOE PACE Exercises 1990) calculations by Birdsell show a large difference between one-, two-, and three-dimensional saturation profiles at the Yucca Mountain site. Such simulations however, need to be taken a step further to see how much these differences in saturation profiles will influence the calculation of cumulative release. Modeling of a non-linear transient, multi-dimensional, heterogeneous system at the space and time scales of interest is obviously complicated, especially with sparse knowledge of the site properties. Therefore, hydrogeologic research at this scale should be focused on determining appropriate simplifications that would produce conservative results. The hydrogeologic system being non-linear, this by no means is an easy task.

Current use of geochemistry in far-field transport of contaminants is limited to using a static and linear retardation process which covers many phenomena such as ion exchange and surface adsorption. While this concept has been used for many years in a number of applications (e.g., hazardous waste disposal), it is by no means accepted. Research ought to focus on whether retardation factors, while not theoretically correct, are sufficient (implicitly, conservative) for estimating performance.

SUMMARY

Regulations recognize that scientific and technical uncertainties will pervade throughout the process of performance assessment of geologic repositories. Since all fundamental issues of hydrogeology (and other disciplines) will probably not be resolved within the schedule, the regulations do not ask for the demonstration of repository performance in the strict sense of scientific proof. Instead, reasonable assurance is sought by forcing the system to be conservative by including multiple barriers, requiring redundancy, and gathering of evidence from diverse sources (laboratory, field, natural analogues). Therefore, while precise prediction of space-time distribution of contaminant plumes should be the long-term goal of hydrogeologic research, approximations may be acceptable for performance assessment. Also, other (including qualitative and subjective) evidence, in addition to performance assessment, will be considered in the licensing process in deciding whether a repository will serve its function.

Because all credible future states of the system must be considered, numerous hydrogeologic analyses must be performed for a complete performance assessment. Since the current system state as well as the future system states will have uncertainties, and also because some of the fundamental issues will remain unresolved, these analyses would most likely be performed in a probabilistic framework, thus adding to the calculational task. While it is important that outstanding fundamental problems be addressed in research, it is equally important to devote effort to simplify and research those issues that have the most impact on performance. Those issues that have lesser impact on performance will need to be shown to be addressed by the redundancy in the system.

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HYDROGEOLOGIC ISSUES AT YUCCA MOUNTAIN: FINDINGS OF A DOE PEER REVIEW TEAM

R. Allan Freeze
University of British Columbia

INTRODUCTION

The Unsaturated Zone Hydrology Peer Review Team (PRT) was established by the Regulatory and Site Evaluation Division of the Yucca Mountain Project Office of the U.S. Department of Energy. The members of the PRT were: Lorne Everett, Allan Freeze (Chairperson), Rien van Genuchten, Gerry Grisak, Jim Mercer, Bill Nelson and Stavros Papadopulos. The technical secretary was Marvin Saines, and DOE liaison was provided by Claudia Newbury. In addition four observers were invited to represent the participating research agencies: Dwight Hoxie (U.S. Geological Survey), Everett Springer (Los Alamos National Laboratory), George Barr (Sandia National Laboratory), and Dwayne Chestnut (Lawrence Livermore Laboratory).

The objective of the peer review was to evaluate the work done within the Yucca Mountain Project in developing an understanding of unsaturated zone hydrology at the Yucca Mountain site, and to provide recommendations to DOE regarding unsaturated zone hydrologic investigations at Yucca Mountain. The PRT was specifically asked to consider: (1) matrix flow, (2) fracture flow, (3) gaseous flow, (4) the presence and effectiveness of capillary barriers, (5) the presence and effectiveness of fracture barriers, and (6) saturated-unsaturated groundwater travel times. It was agreed that the PRT deliberations would emphasize the natural hydrogeological system rather than the response of this system to the emplacement of the repository. Emphasis therefore fell on the flow processes at the expense of detailed consideration of radionuclide transport processes.

The first meeting of the PRT was held in Las Vegas on April 23 - 26, 1990. The output from this meeting was a list of questions and topics to be addressed by the Principal Investigators (PI's) of the Yucca Mountain Project at a second meeting of the PRT. The second meeting was held in Las Vegas on June 4 - 8, 1990. Presentations by the PI's were followed by lengthy discussion periods, and there was considerable interaction between the PI's and PRT, and among the PI's themselves.

The PRT submitted its Peer Review Record Memorandum (PRRM) to DOE in September 1990. In this document the PRT found itself in essential agreement with the conceptual hydrologic model espoused by members of the Yucca Mountain project teams (Montazer and Wilson, 1984; Lin and Tierney, 1986; Hoxie, 1989). The PRT did not identify any conceptual hydrologic paths of fluid flow through the unsaturated zone at Yucca Mountain that have not come under consideration as potential radionuclide migration routes by the various research

teams. The PRT was impressed with the strong motivation of the research teams and with the high scientific quality of the ongoing research programs.

The PRRM includes 24 conclusions and recommendations, divided between those based on Programmatic Issues and those based on Technical Issues. Among the programmatic issues identified were: (1) the need for improved program integration and interagency communication, (2) the need for project prioritization procedures within the project, (3) the negative impacts of the current quality-assurance environment, and (4) the need for closer coordination of construction activities and research activities so as to prevent undue site disturbance. These programmatic issues will not be discussed further; emphasis in this presentation is placed on the technical issues. The technical issues encompassed both the unsaturated zone and the saturated zone; emphasis here will be on the unsaturated zone.

CURRENT UNDERSTANDING OF UNSATURATED HYDROLOGIC PROCESSES AT YUCCA MOUNTAIN

Yucca Mountain presents a complex hydrologic setting to the analyst. The inter-bedded welded and nonwelded tuffs that exist at the site produce a layered stratigraphic sequence of porous fractured rocks in which contiguous layers differ strongly in their unsaturated hydraulic properties and in the spacing and aperture of their fracturing. In addition, the presence of small-scale geologic features such as fracture coatings, and large-scale geologic features such as fault zones, complicate the hydraulics. There is both water flow and gas flow in the mountain, and the latter is likely to be affected by the atmospheric thermal and barometric regime. At the very least, an understanding of unsaturated-zone hydrology requires consideration of non-isothermal, two-phase fluid flow in heterogeneous, fractured, porous materials.

Despite this complexity, there appear to be several aspects of the hydrologic system that are reasonably well understood at this point in the program: (1) Both low-intensity long-duration winter precipitation and high-intensity summer storms provide a source of water for infiltration on the washes, ridges, slopes and upland areas of Yucca Mountain. (2) Large-aperture surface fractures can deliver infiltration water to depths of several tens of meters in a short time. (3) Unsaturated-zone vapor-phase transport can significantly redistribute moisture within the shallow unsaturated zone. (4) There will almost certainly be perched zones of saturated conditions that will develop at depth. (5) Although open fractures undoubtedly act as capillary barriers at the local scale, it is doubtful that horizontal fractures are sufficiently continuous, open and interconnected so as to represent a physical discontinuity capable of creating a significant barrier to moisture infiltration. (6) There are many potential mechanisms that could lead to the generation of preferential saturated flow paths in the vadose zone. (7) There are also many potential mechanisms that could significantly delay and attenuate such flow.

There are still major uncertainties associated with some of the most important processes. These include: (1) the processes describing matrix-fracture interactions and the theoretical basis of current models that quantify these processes; (2) the attenuation potential of bedded nonwelded tuffs; (3) the role of gas flow; (4) the role of faults; and (5) the role of fracture coatings. The first three of these are addressed below.

FRACTURE- MATRIX INTERACTIONS

The most important conceptual issue in unsaturated-zone fractured-rock hydraulics revolves around the processes of matrix-fracture interaction. It is extremely difficult to develop a single, coherent and complete theoretical formulation capable of evaluating non-isothermal multi-phase fluid flow in a dual-porosity medium. As a result, an elegant but approximate theoretical formulation has emerged (Wang and Narasimhan, 1985; Peters and Klavetter, 1988). This approach incorporates fracture-flow in overlapping fracture and matrix continua. The dependent pressure is assumed to be the same in both the fracture and matrix continua. This assumption breaks down across a wetting front that is advancing into an initially drier portion of the system, so for this situation the wetting front is represented as an advancing instantaneous shock wave.

This theoretical formulation is a carefully thought-out and well-documented approach to considering fracture and matrix flow under isothermal conditions. However, it is imperative that there be continued evaluation of the assumptions that underlie this approach, in particular, the assumption of rapid attainment of equilibrium fluid pressure across the matrix-fracture boundary, and the acceptance of the concept of overlapping continua.

This latter concept presumes that the unsaturated characteristic curves for rock can be specified using the types of empirical relationships derived for unconsolidated materials, and that composite values of the hydraulic conductivities and moisture capacity coefficients, expressed as functions of the pressure head, are representative of the combined matrix-fracture system.

Few, if any, examples exist in the literature to guide the experimental plan for measuring these hydraulic properties. Many innovative techniques are under development by scientists involved in the Yucca Mountain project. They will be especially challenged by the determination of hydraulic properties of fractures at relatively high pressure heads ($-50 < h < 0$ cm), and of the rock matrix at relatively low pressure heads ($-10^5 < h < -10^3$). There is little evidence that supports mercury intrusion methods, and there are apparent limitations to both centrifugal methods and psychometry methods.

Even more fundamental than potential laboratory instrumentation problems is the question of whether laboratory measurements on small rock samples are in any way representative of actual field conditions. In particular, they may not reflect

the small-scale spatial variability of hydraulic properties that may lead to the development of preferential flow paths.

It was the opinion of the PRT that further theoretical developments of matrix-fracture interactions are unlikely to be fruitful until the current theories are confirmed or adapted on the basis of controlled laboratory and field experimentation. Although the emerging theories are rigorous under the assumptions involved, meeting some of those assumptions is doubtful enough that careful validation is now required.

ATTENUATION POTENTIAL OF BEDDED NONWELDED TUFF

It has been observed at Yucca Mountain that the fracture density is much lower in nonwelded tuffs that in welded tuffs. One of the most critical features of the conceptual hydrologic model for Yucca Mountain is the postulated ability of nonwelded tuffs to attenuate transient moisture pulses. In particular, it is thought that the vitric tuffs of the near-surface Paintbrush nonwelded unit may significantly attenuate the downward migration of infiltrating water, and the zeolitized tuffs of the Calico Hills nonwelded unit, which lie below the proposed repository horizon, may significantly attenuate downward water percolation at depth.

Development of the attenuation concepts are based on interpretations of results from computer simulations of unsaturated flow that are based on the conceptual model of fracture-matrix interactions described in the previous section. For the reasons outlined there, it is imperative that field experimentation in the Paintbrush nonwelded tuffs of the Calico Hills unit be carried out to investigate the validity of the attenuation mechanism.

GAS FLOW

Recent evidence makes it clear that there is substantial air flow in the unsaturated fractured tuffs near the crest of Yucca Mountain(Thorstenson, et al, 1989). These flows are attributed to convective circulation through larger fractures arising from topographic relief, seasonal temperature variations, pressure changes, and density differences resulting form variations in gas composition. Initial modeling results (Kipp, 1987; Amter and Ross, 1990) have helped to assess the relative importance of the various contributing mechanisms. Further work is needed to determine the depth of active air circulation, and to assess the role of the circulation system in the redistribution and discharge of moisture, and as a potential transport mechanism for radionuclides. In addition, the potential impacts that the natural flow of air through Yucca Mountain will have on field experiments will have to be evaluated. It is possible that gaseous transport is at least partially responsible for the observed inconsistencies between unsaturated-zone travel times calculated on the basis of Darcy's law and those indicated by isotopic ages based on tritium and chlorine-36 determinations.

SITE CHARACTERIZATION PHILOSOPHY

There is no site characterization program that could be expected to remove all uncertainty as to the three-dimensional character of the layered stratigraphy, the location of vertical faults, the continuity and connectivity of fracture systems, and the presence or absence of zones of saturation in the unsaturated zone.

Under these circumstances, the PRT is of the opinion that the traditional approach to site characterization is not likely to be successful. In the traditional approach models accept field-based measurements of the hydrogeological parameters (such as hydraulic conductivity) as input, and produce predictions of state variables (such as hydraulic head) as output. The predicted values of the state variables are compared against values observed in the field, and a calibration process continues in an interactive fashion until relatively accurate predictions of site response to proposed engineering projects can be made.

Instead of this traditional approach, the PRT recommended a hypothesis-testing approach to site characterization, whereby the calibration of hydrologic models is carried out with respect to integrated performance measures rather than a detailed matching of the state variables. The approach emphasizes the collection of field data for the purpose of reducing conceptual uncertainty through the testing of hypotheses, rather than for the reduction of parameter uncertainty per se.

The testing of hypotheses is a statistical procedure, and the acceptance or rejection of a hypothesis is accompanied by a confidence level that can be generated by stochastic modeling. In this case, the output from stochastic modeling is related to an accept/reject, terminate/expand type of decision. The stochastic modeling is not carried out simply to identify the level of uncertainty, rather, it is an aid to decision making.

This philosophy of site characterization could be applied to the issues of fracture-matrix interaction, moisture attenuation by nonwelded tuff, and moisture redistribution by gas flow, as outlined above.

NEED FOR PROTOTYPE STUDIES IN THE FIELD

In the PRRM, the PRT stated its strongly-held view that it is imperative that the Yucca Mountain research teams gain access to suitable field sites on Yucca Mountain, or in similar terrain elsewhere, in order to carry out prototype studies required for equipment testing, concept hypothesis testing, field methodology development, and model validation.

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ON THE RELATIONSHIP BETWEEN INFORMATION CONTENT AND MODEL STRUCTURE: ADVECTIVE TRAVEL (TIME) VERSUS DISPERSION

Shlomo P. Neuman, University of Arizona

In this extended abstract I review some key EPA standards and NRC regulations concerning the role of the geologic setting in barring radionuclide migration from high-level nuclear waste repositories to the accessible environment; I identify some questions (printed in italics) based on these standards and regulations; and I propose a theoretical framework within which at least some of these questions could, in principle, be answered.

EPA STANDARDS (According to Working Draft 2 of 40 CFR Part 191, 1-31-90), NRC REGULATIONS (According to 10 CFR Ch.1, 1-1-90 Edition) AND SOME RELATED QUESTIONS

EPA 191.13 CONTAINMENT REQUIREMENTS: (a) Disposal systems for spent nuclear fuel or high-level or transuranic radioactive wastes shall be designed to provide a reasonable expectation, based upon performance assessments, that the cumulative releases of radionuclides to the accessible environment for 10,000 years after disposal from all significant processes and events that may affect the disposal system shall: (1) have a likelohood of less than one chance in 10 of exceeding the quantities calculated according to Table 1 (Appendix B) [Release Limit per 1,000 MTHM or other unit of waste] ; and (2) have a likelihood of less than one chance in 1,000 of exceeding ten times the quantities calculated according to Table 1 (Appendix B).

"Performance assessment" means an analysis that: (1) identifies the processes and events that might affect the disposal system; (2) examines the effects of these processes and events on the performance of the disposal system; and (3) estimates the cumulative releases of radionuclides considering the associated uncertainties, caused by all significant processes and events. These estimates shall be incorporated into an overall probability distribution of cumulative release to the extent practicable.

EPA is also considering options for INDIVIDUAL AND GROUNDWATER PROTECTION REQUIREMENTS such as

EPA 191.5 ... to provide a reasonable expectation that for X [1,000 or 10,000] years after disposal, undisturbed performance of the disposal system shall not cause the annual commited effective dose equivalent due to all potential pathways from the disposal system to any member of the public in the accessible environment to exceed Y [25 or 10] millirems. These pathways shall include the assumption that individuals consume 2 liters per day of drinking water from any high-yield aquifer outside of the controlled area.

EPA 191.16 (a) ... to provide a reasonable expectation that, for X years after disposal, undisturbed performance of the disposal system shall not cause: (1) any increase in the levels of radioactivity in any portion of a special source of ground water *etc.*

"Committed effective dose equivalent" means the total dose equivalent received over a lifetime by an individual following an intake of radionuclides into the body, multiplied by appropriate weighting factors ...

NRC 60.113(a)(2) ... The geologic repository shall be located so that prewaste-emplacement **groundwater travel time** along the **fastest path** of likely radionuclide travel from the disturbed zone to the accessible environment shall be **at least 1,000 years** or such other travel time as may be approved or specified by the Commission.

NRC 60.122(b)**Favorable conditions(7)** Pre-waste-emplacement **groundwater travel time** along the **fastest path** of likely radionuclide travel from the disturbed zone to the accessible environment that **substantially exceeds 1,000 years.**

How does this travel time relate to measurable site characteristics and to EPA Standards?

NRC 60.102(e)(2) ... The engineered barrier system works to control the release of radioactive material to the geologic setting and **the geologic setting works to control the release ... to the accessible environment. Isolation** means inhibiting the transport of radioactive material so that **amounts and concentrations** of the materials **entering the accessible environment will be kept within prescribed limits.**

How precisely do these amounts and concentrations relate to travel time, measurable characteristics of the geology, and EPA standards?

NRC 60.21(c) The Safety Analysis Report shall include: ... (1)(ii)(C) An evaluation of ... performance ... **giving the rates and quantities of releases** of radionuclides to the accessible environment **as a function of time;**

In what relation to EPA standards? This evidently requires reliance on models of time-dependent transport? The latter must further be validated:

NRC 60.21(c)(1)(ii) **The assessment shall contain:** (F) An explanation of measures used to support **the models used to perform the assessments** required in paragraphs (A) through (D). **Analyses and models that will be used to predict future conditions and changes in the geologic setting shall be supported by using an appropriate combination of such methods as field tests, in situ tests, laboratory tests which are representative of field conditions, and natural analog studies.** NRC 60.101(a)(2) ... For ... long-term objectives and criteria, what is required is reasonable assurance making allowance for ... uncertainties involved, that the outcome will be in conformance with those objectives and criteria. **Demonstration of compliance** with such objectives and criteria **will involve the use of data from accelerated tests and predictive models that are supported by** such measures as **field and laboratory tests, monitoring data and natural analog studies.**

*What must be measured in the field and/or laboratory, **how and on what scale(s)** in space-time, to allow the QUANTITATIVE ESTIMATION of TRAVEL TIME along the fastest path, AMOUNTS and CONCENTRATIONS entering the accessible environment, and RATES and QUANTITIES of releases to the accessible environment AS A FUNCTION OF TIME, as well as the associated ESTIMATION UNCERTAINTY, once release rates from the engineered repository have been specified?*

In what precise way is such quantitative estimation aided by "detailed information" of the kind required in NRC 60.21(c)(1)(i), *particularly* (A) The orientation, distribution, aperture, in-filling and origin of fractures, discontinuities, and heterogeneities; (B) The presence and characteristics of other potential pathways such as solution features, breccia pipes, or other potentially permeable features? *How, in what quantity, and on what scale(s) need such information be collected?*

What "hydrogeologic properties and conditions" [60.21(c)(1)(i)(D)] *must be determined, how,*

in what quantity, and on what space-time scale(s) to make such quantitative estimation possible?

To what extent, if any, can models and analyses which attempt to make such quantitative estimates be validated? What is the meaning and importance of this term? What validation strategy, if any, should the NRC adopt?

A PROPOSED THEORETICAL FRAMEWORK

TRAVEL TIME AND CUMULATIVE RELEASE: Consider the random advective (Eulerian) seepage velocity field

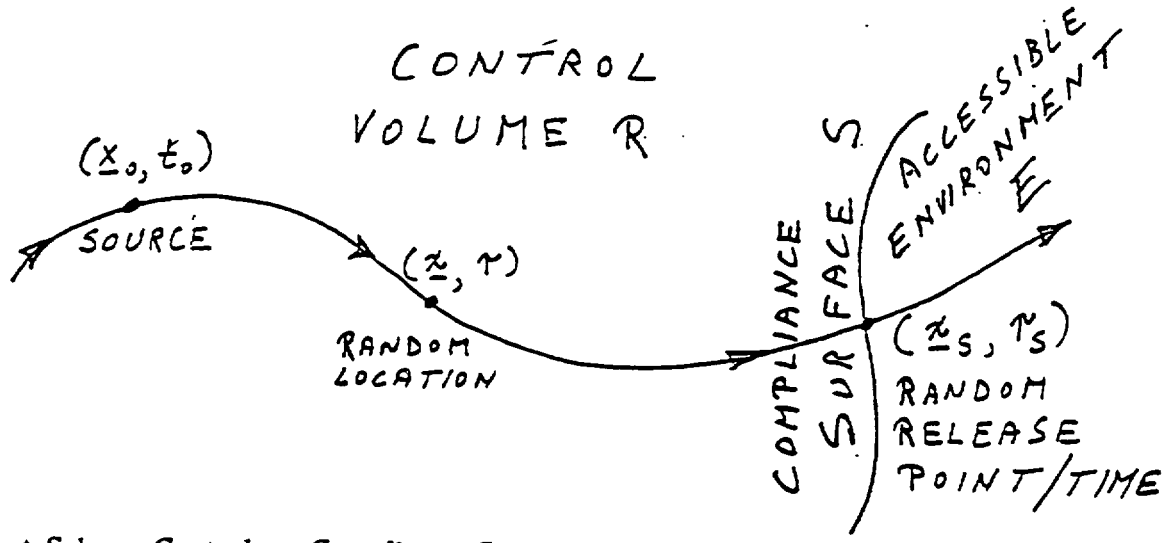
$$v(x,t) = \langle v(x,t)\rangle + v'(x,t) \tag{1}$$

where

$$\langle v(x,t)\rangle = \text{ensemble mean velocity} \tag{2}$$

$$v'(x,t) = \text{zero-mean fluctuation about } \langle v(x,t)\rangle. \tag{3}$$

Randomness stems from ***space-time variability of*** v(x,t) and ***errors in its estimation.***



Let S be a ***Control or Compliance Surface*** enclosing the ***Repository Control Volume*** R from the ***Accessible Environment*** E. Following G.I. Taylor's (1921) *theory of continuous motions*, consider an indivisible solute "particle" of mass M_0 released from the repository to the host rock at point x_0 and time t_0, then traveling along a ***random trajectory (flow path)*** to cross S into E at the ***random point*** x_S and ***random arrival time*** τ_S (***travel time*** $\tau_S - t_0$). Assume for simplicity, and without loss of generality, that all streamlines emanating from the repository intercept S at some random point in space-time.

Following Dagan (1987, 1989) we write

Total (random) particle displacement
= Advective displacement + Brownian Displacement

$$X_t = X + X_B \tag{4}$$

where the Brownian component accounts for classical (local) Fickian dispersion. The *concentration* due to this particle is

$$c(x,t;x_0,t_0) = \frac{M_0}{\theta}\,\delta(x-x_0-X_t) \tag{5}$$

where θ is *water content*. Assuming for simplicity that θ = constant, the *ensemble mean concentration* is

$$<c(x,t|\,x_0,t_0)> = <\frac{M_0}{\theta}\,\delta(x-x_0-X_t)> = \frac{M_0}{\theta}\,f(x;t,x_0,t_0) \tag{6}$$

where

$$f(X_t\,|\,t,x_0,t_0) = \text{pdf of } X_t\text{, evaluated at } x_0+X_t = x. \tag{7}$$

Define

$G(\tau_S;S,x_0,t_0)$ = the *cumulative probability that a particle released from the repository location* x_0 *at time* t_0 *crosses the compliance surface* S *into the accessible environment E during any time* $t_0 < t \leq \tau_S$. Then

$$G(\tau_S;S,x_0,t_0) = 1 - \int_R f(x;\tau_S,x_0,t_0)\,dx. \tag{8}$$

By virtue of (6), this can be written as

$$G(\tau_S;S,x_0,t_0) = 1 - \frac{\theta}{M_0}\int_R <c(x|\,\tau_S,x_0,t_0)>\,dx = \frac{<M_S(\tau_S\,|\,x_0,t_0)>}{M_0} \tag{9}$$

$M_S(\tau_S\,|\,x_0,t_0)>$ = mass having reached the accessible environment E during $t_0 < t \leq \tau_S$.

Dagan thus establishes a ***clear and unequivocal relationship*** **between the** ***cumulative probability*** G **of the (random)** ***travel time*** $\tau_S - t_0$, **as well as the** ***mean cumulative release*** **to the accessible environment,** $<M_S(\tau_S\,|\,x_0,t_0)>$, **and the** ***ensemble mean concentration*** $<c(x,t|\,x_0,t)>$.

We now depart from Dagan's analysis by noting that the ***actual mass*** having reached the accessible environment by time τ_S is

$$M_S(\tau_S\,|\,x_0,t_0) = M_0 - \theta\int_R c(x|\,\tau_S,x_0,t_0)\,dx. \tag{10}$$

We take the view that

$<M_S>$ = ***unbiased estimate*** **of the cumulative release** M_S

which is associated with the zero-mean ***estimation error***

$$M_S' = M_S - <M_S> \qquad <M_S'> = 0. \tag{11}$$

Hence the ***estimation variance*** can be written as

$$\text{Var } M_S'(\tau_S\,|\,x_0,t_0) = \theta^2\int_R <c'(x|\,\tau_S,x_0,t_0)^2>\,dx \tag{12}$$

where

$$c'(x,t) = c(x,t) - <c(x,t)> \qquad <c'(x,t)> = 0. \tag{13}$$

We further take the attitude that

$<c(x,t)>$ = ***unbiased estimate*** **of the real concentration** $c(x,t)$,

$c'(x,t)$ = associated ***estimation error***.

Clearly our ability to estimate M_S **(and, by virtue of (9), also G) depends on our ability to estimate the integral of c over R because errors in estimating concentration translate into errors in estimating cumulative release via (12).**

EULERIAN-LAGRANGIAN THEORY OF TRANSPORT; EFFECT OF INFORMATION CONTENT ON ADVECTION AND DISPERSION: The following recent theory by Neuman (1991) demonstrates, among other things, that ***uncertainties*** (measured via ***estimation variance***) **in c (and hence M_S and G), just like uncertainties in *travel times/paths*, depend on the *uncertainty associated with site-characterization of the advective velocity field*.** The better is this field characterized (***throughout*** RI), the smaller are the resulting uncertainties.

Consider a solute particle of unit mass introduced into an advective velocity field at point x_0 and time t_0. For simplicity, disregard local dispersion (set $d \equiv 0$) and express solute mass balance via the ***stochastic advection equation***

$$\frac{\partial c(x,t)}{\partial t} + \nabla\cdot[v(x,t)c(x,t)] = \delta(x-x_0, t-t_0). \tag{14}$$

Express water mass balance via

$$\nabla\cdot v(x,t) = f(x,t) \tag{15}$$

where $f(x,t)$ is a random fluid source function (which may also include terms such as $\partial h/\partial t$ where h is hydraulic head) whose leading moments with v are known. Then adopt the view that

$$\langle v(x,t)\rangle = \text{unbiased } \textit{estimate} \text{ of } v(x,t),$$
$$v'(x,t) = \text{zero-mean } \textit{estimation error}.$$

The solution of (14) is a random concentration field $c(x,t|\,x_0,t_0)$ whose estimate, $\langle c(x,t|\,x_0,t_0)\rangle$, can be shown to satisfy

$$\frac{\partial\langle c(x,t|\,x_0,t_0)\rangle}{\partial t} + \nabla\cdot[\langle v(x,t)\rangle\langle c(x,t|\,x_0t_0)\rangle + Q(x,t;x_0,t_0)] = \delta(x-x_0, t-t_0) \tag{16}$$

$$Q(x,t;x_0,t_0) = \textit{dispersive} \text{ solute mass flux}. \tag{17}$$

The nature of q depends on ***information*** about the advective velocity field $v(x,t)$:

1. In the improbable case where $v(x,t)$ is perfectly known, $v'(x,t) \equiv 0$, $v(x,t) \equiv \langle v(x,t)\rangle$ = deterministic function, and $Q \equiv 0$.

Note: In reality neither ***strict determinism***, nor the common ***unconditional stochastic approach***, are justified. Viewing $\langle v(x,t)\rangle$ as a (generally variable) unbiased estimate of $v(x,t)$ conditioned on actual space-time data, rather than a constant ensemble mean which is (usually) not so conditioned, constitutes a ***mixed stochastic-deterministic approach*** which is, in our view, much more realistic.

2. Rigorously,

$$Q(x,t;x_0,t_0) = -\int\int_{t_0}^{t} \langle c(x,t|\,\chi,\tau)\rangle\langle v'^*(x,t)v'^T(\chi,\tau)\rangle\nabla_\chi\langle c(\chi,\tau|\,x_0,t_0)\rangle\, d\tau\, d\chi$$

$$-\int\int_{t_0}^{t} \langle c(x,t|\,\chi,\tau)\rangle\langle v'^*(x,t)f'(\chi,\tau)\rangle\langle c(\chi,\tau|\,x_0,t_0)\rangle\, d\tau\, d\chi \tag{18}$$

$$\langle v'(x,t)v'^T(\chi,\tau)\rangle = \text{Eulerian covariance tensor of } v'(x,t)$$

where the star indicates that $v'^*(x,t)$ is immune to differentiation and integration with respect to x and t. Alternatively, Q can be expressed as

$$Q(x,t;x_0,t_0) = -\iint_{t_0}^{t} \langle c(x,t|\,\chi,\tau)\rangle\ \langle v'(x,t)v'^T(\chi,\tau)\rangle \nabla\langle c[x,t|\,x_0+\langle X^d(\tau-t_0|\,x_0)\rangle,\tau]\rangle\ d\tau\ d\chi$$

$$-\iint_{t_0}^{t} \langle c(x,t|\,\chi,\tau)\rangle\ \langle v'(x,t)f'(\chi,\tau)\rangle\langle c[x,t|\,x_0+\langle X^d(\tau-t_0|\,x_0)\rangle,\tau]\rangle\ d\tau\ d\chi \tag{19}$$

$x_0 + \langle X^d(\tau-t_0|\,x_0)\rangle$ = mean position at time τ of particle emanating from (x_0,t_0).

Whereas in (18) $\nabla\langle c\rangle$ must be evaluated at all points in infinite space, in (19) it depends only on points along a single mean trajectory. In either case, Q is given by a ***nonlinear, non-Fickian*** expression which shows that $\langle c(x,t|\,x_0,t_0)\rangle$ is generally ***non-Gaussian.*** The latter is controlled by (17) coupled with (18) or (19) which together constitute a nonlinear integro-differential equation for $\langle c(x,t|\,x_0,t_0)\rangle$. The associated transport process is ***nonlocal*** in that solute balance at (x,t) depends not only on quantities at this point but also on those at other points in space-time.

3. The better does the estimate $\langle v(x,t)\rangle$ represent the true velocity v(x,t), the smaller is generally the variance of the estimation error v'(x,t) and the shorter are its space-time correlation lengths. As soon as the particle residence time $t-t_0$ becomes sufficiently large in comparison to the Lagrangian correlation time of this error, one can approximate (18)-(19) by the ***pseudo-Fickian*** expression (for simplicity, we assume $\langle v'f'\rangle \equiv 0$)

$$Q(x,t;x_0,t_0) = -\,D(x,t;t_0)\ \nabla\langle c(x,t|\,x_0,t_0)\rangle \tag{20}$$

where D is a ***dispersion tensor*** given by

$$D(x,t;t_0) = \int_{t_0}^{t} \langle v'(x,t)v'^T(\tilde{\chi},\tau)\rangle\ d\tau \tag{21}$$

$\tilde{\chi}$ = random location at time τ $(t_0 \le \tau \le t)$ of particle reaching x at time t

$\langle v'(x,t)v'^T(\tilde{\chi},\tau)\rangle$ = Lagrangian covariance tensor of v'(x,t)

$$= \int \langle v'(x,t)v'^T(\chi,\tau)\rangle\langle c(x,t|\,\chi,\tau)\rangle\ d\chi. \tag{22}$$

The tensor D is ***local in space, nonlocal in time,*** and tends asymptotically to a local value

$$D^{\infty}(x,t) = \int_{\infty}^{t} \langle v'(x,t)v'^T(\tilde{\chi},\tau)\rangle\ d\tau \tag{23}$$

as $t-t_0$ continues to grow (or, alternatively, as the Lagrangian correlation time of the velocity estimation error shrinks in comparison to a given $t-t_0$ due to a change in information content). The pseudo-Fickian approximation implies that $\langle c(x,t|\,x_0,t_0)\rangle$ is Gaussian.

4. If additionally v(x,t) is space-time stationary (as when $\langle v\rangle \equiv$ constant = ***unconditional estimate*** of v(x,t)) then

$$Q(x,t;x_0,t_0) = -\,D(t-t_0)\nabla\langle c(x,t|\,x_0,t_0)\rangle \tag{24}$$

where now D depends only on particle residence time and not on location in space.

The nature of $D(t-t_0)$ and the particle ***displacement covariance***

$$\Omega_t = \Omega + \Omega_B \tag{25}$$

$$\Omega = \langle (X - \langle X \rangle)(X - \langle X \rangle)^T \rangle \quad \text{for advection} \tag{26}$$

$$\Omega_B = 2dt \quad \text{for Brownian (local) dispersion} \tag{27}$$

has been investigated based on a *linear* approximation by Dagan (1984, 1987, 1989), and a *higher-order quasilinear* approximation by Neuman and Zhang (1990) and Zhang and Neuman (1990).

Neuman (1991) provides explicit formulae for the *estimation covariance* of the concentration; recall that the variance of this error, $\langle c'^2 \rangle$, is needed to evaluate the estimation variance of the cumulative release M_S' in (12). In the *space-time stationary pseudo-Fickian* case with an arbitrary deterministic solute source, setting $t_0 = 0$ yields

$$\langle c'(y,t)c'(x,t) \rangle = \nabla^T \langle c(y,t) \rangle \Omega(t) \nabla \langle c(x,t) \rangle \tag{28}$$

$$\frac{d\Omega(t)}{dt} = 2D(t). \tag{29}$$

Observe:

a. *DISPERSION DECREASES AS INFORMATION CONTENT INCREASES* (in quantity and quality); *conditioning on real data* causes *information to be transferred* from the dispersive to the advective term. Lack of information (*IGNORANCE*) about $v(x,t)$ *REQUIRES THAT DISPERSION BE RELATIVELY LARGE.*

b. *AS INFORMATION IS TRANSFERRED FROM THE DISPERSIVE (IGNORANCE) TERM TO THE ADVECTIVE* term via conditioning, *ERRORS* associated with estimating unknown real concentrations $c(x,t)$ by means of $\langle c(x,t) \rangle$ *DIMINISH.* These *ERRORS CAN BE QUANTIFIED.*

c. The *SAME IS TRUE ABOUT ERRORS IN* estimating *TRAVEL PATHS, TRAVEL TIMES, TRAVEL TIME DISTRIBUTIONS, RELEASE RATES,* and *CUMULATIVE RELEASES* to the accessible environment.

SCALE EFFECT AND CONCEPT VALIDATION: The *scale effect* has recently been *discussed and interpreted* by Neuman (1990). According to this effect, when tracer experiments are interpreted by means of analytical Fickian models which do not account for medium heterogeneity and its influence on seepage (advective) velocities, the resulting *APPARENT LONGITUDINAL DISPERSIVITY GROWS CONTINUOUSLY WITH MEAN TRAVEL DISTANCE.* The above theory thus implies that *UNCERTAINTY (ABOUT CONCENTRATIONS, TRAVEL PATHS, TRAVEL TIMES, ETC.) GROWS CONTINUOUSLY AS THE DISTANCE OF A PLUME FROM ITS SOURCE INCREASES.* Such behavior is *not consistent with* the traditional notion that medium heterogeneity can be represented by means of *stationary random fields.*

Data suggest (Neuman, 1990) that the *RATE AT WHICH APPARENT LONGITUDINAL DISPERSIVITY GROWS WITH MEAN TRAVEL DISTANCE DIMINISHES WHEN THE INTERPRETATION IS BASED ON NUMERICAL MODELS WHICH ACCOUNT FOR MEDIUM HETEROGENEITY* via model calibration (*i.e., conditioning*). This constitutes a *VALIDATION OF THE FUNDAMENTAL IDEA PRESENTED HERE.*

FURTHER IMLICATIONS OF SCALE EFFECT: The observed increase of apparent longitudinal dispersivity with observation or experimental scale in saturated media implies (Neuman, 1990):

1. Heterogeneous geologic media are not statistically homogeneous with respect to saturated log hydraulic conductivity (there are no unique mean, variance, correlation scales) except, at best, locally. **Heterogeneities may appear on a multiplicity of scales** and their effect must be superimposed. Hence site characterization on one scale does not carry over to other scales; a thorough understanding of geologic conditions in the near field of a repository is not sufficient to predict flow and transport in the far field; *CHARACTERIZATION IS REQUIRED ON ALL SCALES OF THE CONTROL VOLUME*. Where this is not practical, *THE ALTERNATIVE IS TO RELY ON SCALING RULES* such as that of Neuman (1990). No such scaling rules presently exist for unsaturated media; much *theoretical work*, supported by *MULTISCALE EXPERIMENTS AND OBSERVATIONS ARE REQUIRED* to derive them.

2. **Saturated flow and transport properties of fractured media scale, on the average, like those of porous media.** Hence the *validity* of many *distinctions* commonly drawn between these two types of media may be *in question*.

3. Neuman's (1990) scaling rule is derived from apparent dispersivities calculated **without information about flow or transport properties of specific heterogeneities** (*fractures, channels, other pathways*), **taking the advective velocity to be that of a *uniform medium*.** Apparent **dispersivities from calibrated numerical models increase** more slowly with scale; in such models medium **properties vary slowly** (usually remaining constant within zones containing numerous finite difference cells) and advective **velocities show corresponding large-scale fluctuations** which would not show in a uniform medium. Knowledge of these large-scale property and velocity variations means that now **only smaller-scale fluctuations remain uncertain**, allowing the dispersivity which represents them to decrease. This demonstrates that ***information has been transferred from the dispersive to the advective term*** of the transport equation; *THE LESS WELL A SITE IS CHARACTERIZED, THE MORE CRUDE IS THE DESCRIPTION OF ADVECTIVE VELOCITIES (AND TRAVEL TIMES) AND THEREFORE THE DISPERSIVITY MUST INCREASES TO REFLECT THIS LACK OF INFORMATION.*

The data thus *validate the theoretical prediction* that *ADVECTION AND DISPERSION ARE TWO SIDES OF THE SAME COIN* **and treating them as two distinct phenomena is inappropriate;** *DISPERSIVITY* is not a local medium parameter but a ***non-local parameter*** which *DEPENDS ON RESIDENCE TIME* and *REFLECTS ALL THAT IS UNKNOWN ABOUT THE ADVECTIVE FIELD*; transport *MODELS WHICH TREAT DISPERSIVITY AS A CONSTANT INDEPENDENT OF INFORMATION CONTENT UNDERESTIMATE THE UNCERTAINTY IN CONTAMINANT FLUXES, CONCENTRATIONS, AND TRAVEL TIMES.*

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Tracer Transport in Fractures

Y.W. Tsang
Lawrence Berkeley Laboratory

Introduction

A fractured medium represents a strongly heterogeneous system. If the matrix permeability is negligibly small compared to the fracture permeability, the flow and transport approximately take place in 2D fractures in a highly heterogeneous 3D space. However, the whole fracture plane is not uniformly conductive to water, rather, flow channeling occurs, that is, the majority of flow concentrates in flow paths of least resistance as demonstrated in recent experimental studies (Abeline et al., 1985, 1987; Bourke, 1987). These features specific to fluid flow in a fractured medium imply that tracer transport is such a medium cannot usually be interpreted by theories which assume flow in a homogeneous porous medium. In the following I describe a new approach to study tracer transport in fractured media. The approach is based on the concept of the variable aperture channel model (Tsang and Tsang, 1987,1989; Tsang et al., 1988), in which transport through fractured rocks is controlled by a number of channels, each of which has variable aperture along its length. These variable apertures sample the aperture probability distribution function which characterize a single fracture. The flow channels are not physical pipes in the fracture plane, but rather preferred paths of least resistance in the sense of potential theory. Flow and transport through a system of fractures is then envisioned (Figure 1) as occurring through these tortuous channels of flow paths from fracture to fracture in the 3D space. Advective dispersion arises then from the possibility of different channels available for transport, and hence the dispersion displayed in tracer breakthrough measurements can be correlated to the geometric parameters of the fractures. This approach is applied to the analysis of Stripa 3D field data (Tsang et al., 1990).

Stripa-3D Experiment

One of the most comprehensive, multi-year tracer transport experiments in fractured rocks was performed by Neretnieks and co-workers (Neretnieks, 1987; Abelin et al., 1987) in the granitic fracture formation in the Stripa mine in Sweden. The experiment was carried out in two drifts in the form of a cross. The longer drift is 75 m long and the shorter intersecting drift is 25 m long. Each drift is 4.5 m in width and 3 m in maximum height. The roof and walls of the drift were covered by over 300 of 1 x 2 m plastic sheets for collection of water and tracers. Three 75 m vertical boreholes are drilled into the roof and nine tracers were injected into different packered-off (1 m long) sections of large enough local hydraulic conductivity. Apparent tracer transport distances from the injection locations to the collection sheets range from 10 to 45 m. Despite the numerous fracture traces on the drift wall, only a small number of the collections sheets

receive significant flow. During the first 30 months of data collection, five of the nine tracers are retured, aain in a very small percentage of the sheets.

Data Analysis

Our conceptual model of the Stripa-3D experiment is as follows. Because the underground drift is maintained at atmospheric pressure, it is a sink for water from the rock around it. The large range of aperture values in the fracture give rise to flow channeling so that the majority of flow takes place in selected flow paths of least flow resistance which comprise only a small fraction of the total 3D flow region, accounting for the observation that only a small percentage of the collection sheets register measurable flow. When a tracer is injected at a particular location in the flow field, the resultant solution moves downstream along these preferred flow paths toward the drift and emerges in a number of plastic collection sheets. At Stripa, dilution of the injected tracer is clearly present because the tracer injection flow rate is much smaller than the total exit flow rate at the drift. Because the unknown dilution effect of the channel flow, the rate of tracer mass accumulation rather than the more commonly used tracer concentration is adopted as the observed quantity in the following analysis. Due to the strong heterogeneity inherent in the fractured medium, the tracer break through curve from point measurements will be sensitive to measurement location. To remove this data sensitivity to measurement location, the mass accumulation data are spatial averaged over all collection sheets with non-zero mass emergence for each tracer, so that one resultant breakthrough curve is obtained for each tracer as shown in Figure 2. The shape and structure of the breakthrough curves are attributed to two factors: (1) flow channeling from medium heterogeneity, and (2) the non-simple time dependence of injection tracer mass as shown in Figure 3. To separate the effects of the two factors which give rise to the time variation of the breakthrough curves a deconvolution method similar to that used in signal processing and information theories and to the unit hydrograph method of surface hydrology (Eagleson et al., 1966; Dreiss, 1982: Neuman and de Marsily, 1976) is applied to the breakthrough data. The deconvolution transforms the breakthrough data to that of response to a pulse tracer injection, thus filtering out the effect of the complicated time-dependent mass injection, and retaining only the effect of the medium heterogeneities on the break through. The deconvolution is valid if the system response is linear and is stable with time, which it is in the framework of the conceptual model where advective transport is controlled by medium heterogeneities. A simplified formulation which is particularly suited to discretized data (Tsang et al., 1990) involves the use of Toeplitz matrices (Gohberg, 1982; Gray, 1977). Examples of the breakthrough data after deconvolution is shown in Figure 4 clearly unveils the multiple channel nature of the tracer transport in them Stripa-3D data. Over the range of distances and observation time periods, the transport for Eosin B apparently takes place in our major channels, which the breakthrough for the other four tracers display two channels each.

The deconvoluted breakthrough curves of the five tracers show that the standard deviation σ_t of particle arrival times for all the peaks is about the same. This measure

of dispersion σ_t is closely related to the variance of the aperture distribution of the fractures. Estimates of the mean and variance for fracture apertures have been made from the Stripa 3D data (Tsang et al., 1990).

Fracture Network Modeling

The multi-peak response to a pulse injection in the tracer breakthrough curve from the above analysis of Stripa-3D data of tracer transport in a fractured medium display dispersion on two different scales. On the larger scale, the multiple peaks arise from the possibility of different transport routes through the fracture network; on the smaller scale, dispersion around each peaks is caused by the range of aperture values in each fracture in the medium. This interpretation of the tracer breakthrough has been confirmed by recent fracture network modeling studies (Nordqvist et al., 1991). In that work, a 3D variable-aperture fracture network for flow and transport in crystalline rock was developed. The model generates a network of fractures. Then the variable aperture character of the fractures in the network is introduced through a library of single fracture permeabilities and particle transport residence time spectra. Geostatistical methods are used to generate single fractures with spatially varying apertures. The flow pattern, the fracture transmissivities, and the frequency distribution of residence times (Moreno et al., 1988) that constitute the library of single fractures are assigned to the fractures in the network in a random selection, these are then used in the solution of flow through the fracture network and in a particle tracking calculation of solute transport from one side of the network to the other. Figure 5 shows the breakthrough response to a pulse injection for 15 meter transport through a fracture network where the average fracture spacing is on the order of 3 m. The multi-channel response similar to that shown in the Stripa-3D field data is apparent.

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Nonequilibrium Fracture-Matrix Flow During Episodic Infiltration Events in Yucca Mountain

Thomas A. Buscheck and John J. Nitao

Earth Science Department

Lawrence Livermore National Laboratory

1. Introduction

The Yucca Mountain Project (YMP) of the U.S. Department of Energy (DOE) is investigating the suitability of the fractured, tuffaceous rocks occurring in the unsaturated zone at Yucca Mountain, Nevada for nuclear waste storage. Adequate representation of fracture-matrix interaction during episodic infiltration events is crucial in making valid hydrological predictions of repository performance under both nominal and perturbed conditions. Various approximations have been applied to represent fracture-matrix flow interaction. The zeroth order approximation (Klavetter and Peters, 1988) assumes the fracture and matrix porosities to be in capillary equilibrium. The fracture and matrix properties can then be pore-volume-averaged into an Equivalent Continuum Model (ECM) which is also referred to as an effective continuum or as the composite curve model. The dual porosity approach, effectively a first order approximation, assumes that the mass transfer between the fracture and matrix block can be represented by a mass transfer coefficient, implying quasi-steady-state flow from matrix block to fracture. The dual porosity approach has been applied to model single phase flow in fractured reservoirs (Barrenblatt and others, 1960; Warren and Root, 1963). Braester (1986) has applied dual porosity models which treat relative permeability effects arising from multiphase flow. The primary feature of the dual porosity approximation is that the pressure field within a matrix block is represented by an averaged value. The second order approximation (Buscheck and Nitao, 1988; Nitao and Buscheck, 1989; Nitao, 1990) discretely accounts for the fracture and matrix porosities using the Fracture-Matrix Model (FMM). The FMM work has involved numerical modeling, using the V-TOUGH code (Nitao, 1989) which is a modified version of the TOUGH code (Pruess, 1987), as well as the development of analytical and semi-analytical models (Nitao, 1989).

This report examines the impact of nonequilibrium fracture-matrix flow on episodic infiltration events in Yucca Mountain. For both the FMM and ECM calculations, a ponded boundary condition is maintained at the repository horizon until the liquid front has broken through to the water table. The relative impact of matrix imbibition is examined for the five major hydrostratigraphic units between the repository horizon and the water table. We also address the question of what sequencing of infiltration events gives rise to episodic behavior versus behavior which may be time-aggregated. The implications of nonequilibrium fracture-matrix flow on radionuclide transport are also briefly discussed.

2. Discussion of Numerical Models, Physical Data and Assumptions

We consider a two-dimensional system of vertical, parallel, uniformly-spaced fractures extending continuously from the repository to the water table (Figure 1). Due to symmetry, we can consider an infinite periodic two-dimensional system extending from the no-flow boundary at the midplane of the fracture to the no-flow boundary at the midplane of the matrix block. Liquid enters the top of the fracture (which represents the floor of a repository drift) under a constant pressure due to ponding. An example to which these assumptions may be applicable is the "human intrusion drilling scenario" which is currently being considered by the YMP. In this scenario, once an exploratory drilling operation has penetrated a drift, circulation of drilling fluid is lost, thereby introducing enough fluid to maintain a ponded condition for a limited period.

Using the matrix property data listed in Table 1 (Peters and others, 1984; Klavetter and Peters, 1988), we model the five major hydrostratigraphic units lying between the repository horizon and the water table. It is important to note that characteristic curve data are not available for imbibition. Applying the characteristic curves determined by Peters and others (1984) with the use of an oven pschychrometer to imbibition calculations for Grouse Canyon densely welded tuff, Buscheck and Nitao (1987, 1988) found that a reasonable match between modeled and observed data was obtained if matrix

permeability, k_m was reduced by a factor of 40. This discrepancy could be attributed to uncertainty concerning k_m or to capillary hysteresis. Using data for Topopah Spring welded tuff, TSw (Lin and Daily, 1990), we obtained a reasonable match between modeled and observed imbibition data after applying a similar reduction in k_m. In order to approximately account for what is an apparent capillary hysteresis effect, we decided to apply this k_m reduction factor to all of the units listed in Table 1.

Available data for fracture properties in Yucca Mountain is sparse. Montazer and others (1985) measured bulk (air) permeability, k_b, in TSw to a depth of 100 m (obtaining $1\text{x}10^{-11} < k_b < 7\text{x}10^{-13}\ m^2$). For well J-13 Thordarson (1983) reported a bulk hydraulic conductivity of 1 m/day ($k_b = 1.7\text{x}10^{-11}\ m^2$). For fracture spacings listed in Table 2, the hydraulic fracture aperture can be calculated based on the cubic law and the ECM definition of bulk permeability, $k_b = k_m(1-\phi_f) + k_f\phi_f$, where k_f and ϕ_f are the permeability and porosity of the fracture. For the range listed in Table 1, the effect of k_m on this calculation is negligible. Note that we assume all fractures to be parallel. We considered fracture apertures, b of 10, 50, 100 (reference case), 200, 400, and 1000 μm.

The Environmental Assessment (1986) reports from 15-40 fractures per cubic meter for welded units to as few as 1 fracture per cubic meter for nonwelded units. Because many fractures will not lie along fracture pathways which are connected to an overlying source of water, the effective fracture spacing is likely to be considerably greater than the actual (or apparent) fracture spacing. We considered fracture spacings, B of 0.3, 3.0 (reference case), 30, and 100 m.

3. Discussion of Results

Prior to conducting the episodic infiltration calculations it was necessary to initialize the saturation and pressure fields in the model. For the reference case, the saturation at the upper boundary (representing the base of the repository horizon) is fixed at 85 percent and at the lower boundary (representing the water table) is fixed at 100 percent. After reaching steady-state, the vertical saturation profile in Figure 2 is attained, yielding a steady-state flux of 0.045 mm/yr. This procedure is repeated for repository horizon saturations of 95 and 50 percent, yielding steady-state fluxes of 0.132 and -0.003 mm/yr, respectively, along with the associated saturation profiles in Figure 2. For a steady-state flux of 0.00 mm/yr, which corresponds to capillary-gravity equilibrium, the associated saturation profile results in a repository horizon saturation of 68.9 percent. Note that this saturation falls well within the range of saturations measured at the repository horizon. It appears that the existing saturation profile at Yucca Mountain is consistent with zero net infiltration flux. Due to the relatively small k_m of TSw2 and TSw3, the saturation profile within those units is quite sensitive to variations in infiltration flux. Due to its large k_m, CHnv can sustain the steady-state flux at very small saturations ($\approx$ 17 percent). The saturation profiles in the CHnz and PPw are less sensitive to variations in the steady-state flux.

Before further discussing the results of this study it is useful to review a few fundamental concepts of unsaturated fracture-matrix flow in idealized systems. Matrix-dominated flow occurs when the flux into the fracture is sufficiently low such that most of the water is imbibed by the matrix close to the entrance before significant fracture flow can occur (Nitao 1990). Movement of the liquid front in the fracture, if any, will lag behind the front in the matrix, and the speed of the front is dominated by the matrix properties. Fracture-dominated flow occurs when the flux into the fracture is sufficiently high such that the liquid front in the fracture will move in advance of the flow in the matrix which is primarily orthogonal to the direction of flow in the fracture. In fracture-dominated flow, the speed of the front is governed by the interaction between driving forces in the fracture and the suction forces in the matrix.

Nitao and Buscheck (1989) found that fracture-dominated flow can be classified into three physically interpretable, distinctive flow regimes. During flow period I, flow in the matrix is not yet significant enough to affect flow in the fracture. Therefore, the speed of the liquid front is dominated by the driving forces in the fracture: fracture capillarity, the imposed boundary flux or pressure, and gravity. For this study, flow period I is dominated by gravity and the liquid front moves linearly in time. During flow period II, the impact of matrix imbibition is fully developed and the liquid front moves as $t^{1/2}$. During flow period III, the wetting zones from neighboring fractures have fully interfered, thereby reducing the effect of matrix imbibition. The movement of the front is again linear in time (but substantially reduced relative to flow period I) and is the same as that predicted by the ECM.

Buscheck and Nitao (1988) found that matrix imbibition results in insignificant fracture flow subsequent to the removal of a ponded infiltration source. They also found that for welded tuffs the time for the dimensionless liquid saturation, S_e, of the wetting zone in the matrix to relax to within 10 percent of native saturation conditions is on the order of months to a year, where S_e is defined as

$$S_e = \frac{S - S_i}{1 - S_i} \quad \text{where } S_i \equiv \text{ the initial liquid saturation.}$$

For CHnv it is found to take over 10 years. For episodic infiltration events separated by a week or less, the cumulative liquid front movement is nearly the same as would occur had all of the events occurred continuously. For CHnv, episodic events can be separated by a year without affecting the cumulative liquid front movement.

For the episodic infiltration calculations, a ponded upper boundary is maintained at atmospheric pressure until the liquid front breaks through to the water table, located 225 m below the repository. The impact of matrix flow on the liquid front movement is well illustrated by comparing the groundwater travel times, *GWTT*, for liquid front penetration through the relatively impermeable welded units, TSw2 and TSw3, versus the permeable nonwelded unit, CHnv (column 2 of Table 3). For the reference case it takes only 4.5 hours for the liquid front to penetrate the TSw2 and TSw3 while taking an additional 8.3 days to penetrate the CHnv. Figure 3 is a contour plot of S_e at t = 8 hours, shortly after the front has reached the CHnv. Flow in the CHnv is being dominated by the matrix as flow is laterally diverted as quickly as it enters the CHnv. After 20 days the wetting zones from neighboring fractures are starting to interfere (Figure 4). Due to the dominance of matrix flow, the liquid front does not fully penetrate the CHnv, and enter the CHnz, until entirely saturating the CHnv (Figure 5). Due to the small k_m of the CHnz and the very high initial saturation of the PPw, it takes only an additional 3.4 days for the liquid front to penetrate those units and reach the water table (Figure 6).

Tables 3 and 4 illustrate the impact of matrix flow by comparing *GWTT* for the case of no matrix flow (column 1) with the case of fracture-matrix interaction (column 2). Column 3 lists the "retardation" ratio, R_m defined as the ratio of the *GWTT* with matrix interaction to the *GWTT* without matrix interaction. In other words, R_m is the factor by which the liquid front movement is delayed by virtue of matrix interaction. By definition, for flow period I, $R_m \leq 2$. Therefore, in the reference case, as the liquid front is penetrating TSw2 and TSw3, a transition is occurring from flow period I to II (Table 3). As the wetting zones in CHnv begin to interfere, flow in CHnv transitions from matrix-dominated flow to fracture-dominated flow regime III. Fracture-dominated flow period II persists in CHnz and PPw. For b = 1000 μm (Table 4), the large fracture conductivity dominates flow, with flow period I persisting in all but the CHnv which experiences flow period II. Column 4 lists R_m predicted by the ECM. Effectively, the ECM provides instantaneous matrix interaction over all of the matrix porosity lying between wetting fractures. The *GWTT* is drastically overpredicted by the ECM for TSw2, TSw3, CHnz, and PPw. Only for the CHnv (and only for $b \leq 100$ μm) is the ECM found to be sufficiently accurate (Table 3).

While it was necessary for the wetting zones in the CHnv of the reference case (B = 3.0 m) to interfere prior to re-establishing fracture-dominated flow, for wider fracture spacing, fracture-dominated flow is eventually re-established by virtue of the small thickness of the CHnv and decaying matrix imbibition flux. Eventually the total flux into the matrix declines to where the fracture flux is sufficient to penetrate through to the CHnz. For b = 100 μm this occurred after the wetting zone had spread 6.08 m laterally in the CHnv matrix (column 3 of Table 5). Due to model symmetry, Table 5 actually lists the half-width of the wetting zone. For a wide range of apertures, Table 5 gives the maximum lateral spread of the wetting zone in the matrix just as the liquid front has fully penetrated that unit. Table 5 can also be used as an upper bound on the required spacing between wetting fractures in order for the ECM to be reasonably valid for this idealized system of fractures. Notice that for all but the CHnv (and for $b \geq 100$ μm) the necessary spacing is on the order of millimeters to centimeters.

Figure 7 is a log-log plot of the information in Table 5. Notice that the slopes of all of these curves (except for CHnv) vary from a slope of -3 for small b to a slope of -1 for large b. For CHnv the transition to a slope of -1 occurs for b > 1000 μm. Therefore, the sensitivity of the lateral penetration of the wetting zone in the matrix varies from b^{-3} for small b to b^{-1} for large b. This sensitivity is

better understood in light of the analysis of Nitao and Buscheck (1989) who found that the lateral penetration, d_m, of the wetting zone in the matrix is dependent on the matrix wetting diffusivity, D_m

$$d_m \sim \frac{2\sqrt{D_m t}}{\sqrt{\pi}} \tag{1}$$

During flow period I, the liquid front penetration, L, is linearly dependent on the saturated hydraulic conductivity of the fracture, K_f

$$L \sim K_f t \quad \text{where} \quad K_f \sim b^2$$

Substituting into (1), we get

$$d_m \sim \frac{2\sqrt{D_m}}{\sqrt{\pi}} \frac{\sqrt{L}}{b} \tag{2}$$

yielding a b^{-1} dependence of lateral matrix penetration during flow period I which is consistent with the observation concerning large b in Figure 7. During flow period II

$$L \sim K_f \sqrt{t_b t} \quad \text{where} \quad \sqrt{t_b} \sim b$$

Substituting into (1), we get

$$d_m \sim \frac{2\sqrt{D_m}}{\sqrt{\pi}} \frac{L}{b^3} \tag{3}$$

yielding a b^{-3} dependence of lateral matrix penetration during flow period II which is consistent with the observation for small b in Figure 7.

Because it smears liquid fronts over the entire fracture and matrix porosity, and because it also smears the effect of episodic events by virtue of time-averaging them into an "effective" steady-state flux, the steady-state ECM overpredicts *GWTT* (usually quite substantially), relative to the nonsteady-state FMM. This smearing artificially retards the movement of the liquid front, but it may also lead to substantially underpredicting the time for radionuclide breakthrough, relative to the FMM. Shortly after the end of an episodic event, liquid in the fracture will be totally imbibed by the matrix along with any dissolved radionuclides. Although subsequent events may transport "additional" radionuclides, their ability to further displace radionuclides imbibed in the matrix during earlier events will be limited. This limited ability to further vertically displace radionuclides stems from the matrix wetting diffusivity, D_m (of the low matrix permeability units) being at least as great as the molecular or ionic diffusivity. For the high matrix permeability units, D_m is at least two orders of magnitude greater than the molecular or ionic diffusivity. Hence, advection by imbibition away from the fracture will tend to dominate diffusion of radionuclides toward the fracture, limiting the re-entrainment of previously imbibed radionuclides. Because it bulk-averages flow in the fracture and matrix, the ECM cannot account for the partitioning of radionuclides in the fracture and matrix porosities.

Based on the analysis of existing saturation profile data, there appears to be a zero net infiltration flux through Yucca Mountain. However, bomb-pulse ^{36}Cl measurements reported by Norris (1989) are consistent with episodic fracture flow from the groundsurface to considerable depths. To resolve this apparent contradiction, mechanisms (other than percolation to the water table) are required to remove water from the vadose zone. These mechanisms may include vapor flow (Thorstenson and others, 1989) as well as lateral liquid flow along high permeability units such as the CHnv. The capacity of these mechanisms may be considerably in excess of what is currently required to provide a net zero flux. For scenarios in which Yucca Mountain is not gradually saturating, the key consideration in analyzing radionuclide transport is the intensity and duration of the maximum possible infiltration episodes (i.e. an event or a group of events which effectively act as a single event). If a radionuclide front is not driven to the water table during the course of a maximum infiltration episode, then subsequent movement of that front will be governed by matrix-dominated flow (which may be negative).

4. Conclusions

Using the V-TOUGH code episodic infiltration events were modeled using two different conceptual models: (1) discretely representing the fracture and matrix properties (FMM) and (2) pore-volume-averaging their properties through the use of an equivalent continuum model (ECM). For the five major hydrostratigraphic units between the repository and the water table, the discrete accounting of fracture and matrix flow is found to be critical to accurately predicting the liquid front movement in an idealized system of fractures. Moreover, it is argued that discrete accounting of the partitioning of radionuclides in the fracture and matrix porosities is also critical to accurately predicting radionuclide transport.

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Table 1
Yucca Mountain Tuff Matrix Properties
(Klavetter and Peters, 1988)

Unit	Sample Code	Porosity	Permeability m^2	S_r	α $10^{-2}m^{-1}$	β
TSw2	G4-6	0.11	1.9×10^{-18}	0.080	0.567	1.798
TSw3	GU3-11	0.07	1.5×10^{-19}	0.080	0.441	2.058
CHnv	GU3-14	0.46	2.7×10^{-14}	0.041	1.60	3.872
CHnz	G4-11	0.28	2.0×10^{-18}	0.110	0.308	1.602
PPw	G4-18	0.24	4.5×10^{-16}	0.066	1.41	2.639

w ≡ welded nv ≡ nonwelded vitric nz ≡ nonwelded zeolitized

Table 2
Calculated Fracture Apertures Based on Reported Bulk Hydraulic Conductivities
(Montazer and others, 1985; Thordarson, 1983)

assumed fracture spacing, B (m)	calculated fracture aperture, b (μm)
1.00	203 to 587
0.3	141 to 407
0.1	94 to 273
0.01	43 to 127

Table 3
b = 100 μm; B = 3.0 m (Reference Case)

	GWTT (FMM) (w/o matrix) (sec)	*GWTT* (FMM) (w/ matrix) (sec)	R_m (FMM)	R_m (ECM)
TSw2 & TSw3	7359.	1.62×10^4	2.2	455.
CHnv	551.	7.18×10^6	13028.	13720.
CHnz & PPw	1.96×10^4	2.94×10^5	15.	373.
TOTAL	2.76×10^4	7.46×10^6	270.	662.

Table 4 b = 1000 μm; B = 3.0 m				
	GWTT (FMM) (w/o matrix) (sec)	*GWTT* (FMM) (w/ matrix) (sec)	R_m (FMM)	R_m (ECM)
TSw2 & TSw3	70.	70.	1.0	45.6
CHnv	5.5	30.	5.4	1372.
CHnz & PPw	200.	245.	1.2	37.5
TOTAL	276.	345.	1.3	66.1

Table 5 Maximum Lateral Spread of the Wetting Zone in the Matrix (m)						
	10 μm fracture	50 μm fracture	100 μm fracture	200 μm fracture	400 μm fracture	1000 μm fracture
TSw2	4.15	3.54×10^{-2}	6.26×10^{-3}	2.32×10^{-3}	1.08×10^{-3}	4.48×10^{-4}
TSw3	0.90	5.47×10^{-3}	9.68×10^{-4}	3.59×10^{-4}	1.61×10^{-4}	6.92×10^{-5}
CHnv	5.92×10^{3}	47.3	6.08	0.80	0.11	6.74×10^{-3}
CHnz	68.7	0.55	6.97×10^{-2}	9.27×10^{-3}	2.06×10^{-3}	1.01×10^{-3}
PPw	700.	5.60	0.71	9.0×10^{-2}	1.28×10^{-2}	5.3×10^{-3}

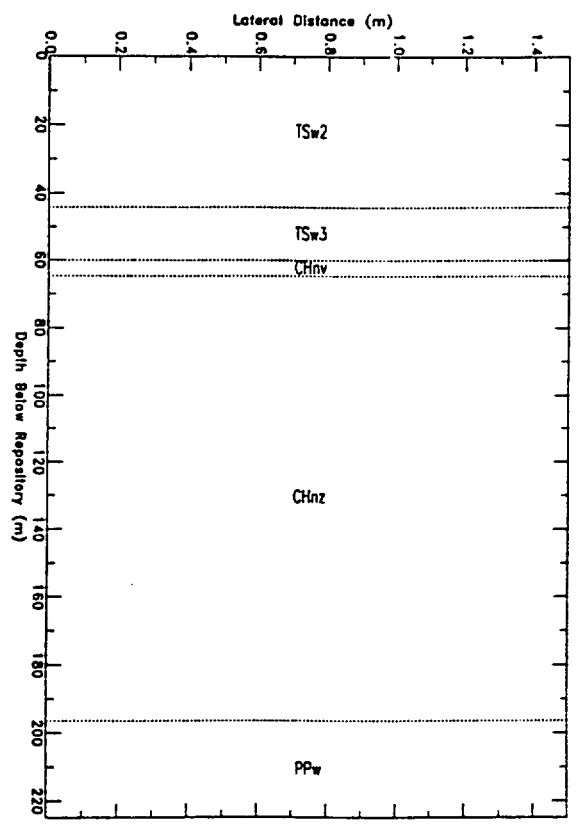

Figure 1. Schematic of the FMM. The fracture midplane is located at $x = 0$ and the matrix midplane is located at $x = 0.15\ m$. Note that horizontal distances are exaggerated by a factor of 100.

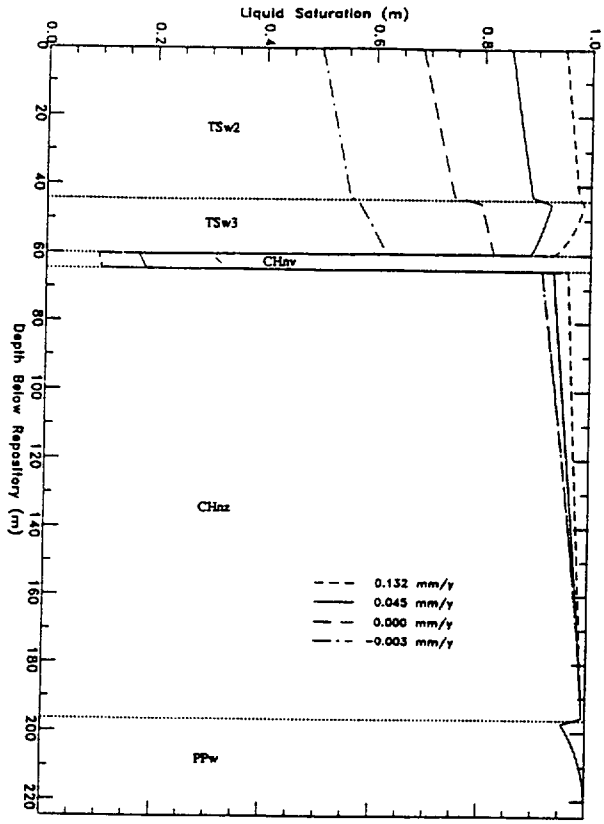

Figure 2. Vertical liquid saturation profile under various steady-state infiltration fluxes.

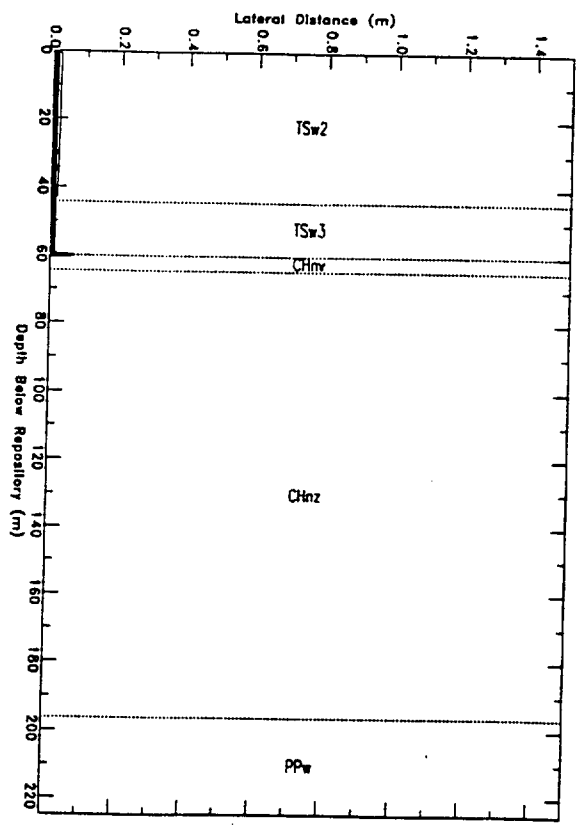

Figure 3. Contour plot of S_e at $t = 8\ hrs$. Horizontal distances are exaggerated by a factor of 100.

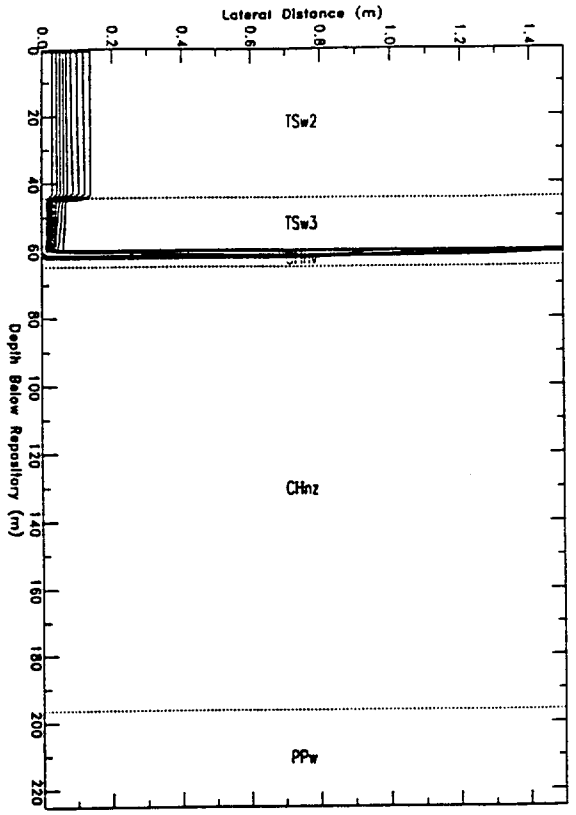

Figure 4. Contour plot of S_e at $t = 20$ *days*. Horizontal distances are exaggerated by a factor of 100.

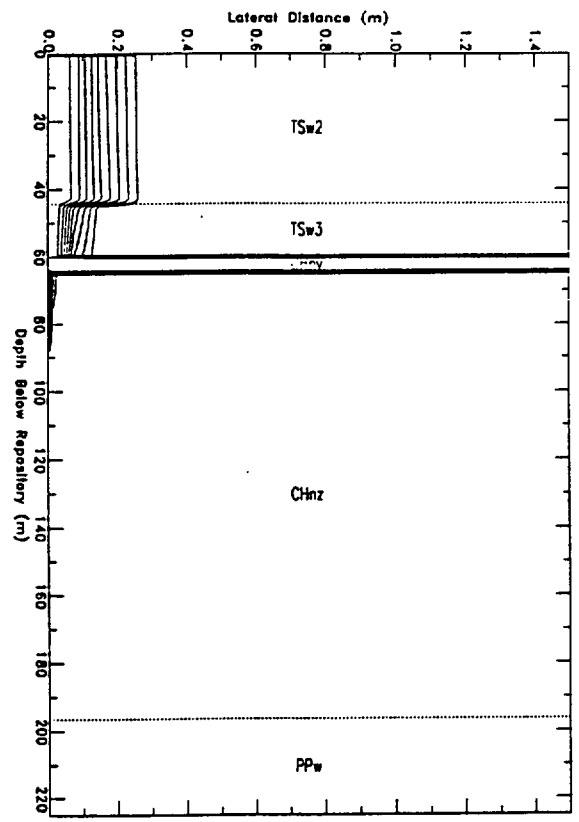

Figure 5. Contour plot of S_e at $t = 84$ *days*. Horizontal distances are exaggerated by a factor of 100.

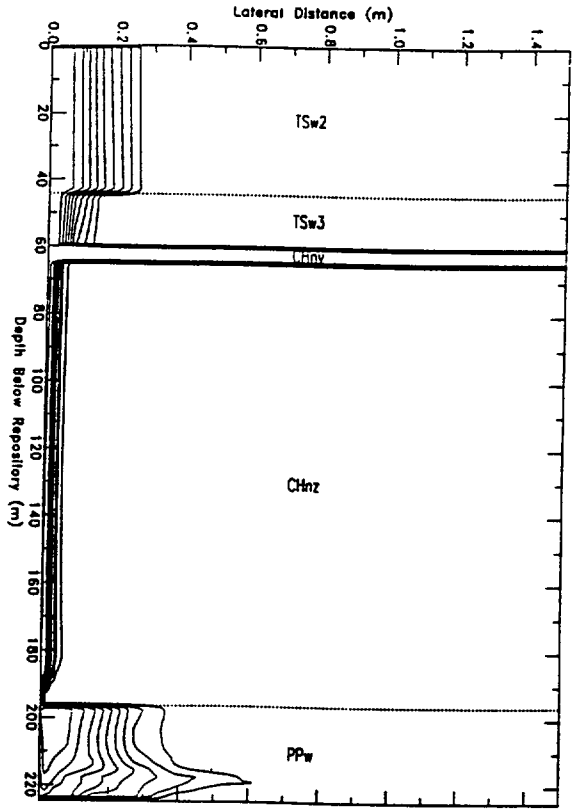

Figure 6. Contour plot of S_e at $t = 87$ *days*. Horizontal distances are exaggerated by a factor of 100.

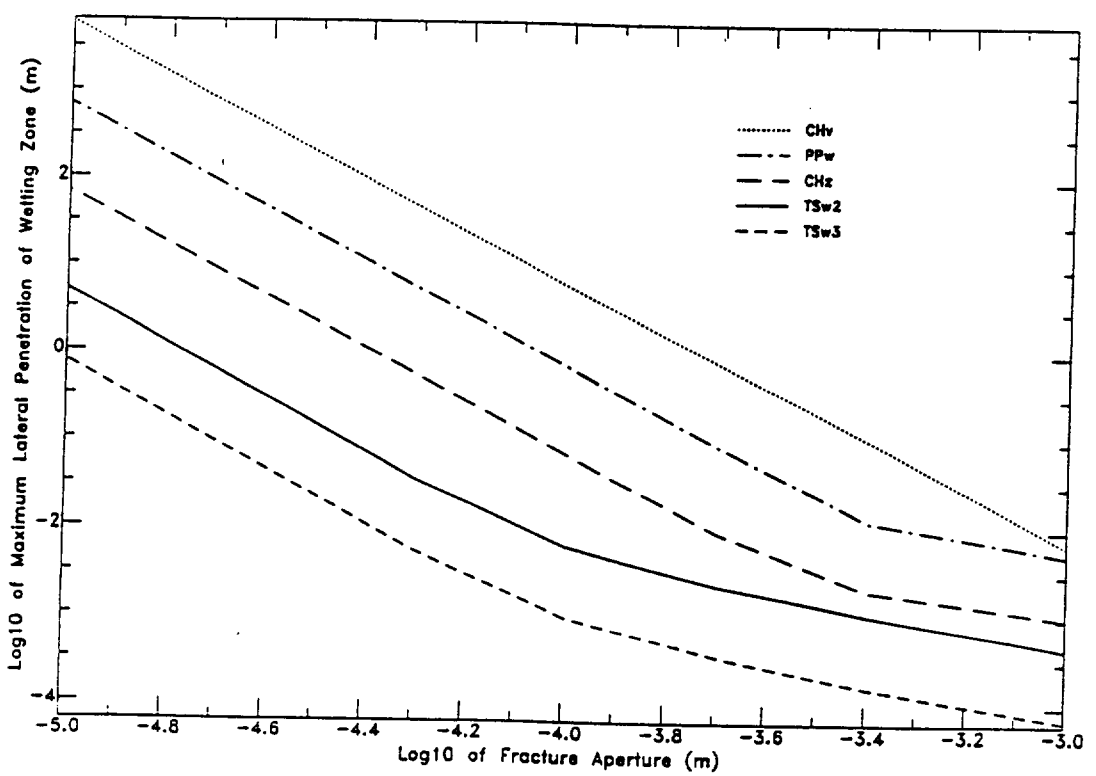

Figure 7. Log-log plot of maximum lateral penetration of wetting zone versus fracture aperture.

UPDATE ON INTRAVAL-PHASE II TEST CASES

Thomas J. Nicholson
Office of Nuclear Regulatory Research
U.S. Nuclear Regulatory Commission

1. Introduction

The issues being discussed at this workshop, specifically flow and transport through unsaturated rock related to high-level radioactive waste (HLW) disposal are also being addressed in the INTRAVAL Project. The INTRAVAL Project is an international cooperative project for studying validation issues associated with geosphere transport models[1]. The INTRAVAL effort has evolved from two earlier international cooperative studies, INTRACOIN[2,3], dealing with analysis of transport models, HYDROCOIN[4,5], dealing with analysis of hydrogeologic flow models, and international symposia devoted to model validation, GEOVAL87[6], and GEOVAL90[7]. The INTRAVAL Project is managed by the Swedish Nuclear Power Inspectorate. The central theme to INTRAVAL is the critical examination of validation issues for evaluating geosphere transport models that may be used in performance assessment of HLW facilities.

2. Project Structure

The purpose of INTRAVAL is to increase the understanding of how various geophysical, hydrogeologic and geochemical processes of importance to radionuclide transport can be described by specially formulated numerical models. This objective is being realized through simulations and analyses of laboratory and field experiments and natural analogue studies chosen as validation test cases.[1] The INTRAVAL test cases cover a range of spatial and temporal scales, hydrogeologic conditions and media, as well as, transport phenomena. These laboratory and field experiments provide site and contaminant specific data sets to the various 33 modeling groups (e.g., University of Arizona, CNWRA, SNL, PNL, USGS, etc.) established by 21 funding organizations (e.g., DOE, NRC, AECL) from 12 countries (e.g., USA, Canada, France, Japan, etc.).[1]

INTRAVAL was established in October 1987 as a three year project (Phase I) with an additional three-year extension approved in October 1990 (Phase II). The Phase I effort included 17 test cases as shown in Table 1. The selection criteria for these test cases were developed by an ad-hoc technical group involved in preparing the INTRAVAL technical proposal.[8] Generally, the criteria were: (1) the phenomena involved in the experiment should be relevant to the process of transport of radionuclides in the geosphere surrounding a repository; (2) the experiments should be well documented in order to make the modeling teams acquainted with the experiment and to make it possible to achieve as comprehensive a database as posible, (3) the experiment should include as many independently determined data as possible so as to allow meaningful model selection and validation.[9] The Phase I test case experiment were helpful in development of conceptual models and examination of ground-water flow and transport processes relevant to below ground disposal of radioactive waste.

Phase II effort began in April 1991 includes 10 test cases (see Table 2)[1]. Separate data sets for model calibration and subsequent model validation are being developed for many of the test cases. Phase II selection criteria were developed by the VOIC and assited the Coordinating Group in their deliberations.

Table 1: INTRAVAL Phase I Test Cases[1]

1a: Radionuclide migration in intact rock and clay samples by diffusion and advection based on laboratory experiments performed at Harwell, U.K.

1b: Uranium migration in crystalline bore cores based on experiments performed at PSI, Switzerland.

2: Radionuclide migration in single natural fissures in granite, based on laboratory experiments performed at KTH, Sweden.

3: Tracer tests in a deep basalt flow top performed at the Hanford, reservation, Hanford, USA.

4: Flow and tracer experiments in crystalline rock based on the Stripa 3-D experiment performed within the International Stripa Project.

5: Tracer experiments in a fracture zone at the Finnsjon research area, Sweden.

6: Synthetic database, based on single fracture migration experiments in Grimsel Rock Laboratory in Switzerland by NRC/NAGRA/PNL.

7a: Redox-front and radionuclide movements in an open pit uranium mine. Natural analogue studies at Pocos de Caldas, Minas Gerais, Brazil by SKB/NAGRA/U.K.DoE/U.S. DOE.

7b: Morro de Ferro colloid migration studies. Natural analogue studies at Pocos de Caldas, Minas Gerais, Brazilby SKB/NAGRA/U.K.DoE/U.S. DOE.

8: Natural analogue studies at the Koongarra site in the Alligator River area of the Northern Territory, Australia by the internal ARAP Project.

9: Radionuclide migration in a block of crystalline rock based on laboratory experiments performed at AECL, Whiteshell, Canada by AECL/U.S. DOE.

10: Evaluation of unsaturated flow and transport in porous media using an experiment with migration of a U.S. NRC trench study in Las Cruces, New Mexico, U.S.A. by University of Arizona (UAz).

11: Evaluation of flow and transport in unsaturated fractured rock using studies at the U.S. NRC Apache Leap Tuff Site near Superior, Arizona, U.S.A. by UAz.

12: Experiments with changing near-field hydrologic conditions in partially saturated tuffaceous rocks performed in the G-Tunnel Underground Facility at the Nevada Test Site performed by the Nevada Nuclear Waste Storage Investigation Project of the U.S. DOE.

13: Experimental study of brine transport in porous media performed at RIVM, Netherlands.

14a: Pumping test in highly saline ground water performed at the Gorleben site, FRG.

14b: Saline ground-water movement in an erosional channel crossing the salt dome at the Gorleben site, FRG.

Table 2. INTRAVAL Phase II Test Cases

1: Flow and tracer experiment in crystalline rock based on the Stripa 3-D experiment by SKB, Sweden (extension of Test Case 4, Phase I).

2: Flow and tracer experiments in crystalline rock fracture zone at the Finnsjon site by SGC/SKB (extension of Test Case 5, Phase I).

3: Ground-water flow associated with salinity effects in the vicinity of the Gorleben Salt Dome by BGR/GSF, Federal Republic of Germany (transfer of Test Case 14, Phase I previously not defined fully).

4: Natural analogue study of radionuclide migration in the weathered zone of the Koongarra uranium deposit, Northern Territories, Australia (extension of Test Case 8, Phase I).

5: Field experiments of unsaturated flow and transport through heterogeneous soils at the Jornada Experimental Ranch, Las Cruces, New Mexico by UAz/NMSU (extension of Test Case 10, Phase I).

6: Coupled flow and transport experiments in unsaturated fractured tuff rock at the Apache Leap Tuff site, Superior, Arizona by UAz/NRC (extension of Test Case 11, Phase I).

7: Migration of tritium in a thick clay sequence at Hades underground research facility, Mol, Belgium.

8: Tracer field experiments in a sandy to gravel shallow aquifer at the Twin Lake site, Chalk River National Laboratory by AECL.

9: Brine flow through bedded evaporites at the Waste Isolation Pilot Plant (WIPP) Site, New Mexico by SNL/U.S. DOE.

10: Ground-water flow in a fractured carbonate aquifer at the WIPP Site, New Mexico by SNL/U.S. DOE.

Phase II Test Case Selection Criteria

Active Phase I test cases which demonstrated significant accomplishments were reviewed using the following list of favorable criteria developed by VOIC:[9]

1. The test cases should be ongoing experiments that would continue through the Phase II period (April 1991-April 1994).

2. The test cases should have an experimental design oriented toward a problem that has both scientific and performance assessment relevance.

3. The test cases should be interactive, allowing for input from the INTRAVAL modeling groups on experimental design and types of data collected.

4. The test cases should already contain sufficient data sets to allow initial modeling efforts for evaluating theories and/or concepts.

5. The test cases should be comprehensive enough to cover relevant flow and transport issues presently missing from the Phase I efforts. These may include:

   a. colloidal transport,
   b. vapor-gas transport,
   c. coupled processes which include thermo-hydrochemical, hydromechanical, and thermo-hydromechanical processes,
   d. microbial-induced transport,
   e. large salinity variations,
   f. density dependent flow (both temporal and chemical effects),
   g. density dependent transport,
   h. effect of large ionic strengths on transport.

Further, it was considered essential that the test cases should cover various geometric, temporal and process ranges, especially;

range of geologic scales	cm, m, 100's m, to kilometers
range of time scales	less than a week, weeks to year, much greater than a year
range of variabilities	homogeneous properties, isotropic to anisotropic variations, variable properties as function of other parameters or processes, systematic vs. non-systematic variations
coupled effects	thermo-hydromechanical, etc.
multiple discontinuties	fracture zones, dykes, faults, etc.

Phase II Validation Issues

The ultimate objective of INTRAVAL is to learn about the validation process using data sets developed from specially designed field experiments. The Validation Integration and Coordination Committee (VICC) composed primarily of the Working Group Chairmen was established by the Coordinating Group to examine the following questions and to integrate all of the modeling groups' results into an integrated validation strategy or lessons learned.

1. What are the relevant processes of the experiment and how does the model

consider them ?

2. What are the geometric and spatial framework of the hydrogeologic system and do the modeling assumptions conform to them ?

3. Are the simplifying assumptions inherent in the model compatible to the hydrogeologic, hydraulic, and geochemical components of the system being modeled and consistent with the model used ?

4. Are the model inputs representative of the system ?

5. Are the field and laboratory experiments detailed enough to provide unique sets of databases that characterize the governing processes ?

6. Is the measurement scale compatible to the scale of the relevant processes ?

7. Is there a coherent validation strategy that allows for additional data collection and determination of "good-of-fit" criteria for comparison of the simulation results versus the independent experimental databases ?

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Does the wind blow through Yucca Mountain?

E. P. Weeks
U.S. Geological Survey

Beginning in February 1986, substantial net discharge of rock gas has been observed from a well located on the crest of Yucca Mountain, Nevada, that taps unsaturated fractured rock. Until recently, this net discharge was attributed entirely to a density contrast between slightly geothermally heated water-vapor saturated rock gas and cooler, much drier atmospheric air (Weeks, 1987; Thorstenson et al., 1990). However, as noted by Thorstenson et al., the net discharge is too large to be explained by the temperature and water-vapor induced density contrast alone. A portion of this excess flow is now attributed to a wind effect. Hypothetically, at least, as the wind blows against the mountain, the pressure increases along the flank due to a bluff or form-drag effect, and decreases at its crest due to an airfoil effect. This pressure differential results in air discharge from the well. Although measurements are not available to confirm the hypothesized pressure distribution at Yucca Mountain, Chepil (1958) has demonstrated both the drag and lift effects on instrumented hemispheres in a wind tunnel experiment. In another set of experiments, Vanoni and Hwang (1967) have measured the pressure distribution across a stabilized sand ripple in a laboratory flume that clearly demonstrates such a phenomenon.

This effect of wind on airflow from wells on Yucca Mountain was not recognized at the time the airflow data at well UZ6S were collected. Fortunately however, the National Weather Service (NWS) Nuclear Support Office had installed a weather station about 20 m north of well UZ6S in 1985, and data on wind speed and direction at a height of 10 meters above ground surface are available from that station for the entire period of airflow record. During the 17-month period for which flow records were available (April 1988-August 1989), 17 periods of anomalously high airflow from well UZ6S were identified that correlated precisely with periods of strong westerly winds. Such a qualitative dependence of air discharge from a well due to wind effects had also been observed (Woodcock, 1987) for a borehole located on a cinder cone at the summit of Mauna Kea, Hawaii.

Data on average hourly air-discharge velocity based on use of a hotwire anemometer were collected from well UZ6S for 4,748 hours during the period November 1988 to August 1989. These data, based on calibration before and after the measurement period, should be accurate within about ± 5 percent for flow velocities greater than 0.5 m/s (meter per second). Simultaneous records of barometric pressure were collected as part of the study, and air temperature, relative humidity, wind speed, and wind direction are available for that period from the NWS weather station and a station maintained by U.S. Geological Survey (USGS). These data were analyzed by linear multiple regression analysis to determine the relative contribution of barometric, temperature, and wind effects to airflow.

Use of linear multiple regression in this manner is predicated on the assumption that each of these factors (barometric pressure change, air temperature, and wind) creates a pressure difference between rock gas in the formation and in the atmosphere at the wellhead that is linearly related to gas flow in the well. Such linear relations allow invocation

of the Law of Superposition and straightforward separation of effects. Strictly speaking, Darcy's Law for gas flow, on which the analyses are implicitly based, is linear in terms of pressure squared. However, for pressure fluctuations less than 0.01 about the mean, the relations is very nearly linear (Weeks, 1978).

The regression-analysis-based empirical coefficients have physical bases that can be used to select proper forms for the regression equation terms. As an example, barometrically-induced air intake and exhaust from a well open through the unsaturated zone arises from the compressibility of air within the unsaturated materials, and is quite transient. This is particularly true for a well tapping a fractured rock mass of limited areal extent, such as that represented by the Tiva Canyon unit tapped by well UZ6S, as barometric pressure equilibrates with that downhole not only by flow through the well and leakage through the caprock, but also from outcrop exposures on both sides of the mountain. Hence air flow to or from the well at any time should be induced by barometric changes occurring only during the previous few hours.

Based on this premise, several trial-and-error regression analyses were made of the form:

$$V_B = a_0 + a_1(P_0-\bar{P}) + a_2(P_0-P_1) + a_3(P_1-P_2)\ldots + a_n(P_{n-2}-P_{n-1}), \quad (1)$$

where V_B = hourly flow velocity due to barometric effects, m/s;

a_0 - a_n = regression coefficients, m/s kPa;

P_0 = barometric pressure at end of hour, kPa;

$\bar{P}$ = mean barometric pressure, kPa;

P_1 = barometric pressure one hour previously, kPa;

and other P subscripts represent the number of hours before present.

Overall, the joint criteria of obtaining a large correlation coefficient while minimizing the number of variables involved in the regression resulted in the equation:

$$V_B = a_0 + a_1(P_0-\bar{P}) + a_2(P_0-P_2) \quad (2)$$

for the final analysis.

In hilly or mountainous terrain, a pressure difference between air or rock gas in the well bore and the atmosphere is generated at the well head by a temperature- and composition-induced density contrast whenever the air temperature and relative humidity vary from those of the rock gas. This pressure difference, which induces flow to or from the well, is given, assuming that the atmosphere and the rock gas in the fracture network represent separate isothermal columns, by the equation (Sanford, 1982):

$$\Delta P = P_W[\exp(\frac{-g\Delta z}{R_A T_{RV}}) - \exp(\frac{-g\Delta z}{R_A T_{AV}})], \quad (3)$$

where ΔP = pressure difference at wellhead, Pa;
P_W = atmospheric pressure at wellhead altitude, Pa;
g = acceleration due to gravity, m/s^2;
Δz = difference in altitude between hillslope fractured rock outcrop and well head, m;
R_A = air-specific gas constant, J/kgK;
T_{RV} = virtual temperature of rock gas, K;
and T_{AV} = virtual temperature of atmospheric air, K.

Virtual temperature is defined as the temperature at which dry air would have the same density as air with its prevailing moisture content and temperature.

Temperature-induced density effects result in airflow between hillside outcrops and the well, and are much less dependent than barometric effects on the compressibility of air in the unsaturated zone. Hence, flow due to temperature effects are well-described by current air temperature, rather than by changes in temperature. Hence, the temperature effects are modeled as:

$$V_T = a_0 + a_1 T_c \quad (4)$$

where V_T = hourly velocity due to temperature effects, m/s; and
T_c = (20°C - T) [293.2/(273.2 + T)
where T = mean air temperature for that hour, °C,
and 20°C = the approximate virtual temperature of the rock gas.

Multiplying (20°C-T) by the bracketed term results in an adjusted temperature difference that is almost linear with the density-induced pressure difference, as described by equation 3.

Wind is hypothesized to produce a pressure drop at the crest of the mountain due to an airfoil effect. For the flow of an ideal (frictionless) fluid over an ideal airfoil shape, the pressure drop at a selected point would be given by the Bernoulli equation:

$$\Delta P_D = C_L \rho u^2/2, \quad (5)$$

where ΔP_D = pressure drop due to airfoil effect, Pa;
C_L = position-dependent lift coefficient, dimensionless;
ρ = air density, kg/m^3;
and u = free air stream velocity, m/s.

In addition to the generation of a pressure drop at a mountain crest, wind creates a pressure buildup along the upwind flank of the mountain due to a

form drag effect, again given for an ideal shape and fluid by the equation:

$$\Delta P_B = C_D \rho \, u^2/2, \tag{6}$$

where ΔP_B = pressure buildup due to drag effect, Pa;

and C_D = position-dependent drag coefficient, dimensionless.

Undoubtedly, pressure differences due to both the lift and drag effects contribute to the wind-generated flow from well UZ6S, as both would increase air exhaust from the well. However, no attempt was made to separately identify their contributions in this study.

For real fluids flowing over natural surface features, pressure differences resulting from lift and drag effects are more complicated, depending on Reynolds number and, hence, wind speed, and on whether boundary layer separation (Schlicting, 1968) occurs that destroys the u^2 relations between wind speed and lift or drag. Under these conditions, both drag and lift coefficients and the exponent of u become dependent on wind speed, and the coefficients are not dimensionless.

Wind effects, like temperature effects, result in flow between the hillside outcrops and well UZ6S, again resulting in the magnitude of wind-generated flow being dominated by current values. Thus, the regression analyses were made using wind data only for the hour that flow measurements were made.

For Yucca Mountain and well UZ6S, the magnitude of the wind effect is highly dependent on wind direction, as the pressure differences generated by lift and drag effects are dependent on the mountain slope and curvature in the upwind direction. Consequently, combined files of wind and flow data were sorted by wind direction and divided into subsets of 20° sectors centered on 10° increments to provide 36 overlapping data sets. Separate values for the wind-function multiplier were determined for each sector for selected values of u^n.

Because pressure differential, due to lift and drag are ideally described by the Bernoulli equation, it was initially assumed that

$$V_u = g(\theta)u^2, \tag{7}$$

where V_u = wind-generated flow velocity, m/s;

$g(\theta)$ = a regression-coefficient constant for a given wind direction sector, s/m;

θ = wind direction, measured clockwise from north, degrees;

and u = mean wind speed, m/s.

Regression analyses for the 36 sectors indicated that a very good regression fit was determined using the above equation for data sets representing wind direction from the northeast and southeast, characterized by a fairly smooth mountain slope in the upwind direction.

However, the fit was much poorer for data sets representing winds across the sharp break in slope along the west face of Yucca Mountain crest, and from due east across the sharp break created by the cut bank of the UZ6 drill pad. For winds from these directions, the increase in air flow from well UZ6S caused by wind effects is substantially better described by a linear function of wind speed than by the wind velocity squared. Under these conditions, "boundary layer separation" and back-flowing eddies (Schlicting, 1968) probably are generated by the sharp break in slope.

The data analyses clearly indicate that the form of the wind function depends on wind direction. However, a comparison of coefficients using an approximate wind function common to all sectors is useful to provide insight on the directional dependence of the wind effect. Hence, in the final analysis, flow was computed as

$$V_u = g(\theta)u^{1.5}. \tag{8}$$

This compromise value of the wind speed exponent provided a better fit to the entire suite of data than did either the squared or linear velocity terms, and it always produced either the best fit or the second best fit to data for individual sectors.

The magnitude of the effect on wind from any direction on flow from well UZ6S was computed as follows. A smooth curve was fit through the 36 coefficients using a cubic-spline routine, and a coefficient value $g(\theta)$ for each degree of wind direction was interpolated. The results of these computations are shown in figure 1 as a plot of the magnitude of the coefficients in polar coordinates centered on well UZ6S. The plot shows a remarkably good fit to the topography of Yucca Mountain (figure 1). For example, the largest coefficients (about 0.18) occur for west winds which strike head onto the bluffs forming the east side of Solitario Canyon. As wind direction is rotated clockwise, the coefficient magnitude declines at a fairly uniform rate until the wind is out of the north and striking the bluffs quite obliquely. The coefficient is near its minimum for wind blowing directly along the ridge crest from the NNE or SSE. The actual minimum coefficient is for wind from due east, and is likely due to the cutbank of the UZ6 drill pad, rather than the natural contour of the mountain shown in the figure.

Examination of the results of the regression analysis indicated that high exhaust and intake velocities predicted by the regression equation were larger in absolute value than the measured values. This phenomenon was attributed to the effects of frictional pressure losses in the wellbore at high flow velocity. Consequently, corrections for these pressure losses were made based on the theory of flow through pipes (Streeter, 1962, p. 217). For a Reynolds number representative of the typical flow velocity range, these pressure losses are proportional to the velocity raised to the 1.75 power. Relating the frictional pressure loss to an estimate of the temperature-induced driving pressure potential, the velocity in the absence of well losses would be related to the measured velocity as

$$V_{WLC} = V + 0.25V^{1.75} \tag{9}$$

where V_{WLC} = well-loss corrected velocity, m/s;
and V = measured velocity, m/s.

Absolute values are implied and the sign of flow is retained. This equation was determined from theoretical considerations. However, the resulting corrected flows appear to be quite linear relative to the appropriate driving weather parameters, suggesting that the linearized correction is appropriate.

The final multiple linear regression equation is

$$V_{WLC} = a_0 + a_1(P_0-\bar{P}) + a_2(P_0-P_2) + a_3T_c + g(\theta)u^{1.5} \quad (10)$$

where $g(\theta)$ is the cubic-spline fit value of the wind-effect coefficient.

The adequacy of the regression equation is demonstrated by a comparison of measured and computed flow, as shown in figure 2 for a relatively windy two-day period in November 1989. For this comparison, computed flow is given by the equation:

$$V_{WLC} = 0.523 - 0.313\ (P_0-\bar{P}) - 9.81\ (P_0-P_2) - .204\ T_c + g(\theta)u^{1.5}. \quad (11)$$

The comparison between computed and measured flow is reasonably good for both calm and for windy periods, particularly considering the degree of approximation used in modeling the effects of wind on flow. Also shown in figure 2 are predictions based on regression of flow in well UZ6S against barometric pressure changes and temperature only. This regression results in the equation:

$$V_{WLC} = 1.53 - 1.33\ (P_0-\bar{P}) - 9.53\ (P_0-P_2) - 0.191\ T_c. \quad (12)$$

Values of V_{WLC} thus computed are somewhat larger than those measured during calm periods, and substantially smaller during windy periods. The predictions are clearly poorer than those obtained when wind speed is included as a prediction variable. In addition, because of the large intercept, the equation indeed overpredicts net exhaust due to temperature effects, accounting for part of the discrepancy noted by Thorstenson et al. (1990).

The hourly predictions demonstrate the adequacy of the regression equation to predict flow, but do not clearly show the effects of temperature-induced density differences on flow. For this comparison, hourly values of temperature-affected flow velocity were computed by subtracting regression-equation based estimates of the wind and barometric effects from the measured well-loss-corrected flow velocity. The hourly values

resulting from these corrections include the effects of temperature on flow, as well as errors in flow measurement and the residual errors in estimating wind, barometric, and temperature effects. Daily average values of flow and of density-adjusted temperature, T_c, were determined to minimize errors resulting from diurnal variations in temperature and diurnal and semidiurnal variations in barometric pressure.

The resulting data were plotted and a regression equation between flow and temperature was obtained (figure 3). This analysis shows an excellent fit between flow and temperature (r=0.989), but indicates that temperature-induced flow would be zero at a virtual air temperature of 22.5°C, rather than a value of 20°C that corresponds to the virtual temperature of water-vapor-saturated air at the measured rock-gas temperature of about 17.5°C. This offset is smaller than that reported by Thorstenson et al. (1990), because in their analysis, some wind-affected flow was inadvertently incorporated into computed temperature effects. Thus part, but not all, of the previously noted discrepancy between measured and theoretically estimated temperature-induced flow is now explained.

Estimates of the separate contributions by wind and temperature effects to net annual gas discharge from well UZ6S for the year 1988 were made from hourly measurements of air temperature, wind speed, and wind direction, based on the appropriate regression-equation constants. These estimates provide an assessment of the relative importance of the two flow-producing mechanisms, both in terms of natural circulation through the mountain in the absence of boreholes, and in terms of assessing the effects on the gas chemistry of enhanced circulation due to installation of the boreholes.

The regression-based estimates of flow from the well bore represent those that would occur in the absence of well losses. However, it is these estimates, rather than those of actual flow, that may more accurately reflect the relative importance of temperature versus wind effects on natural rock gas circulation through Yucca Mountain. This should be true because natural flow velocities would be slow enough and fracture apertures through which the flow occurs small enough that flow remains laminar and hence linear with respect to the pressure differences that are also linearly related to well-loss corrected flow velocities. The regression estimates indicate that, for 1988, the total flow due to temperature effects, including both discharge from the well in winter and from the mountain-flank outcrops in summer, would have been about 1,500,000 m^3. Flow without well losses due to wind would have been about 700,000 m^3, but wind effects cancel about 100,000 m^3 of summertime temperature-induced flow from the outcrops. Thus, flow of about 1,400,000 m^3 would have occurred due to temperature effects and 600,000 m^3 due to wind effects, and wind effects account for about 30 percent of the total flow.

Annual net discharge estimates are also needed to evaluate any changes in chemistry that the gases exhausting from well UZ6S might show with time. For these flow estimates, values of hourly flow were corrected for well-loss effects by an iterative solution to the nonlinear well-loss equation, with the correction proportionally assigned to the temperature-affected and wind- affected velocities if they were both positive, or entirely to the dominant effect if air temperatures were such that density-driven

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Table 1. Monthly summary of temperature-based and wind-based flow of rock gas from well UZ6S during 1988. Positive values are for exhaust from the well.

Month	Flow, cubic meters × 10^{-5} Temperature-affected	Wind-affected	Total[1/]
JAN	1.8	0.3	2.1
FEB	1.4	0.3	1.7
MAR	1.2	0.5	1.8
APR	1.0	0.4	1.4
MAY	0.5	0.6	1.1
JUN	-0.2	0.6	0.5
JUL	-0.7	0.5	-0.2
AUG	-0.4	0.4	0.0
SEP	0.0	0.3	0.3
OCT	0.2	0.3	0.4
NOV	1.3	0.4	1.7
DEC	1.7	0.4	2.0
Total	7.8	5.0	12.8

Totals do not always reflect the algebraic sum of temperature- and wind-affected flows due to rounding.

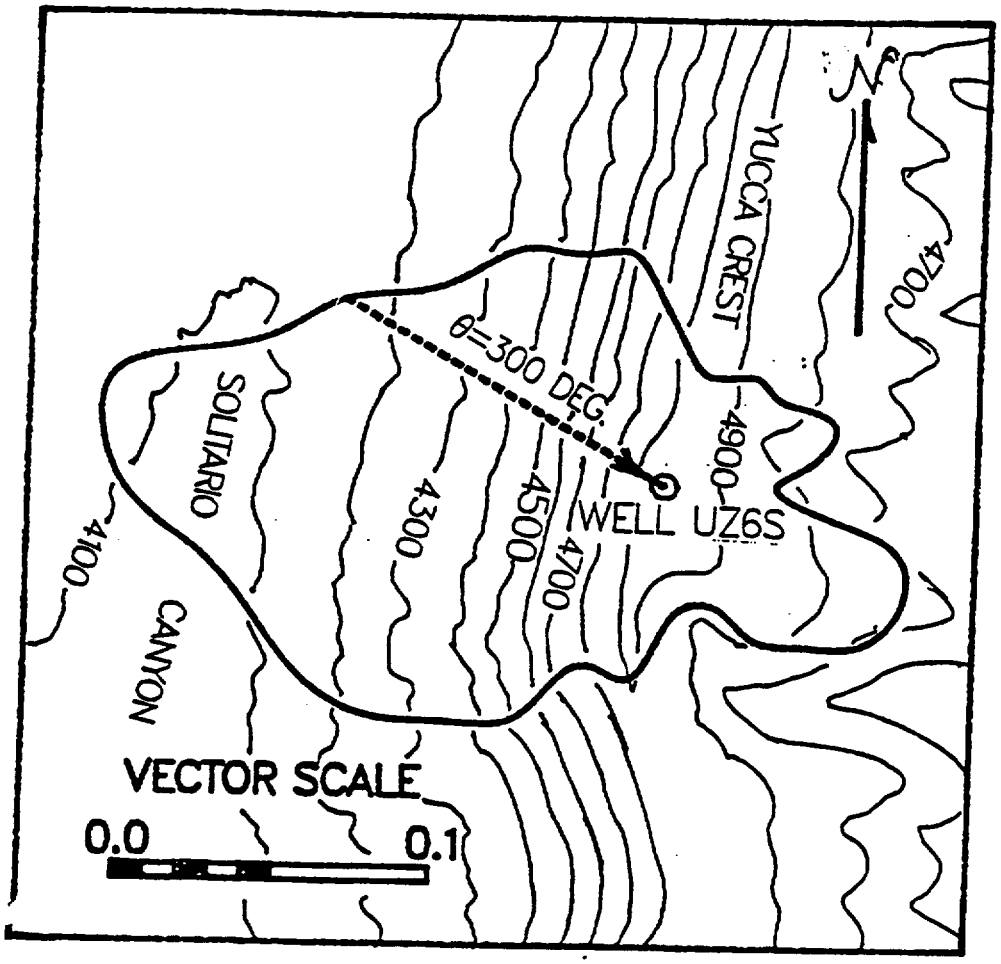


Figure 1. Polar-coordinate plot of the multiplier by which wind velocity to the 3/2 power is multiplied to obtain wind-effect flow from well UZ6S. The vector for $\theta = 300°$ (wind from the west-northwest) is shown as an example, and has a magnitude of 0.115. Superimposed are 100-foot contours for Yucca Mountain.

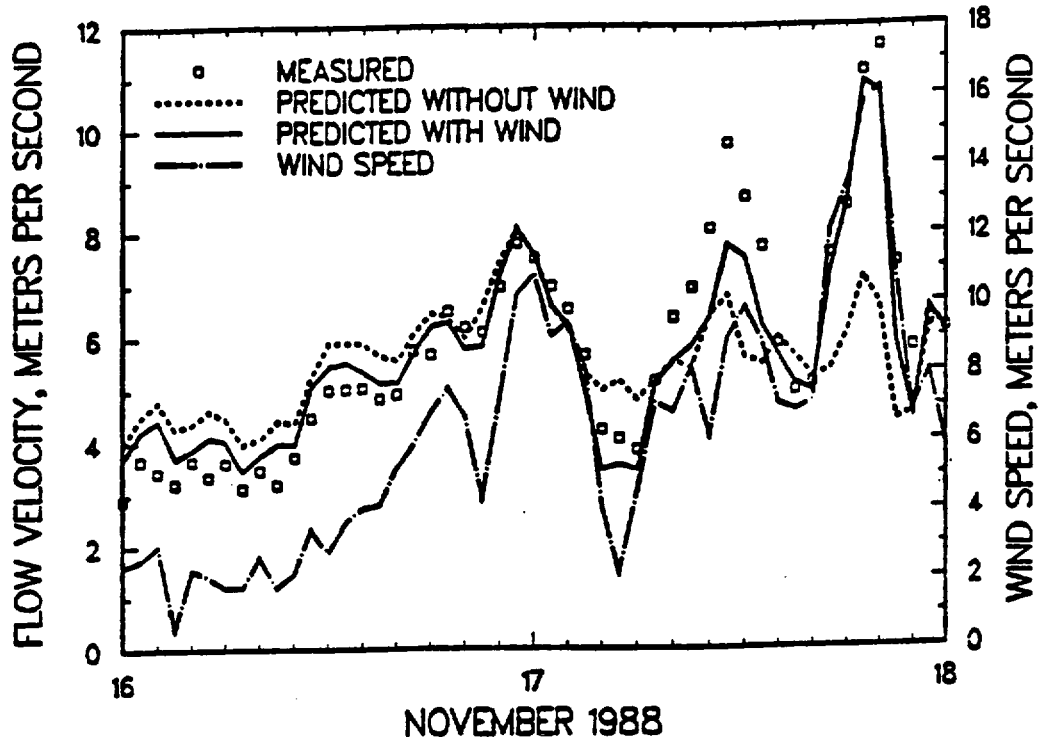


Figure 2. Regression-equation predicted hourly flow, with and without wind effects, and corresponding measured well-loss corrected flow from well UZ6S for a two-day period.

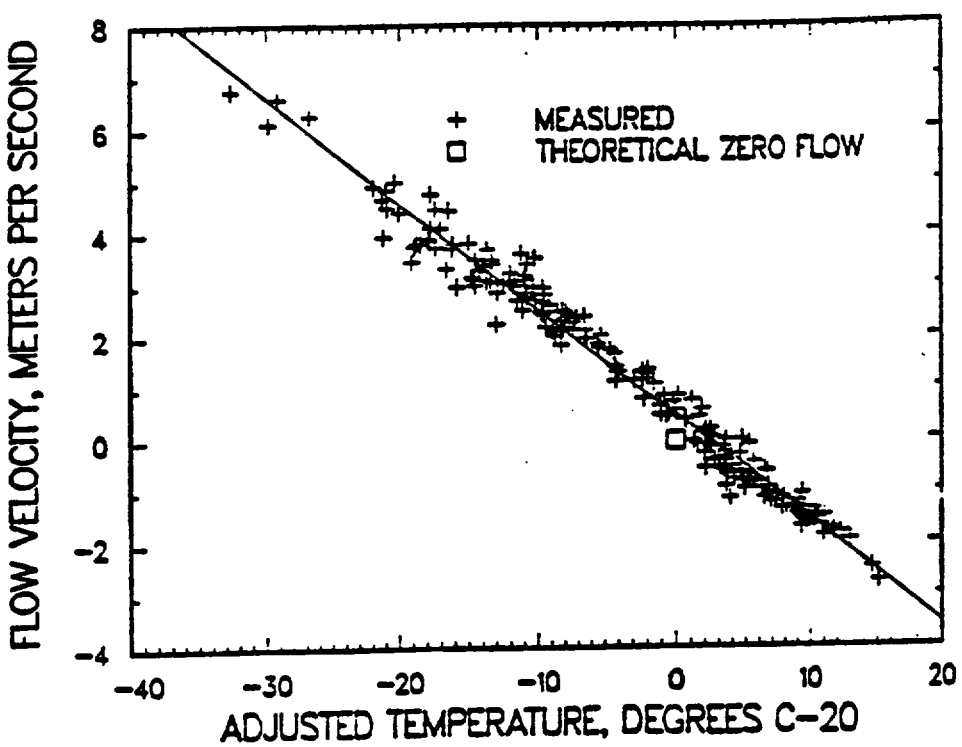


Figure 3. Regression of daily average flow from well UZ6S corrected for well losses and with predicted barometric-induced and wind-induced flow subtracted, against density-adjusted temperature difference from 20°C, the approximate virtual temperature of the rock gas. Data are for 1988-1989.

Nonisothermal Hydrologic Transport Study at the Apache Leap Tuff Site

Todd C. Rasmussen
University of Arizona

A field-scale heater test is proposed for investigating coupled hydrologic, thermal and mechanical processes in unsaturated fractured rock related to the disposal of high-level radioactive waste (HLW) in an underground repository. Observations of fluid flow and solute transport in nonisothermal, unsaturated, fractured rock under controlled, experimental conditions are limited, and the proposed experiment will provide data sets for use in verifying conceptual and computer models related to HLW isolation in an environment where substantial quantities of heat energy are produced by the HLW. Previous nonisothermal experiments in tuff have demonstrated the need for additional field-scale experiments conducted under controlled initial and boundary conditions using more sophisticated and reliable monitoring systems.

An experimental plan is being developed which describes the long-term, field-scale nonisothermal experiment. The plan also describes the justification for conducting the experiment, a summary of related previous experiments, important processes expected to dominate coupled heat, liquid, vapor, gas, and solute flow during the experiment, material properties at and near the proposed heater site, predictions of water movement, water content changes, temperatures, gas fluxes and solute movement during the course of the experiment, and critical design parameters which will be used to control expected outcomes of the experiment and to maximize the ability to distinguish between alternate conceptual model forecasts. The details of the experimental plan have not yet been finalized, and are expected to result from interaction between modelers and experimentalists during the design phase.

The planned heater experiment is being designed to evaluate and confirm existing conceptual and computer simulation models related to fluid flow in a nonisothermal environment. The processes to be investigated include two-phase flow, solute transport, rock deformation due to heating, fracture and matrix flow. Important characterizations parameters include: unsaturated hydraulic, pneumatic, and thermal conductivities; air, vapor and solute diffusivities; vapor pressure reduction due to osmotic potential; and fracture and matrix permeability as a function of stress fields generated by rock thermal expansion and contraction.

Previous laboratory, field and laboratory nonisothermal experiments have demonstrated the complexity associated with fluid flow in unsaturated fractured rock. To avoid ambiguous and inconclusive experimental results it is important that simulation modeling and site characterization be performed prior to conducting the field experiment. The design and implementation of the proposed nonisothermal hydrologic transport study requires a concise and explicit statement of objectives, procedures, and tasks. This section summarizes the phases that will be required during the course of the study, as well as the specific tasks related to the study phases. The details of the experimental plan will be developed in consultation with INTRAVAL participants. (The INTRAVAL program is a multinational effort to compare numerical methods with field observations.)

Study Phases

Six study phases are planned which lead to the evaluation of the current capability to model and predict nonisothermal hydrologic transport in unsaturated fracture rock at the Apache Leap Tuff Site. The various phases, summarized in Table 1, begin with computer modeling activities related to the determination of an initial experimental design. The simulation studies will use existing characterization data from the heater site along with more complete characterization data sets from the nearby injection site. Design issues related to borehole construction and monitoring techniques will be examined during Phase 1.

Phase 2 activities will focus on installation of boreholes as determined during Phase 1 simulation studies. Additional site-specific characterization data will be obtained based upon information obtained from borehole logging, borehole permeability tests, and laboratory characterization tests using oriented cores. Monitoring of moisture and thermal conditions will also begin in this phase.

During the third phase, additional simulation modeling will be employed using the site-specific characterization collected data in Phase 2. The simulations will be used to refine the placement of sensors, the heater, packers and surface cover. After completion of the simulation studies, the placement of the instruments and other components will be performed.

The fourth phase will consist of baseline data collection at the site from the sensors placed during the third phase. The baseline data will be used to determine the initial and boundary conditions as input to computer simulation models for the purpose of determining the optimal heater schedule. Once the optimal heater schedule has been determined and sufficient baseline data have been collected, Phase 5 will begin.

The fifth phase consists of 1) Generating simulation forecasts and confidence intervals for the heater experiment, and 2) Conducting the heating experiment. The two components will be conducted independently and without any cross-communication between the two. Field data will be collected, processed and archived until such time as the simulation studies have been completed. The only exception to this rule will be if there are changes in boundary conditons or if additional characterization data become available.

Simulation results will be compared with experimental results during the final phase. The performance of the simulation models will be evaluated based on their ability to predict field observations. No calibration against the experimental results is expected, and the comparisons will be a test of model accuracy. Confidence intervals will be inspected to determine if the model projections include the observed range of system responses. The forecasts can then be used to evaluate alternate conceptual models.

TABLE 1: Nonisothermal Hydrologic Transport Study

Phase 1	Perform simulations using existing characterization data from the nearby Apache Leap injection site for the purpose of obtaining a preliminary experimental design. Evaluate alternate characterization and monitoring techniques at the injection site. Issues such as borehole locations, orientations and drilling methods will be resolved during this phase.
Phase 2	Install boreholes and further characterize the heater site using in situ and laboratory core measurements. Obtain *in situ* conditions for water contents and temperatures. Select and calibrate measurement devices.
Phase 3	Refine the experimental design based on data collected in Phase 2 and additional simulation studies. Using this information, install sensors, heater, packers and surface cover. Also, install additional boreholes if needed.
Phase 4	Collect baseline data from sensors installed in Phase 3, and continue monitoring water contents which were started in Phase 2. Use data sets in conjunction with computer modeling activities to refine heating schedule.
Phase 5	Perform heater test and measure responses. Concurrently and independently simulate responses using baseline and characterization data, as well as observed initial and boundary conditions.
Phase 6	Compare experimental and simulation results. Determine whether the observed response lies within forecasted confidence intervals. Obtain and test core samples to confirm final conclusions.

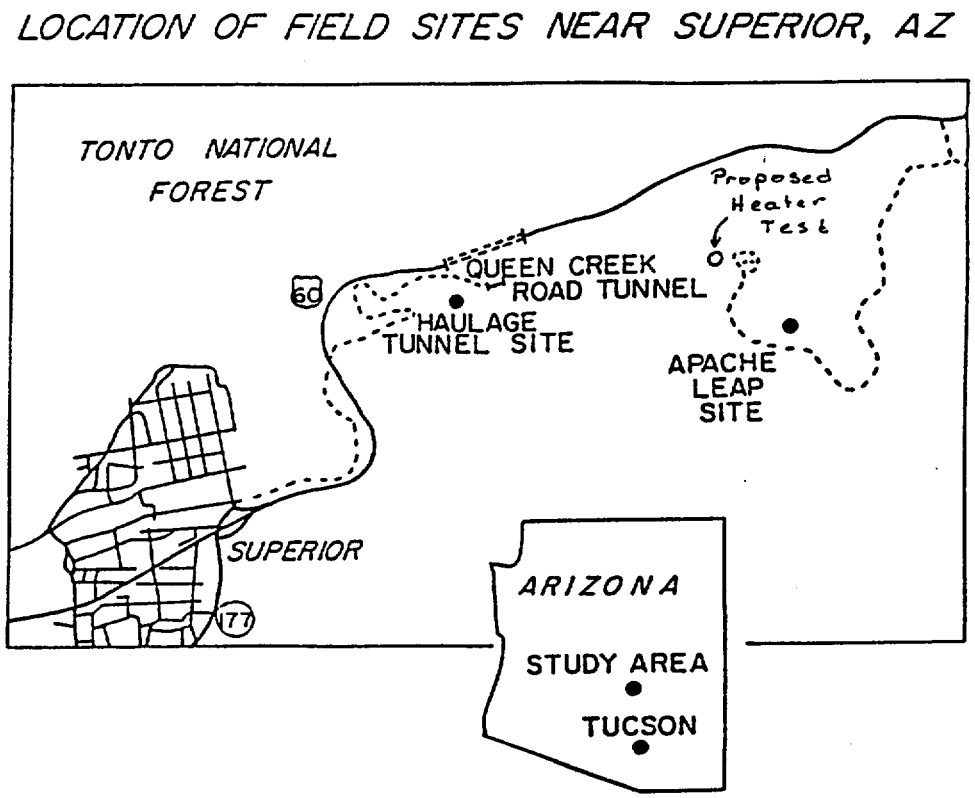


Figure 1: Proposed location of field heater test. Not drawn to scale.

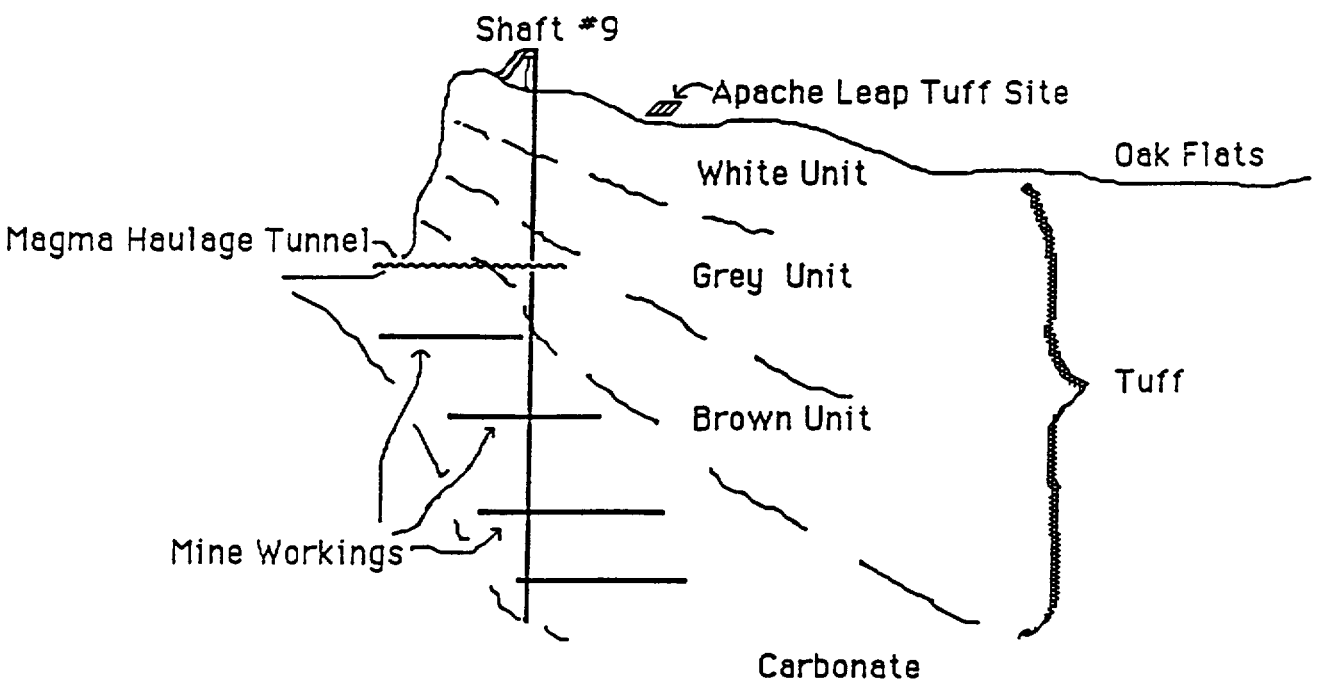


Figure 2: Cross-sectional view of Apache Leap Tuff. Not drawn to scale.

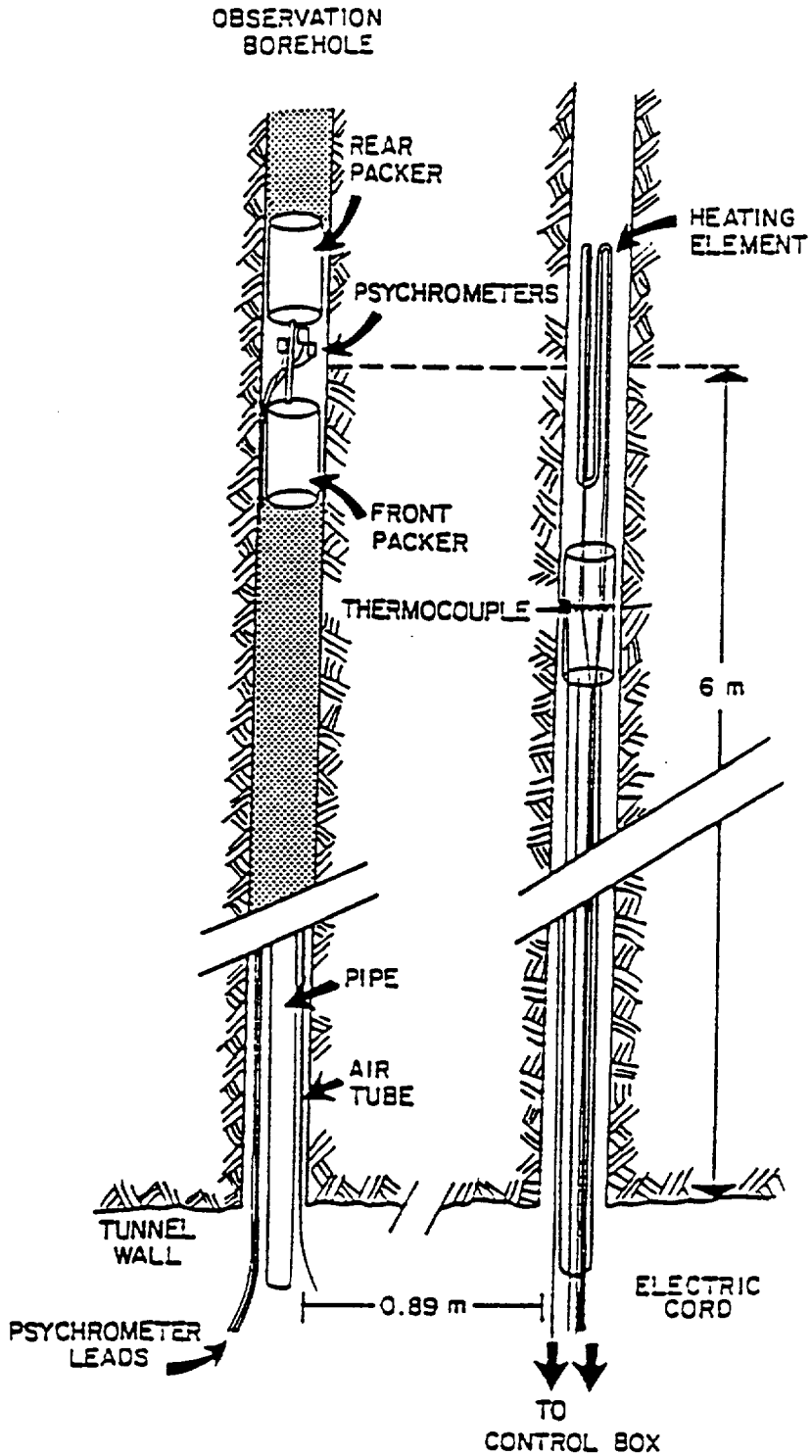


Figure 3: Diagram of heating element and thermocouple located behind packer (right borehole) and packers isolating psychrometers (left borehole) at Queen Creek Road Tunnel Site.

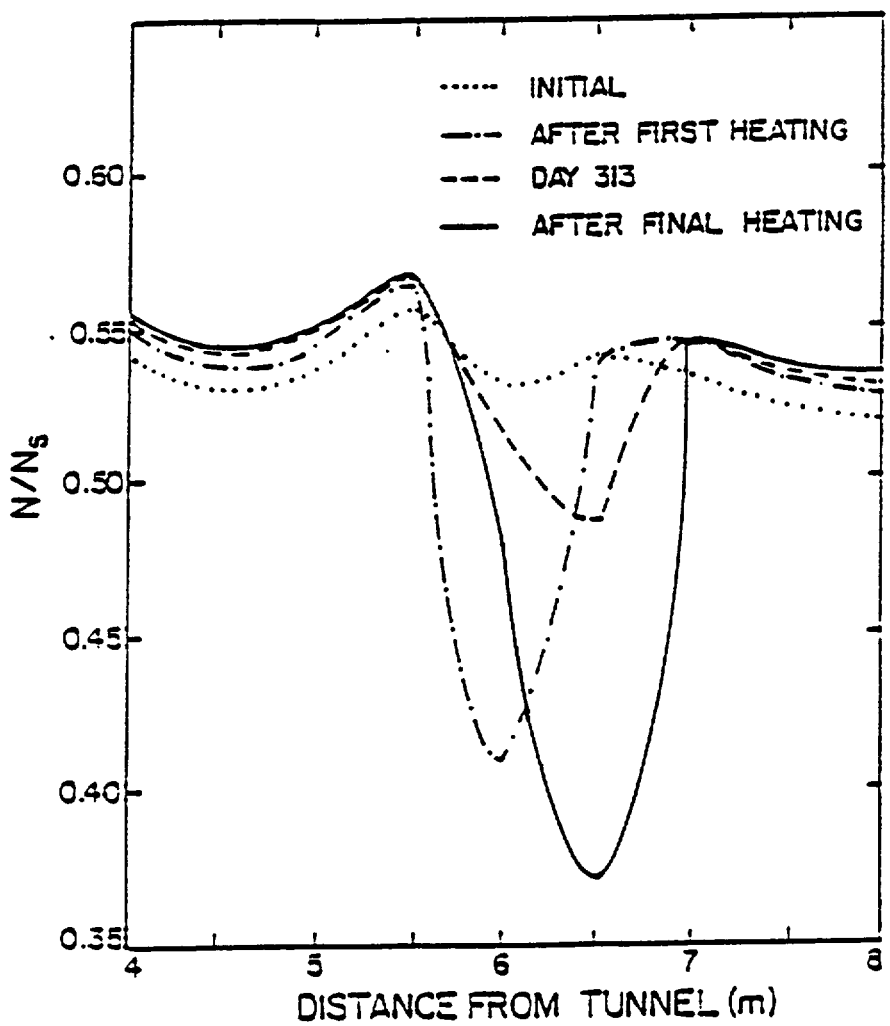


Figure 4: Observed water content in tuff around the heater borehole as a function of time and distance along borehole for heating experiment in Queen Creek road tunnel.

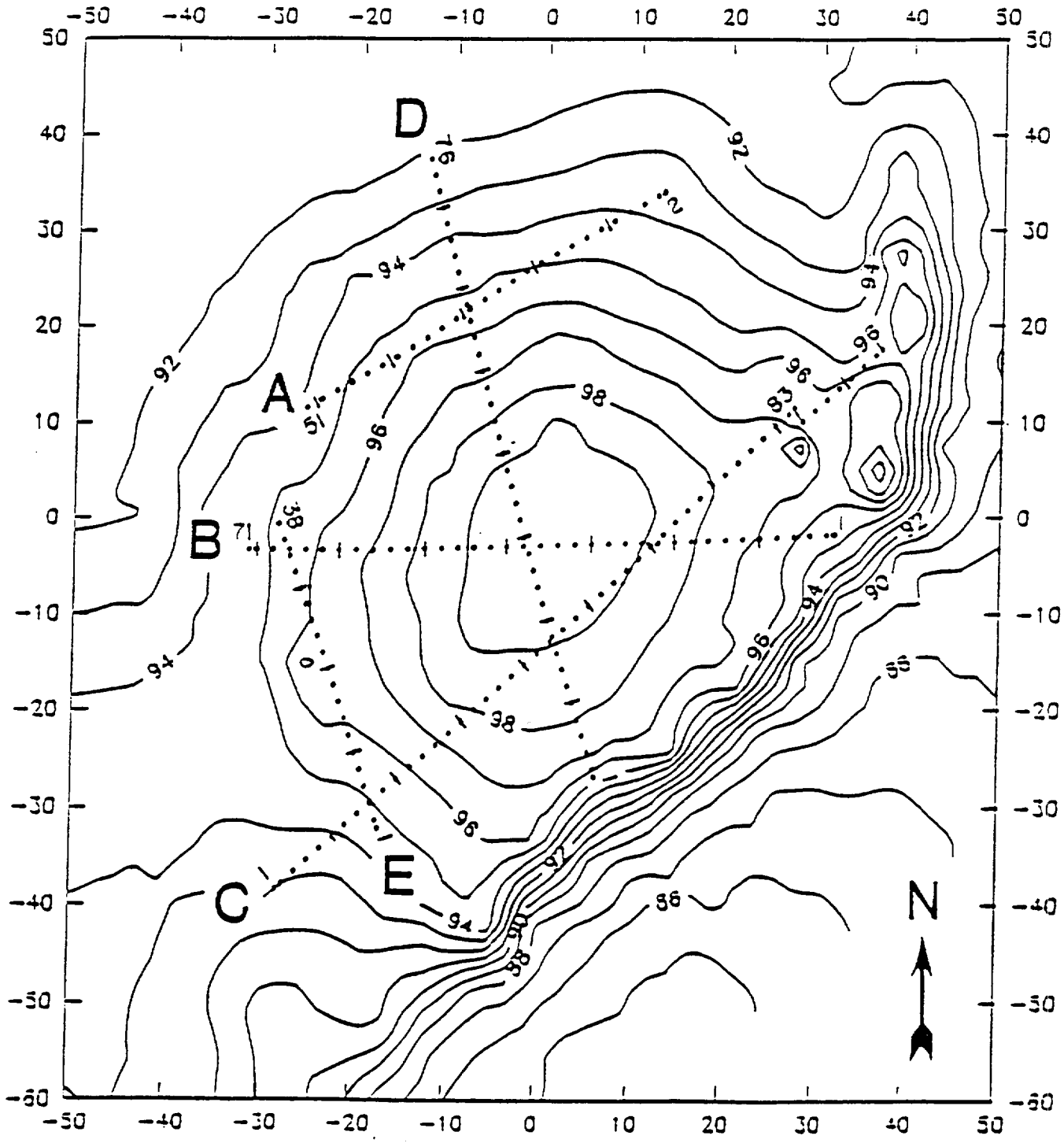


Figure 5: Topography of proposed heater site showing locations of electrical resistivity profiles.

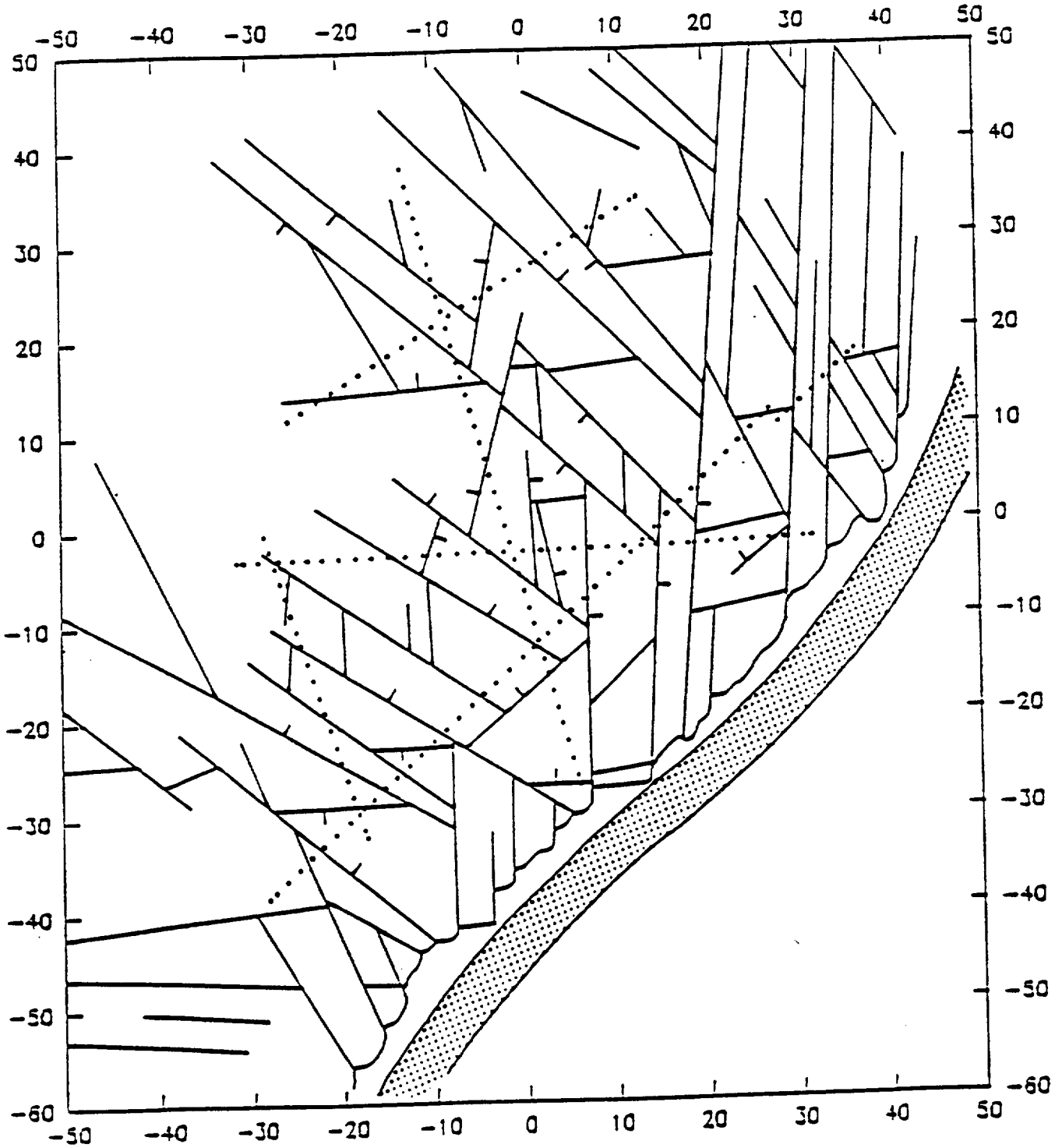


Figure 6: Structural lineaments interpreted from aerial photographs of fracture planes exposed in outcrop at Apache Leap Heater Site.

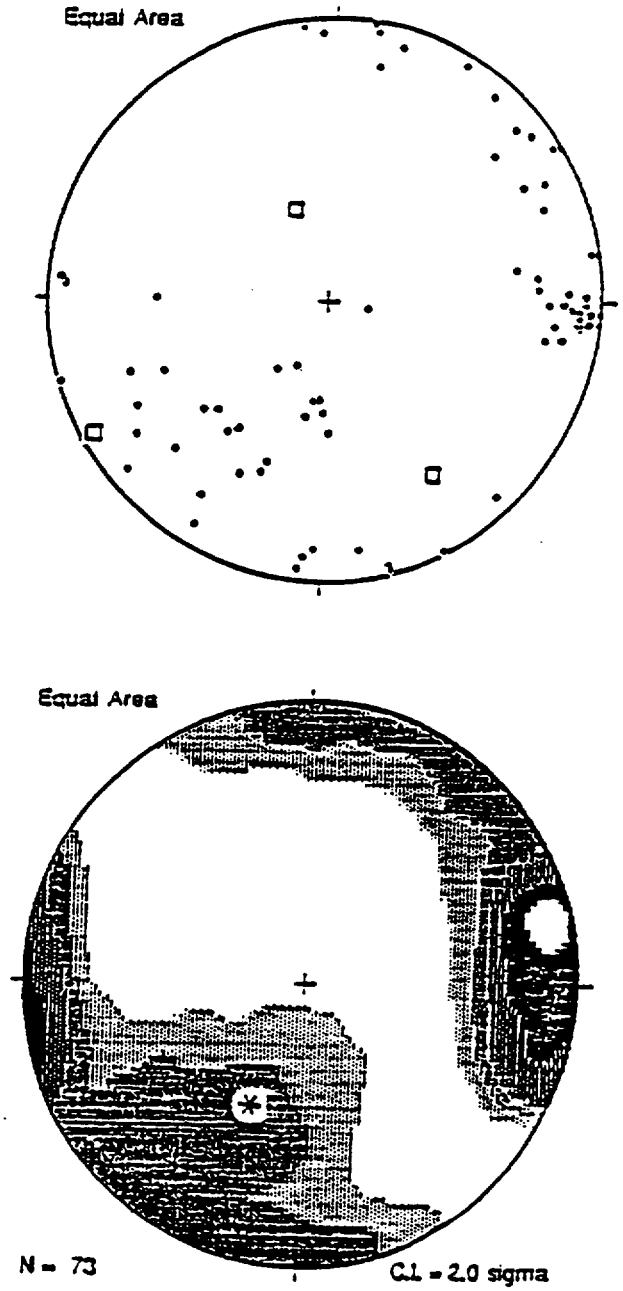


Figure 7: Fracture orientation data at the Apache Leap Heater Site. Equal-area, stereonet projections of poles to fracture planes, collected from a roadcut along the southeastern boundary of the heater knoll.

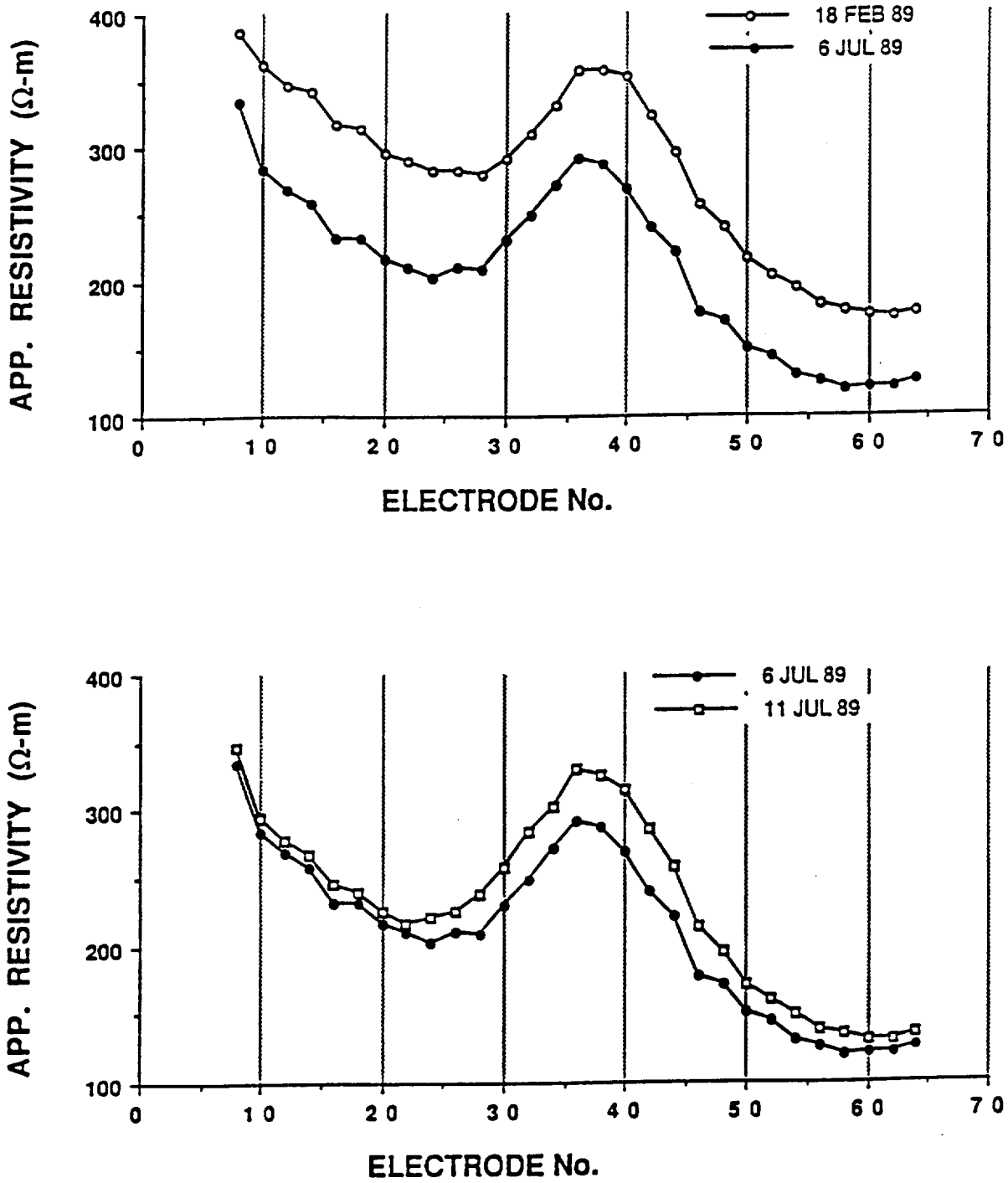


Figure 8: Electrical resistivity along B profile. Electrode spacing (horizontal scale) is one meter, and profiles depicted heare were collected at two meter spacings, with an assumed pnentration depth of approximately one meter. Profiles of upper diagram were surveyed under dry conditions, the difference between dates attributed to temperature effects on pore-fluid resistivity. Profiles of lower diagram were collected before and after a 12 mm rainfall event.

Apache Leap Watershed Study

Ingrid Anderson,
University of Arizona

The fate of rainfall once it reaches the ground surface is an important characterization parameter due to the importance of precipitation as the source term for flow of water through the subsurface. The objective of this study is to provide data sets which will allow estimates to be made of the potential for infiltration, deep percolation and recharge as the result of rainfall. The data sets obtained from this field study provide useful input parameters for computer simulation models. The parameters are used to prescribe the flux boundary condition at the upper surface of the hydrogeologic system.

To obtain meaningful characterization data sets, all elements of the water budget must be examined, including rainfall, interception, surface runoff, infiltration, surface storage, evapotranspiration, and deep percolation. The field site selected for this study is located approximately 400 m to the west-northwest of the Apache Leap Tuff Site. Two catchments have been instrumented, with areas of 1.73 and 0.24 ha. The vegetation at the site is sparse, with over fifty percent exposed rock surfaces and little to no soil cover. Average slopes are 26 and 17 percent for the large and small catchments, respectively.

Precipitation at the site is measured using a tipping bucket raingage which provides rainfall intensity and total rainfall accumulation. Additional rain collection devices are used to measure the spatial variability of cumulative rainfall. The resolution of the tipping bucket raingage is one mm. Temperatures are measured within a sheltered weather station using a thermistor. Runoff from the catchments is measured using 1-foot HS-type flumes. The flumes are instrumented with pressure tranducers. Published rating tables are available which allow the determination of flow rates of less than 1 cfs.

Data are collected on a CR-10 data logger installed at the field site and powered by solar panels connected to an automotive battery. Data are collected on an hourly basis when no runoff through the flume is present, and at five-minute intervals when flume flow greater than a depth of 0.05 ft is measured.

Table 1

Expected maximum rainfall depths (inches) at the Apache Leap Tuff Site.
Source: Miller et al., 1973

Duration	Recurrence Interval			
	2 yr	5 yr	25 yr	100 yr
15 min	0.70	0.74	0.97	1.21
30 min	0.96	1.03	1.34	1.68
1 hour	1.22	1.30	1.70	2.13
2 hour	1.42	1.64	2.21	2.70
3 hour	1.61	1.87	2.55	3.08
6 hour	1.80	2.30	3.20	3.80
12 hour	2.20	2.80	3.70	4.50
24 hour	2.50	3.25	4.20	5.25

Miller, J.F., and R.H. Frederick, and R.J. Tracey, "Precipitation-Frequency Atlas of the Western United States: VII - Arizona", NOAA, 1973.

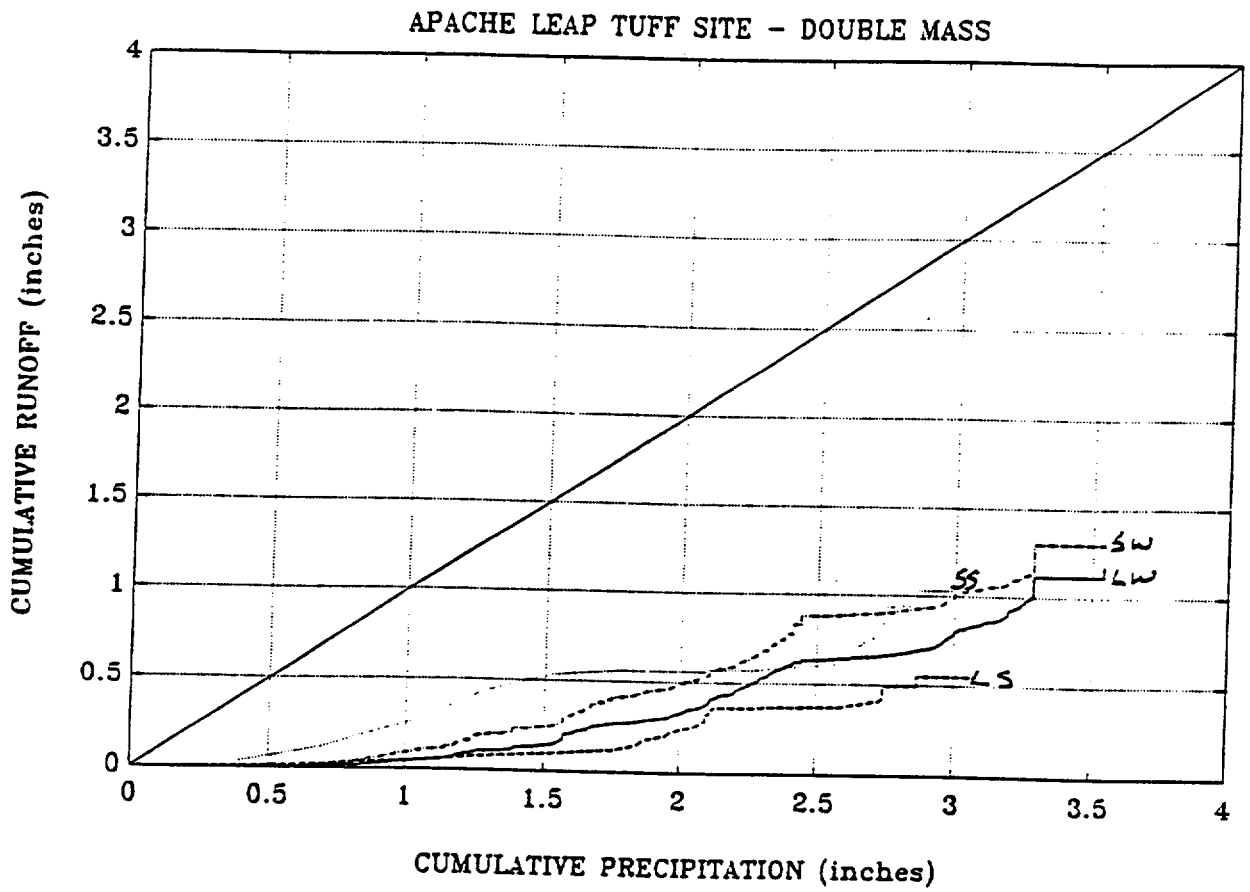
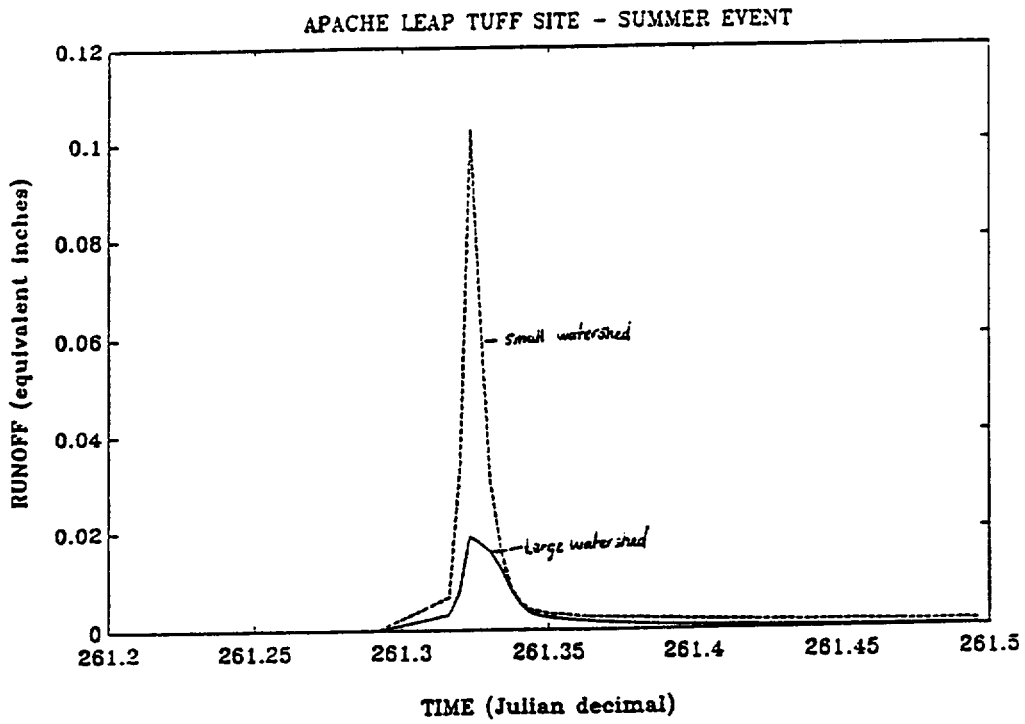


Figure 2. Cumulative runoff vs. cumulative precipitation at ALTS watershed study site. Where SS is data from small watershed during summer event, SW is small watershed during winter event, LS is large watershed data during a summer event and LW is large watershed data during a winter event.



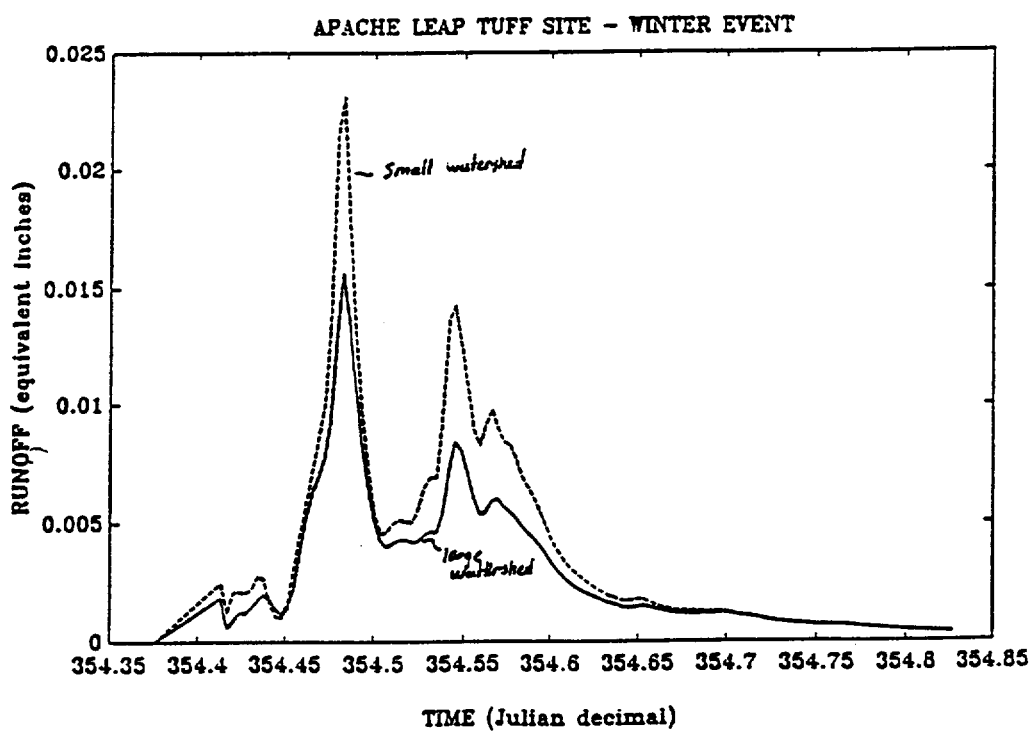


Figure 3. Runoff data for large and small watersheds during a winter and summer rainfall event. (Note 1 hour = .042 days).

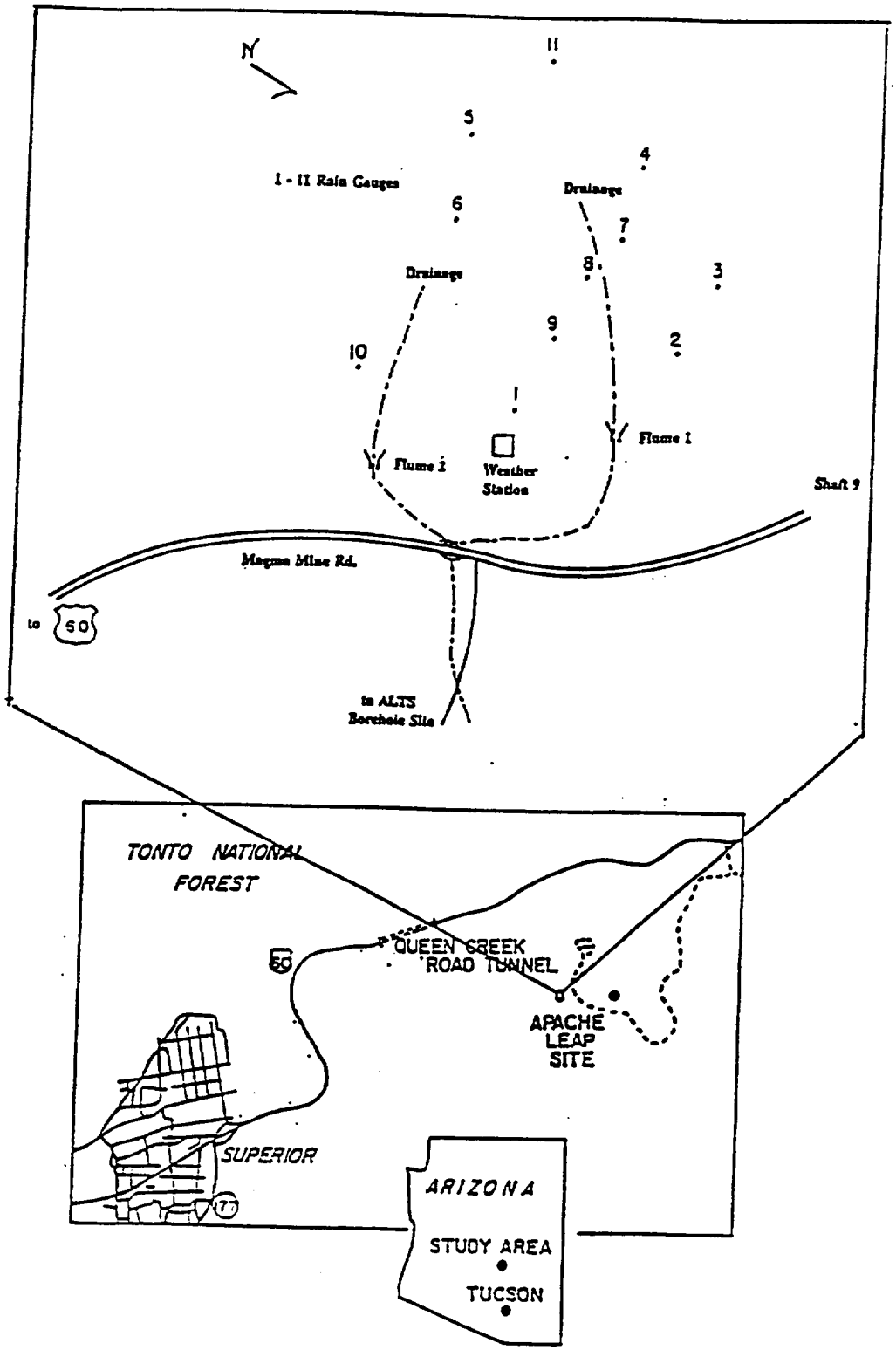


Figure 1. Location of Apache leap tuff site and watershed study area.

Pneumatic Permeability Measurements in a Fractured, Partially Saturated Environment

Amado Guzman, Michael Sully, Shlomo Neuman, and
Charles Lohrstorfer

University of Arizona

Research Synopsis

In the context of underground disposal of high level nuclear waste, the hydraulic conductivity of the host environment is an extremely important parameter. Underground disposal is being considered because of its assumed isolating capacity. This isolating capacity is highly dependent on an overall low hydraulic conductivity.

In order to statistically characterize the distribution of hydraulic conductivity of a candidate nuclear waste site, numerous water permeability tests would need to be performed. Such tests are extremely time consuming and not very likely to be conducted. An alternative is to characterize the permeability of the host rock by using a faster-permeating fluid. Gas permeability determinations, thus, become an attractive alternative.

Our research task comprises the technical design of instrumentation and the theoretical aspects of air flow through fractured, unsaturated rocks including both injection and extraction. There are a number of physical phenomena that need to be addressed. These include the effect of liquid saturation on air permeability, the definition of the flow geometry to establish criteria to select the appropriate mathematical flow models and, the determination of the otherwise hard-to-estimate relative permeability.

To address these issues field determinations of the pneumatic permeability are being conducted at different scales; single borehole at different active interval lengths and cross-borehole tests. Tests are being conducted in selected boreholes located in unsaturated tuff at the Apache Leap Tuff Site located near Superior Arizona. Each test consists of four discharge steps and their corresponding recovery periods. An example of a test is shown in Figure 1.

Effect of Saturation

Liquid saturation has a major impact on gas permeability measurements. Drying of the fractures during injection/extraction may produce pressure responses which suggest increasing permeability during the tests. Analysis of these pressure transients could indicate the critical pressure differential at which the fracture network starts desaturating. This critical pressure diffierential would be the air entry value of the fracture network. This value is also characteristic of the suction at which flow through the fractures ceases to be the dominant component of flow.

Flow Geometry

In a homogeneous, isotropic reservoir the geometry will be completely dependent on the type of source used during the test (i.e., point or line source). In a fractured medium, however, the flow may be controlled to a great extent by the geometry of the fracture network. Analysis of transient data from the ongoing field tests will, hopefully, suggest a better approach for the selection of the appropriate mathematical flow model. Currently, either radial or spherical flow models have been used to interpret the field tests.

Relative Permeability

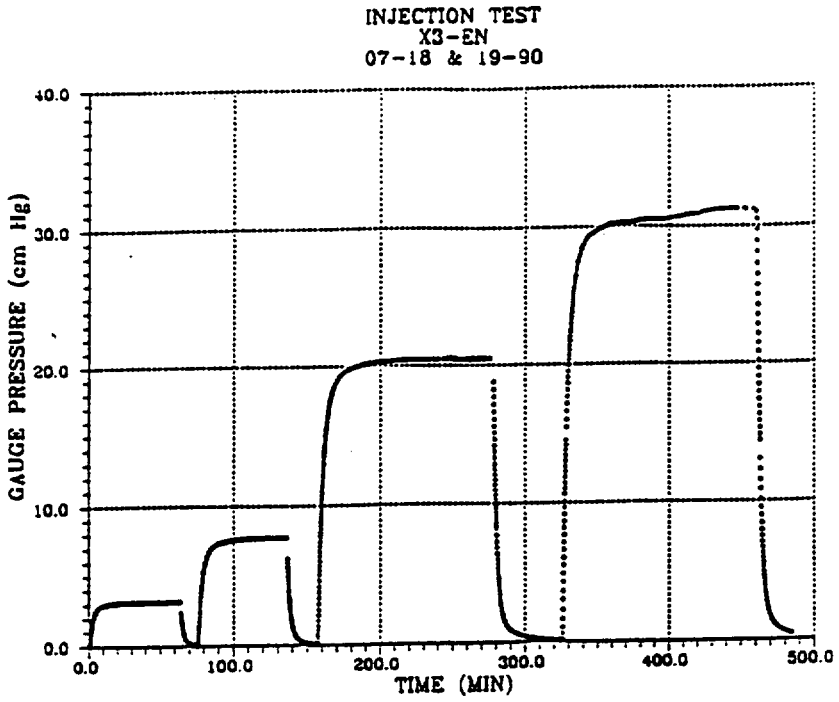
With the permeability measurements obtained over a range of liquid saturations in selected boreholes, relative permeability estimates can be made. These results will be compared with the air permeability results obtained in the laboratory by Evans and Rasmussen (1989). Previously these authors have shown good agreement between liquid relative permeability measured on cores in the laboratory and measured in situ.

In addition, comparisons of the data obtained from the in situ tests would indicate whether or not the fracture network is the dominant structure in terms of flow, and when, if at all, the onset of inertial effects takes place.

Expected Research Results

Field procedures for the borehole tests have been developed. Field experiments are being performed and will continue at the Apache Leap Site in collaboration with Dr. Evan's group. The physical variables being measured are: straddle-packer location, active interval length, air flow rate, and injection pressure. A relative humidity sensor will be installed in the instrumentation in the near future. The outcome of our research will be the following:

1. Criteria to select the appropriate model for data interpretation.
2. Pneumatic permeabilities at a number of scales and liquid saturations.
3. Air entry values for the fracture network (depending on time restrictions)



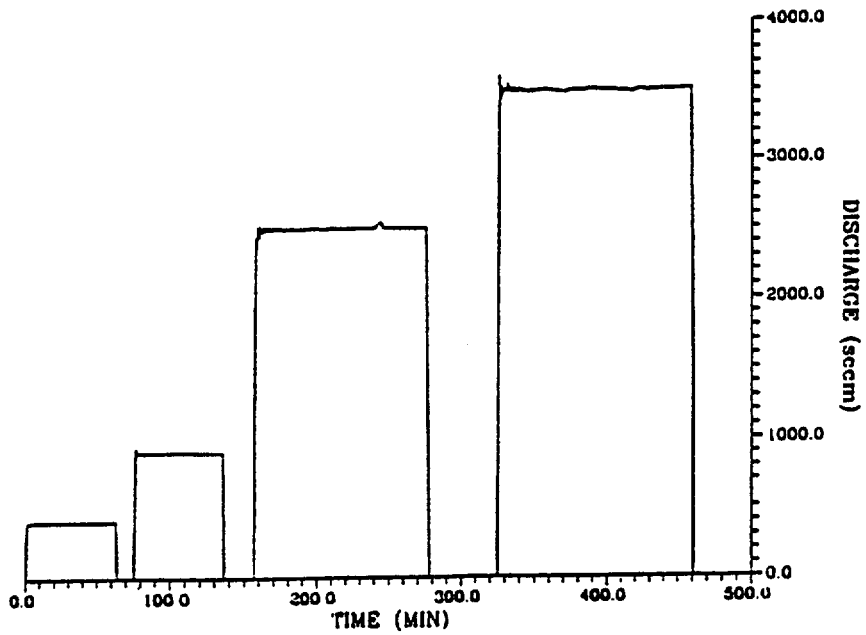


Figure 1. a. Plot of gauge pressures in the injection interval with time for four injection rates. b. Plot of the corresponding injection rates with time.

GEOCHEMICAL AND ISOTOPIC STUDIES IN THE APACHE LEAP REGION

E. A. Lyons and R. L. Bassett
University of Arizona

Classical and isotopic geochemistry, as well as mass balance reaction modeling, are useful tools for understanding the flow and chemical processes in unsaturated fractured rock. In this paper geochemical and isotopic research in progress at the Apache Leap study area is summarized with presentation of preliminary results.

The Apache Leap Tuff, in south central Arizona, is an ash-flow sheet exhibiting the characteristic zones of welding and of recrystallization associated with a simple cooling unit (figures 1 & 2). Based primarily on these properties, Peterson (1961) designated a system of zoning based on practical field identification and defined the basal tuff, the vitrophyre, and brown, gray and white units. The tuff is highly fractured. Vertical and horizontal joints as well as fault zones compose fracture networks that serve as conduits through the rock.

Based on chemical composition the tuff is a quartz latite, and spatially chemical composition is quite uniform. Phenocrysts comprise 35 to 45 percent of the rock. Plagioclase is the most abundant phenocryst mineral with lesser amounts of quartz, biotite, sanidine, magnetite, and others (Peterson, 1961). Groundmass minerals are cristobalite, K-feldspar, quartz and plagioclase (Weber and Evans, 1988).

Magma Mine lies below the Apache Leap region. Although most mine workings are in underlying rocks, several shafts and one haulage tunnel, Never Sweat Tunnel, provide access to the interior of the tuff. Never Sweat Tunnel has been integral to this study. The tunnel follows a curved path from Superior to #9 shaft, its eastern half passing through Apache Leap Tuff (figure 3). Along its course, it parallels and crosses Queen Creek, the primary drainage in the region and a potential source of recharge water for fracture flow systems within the tuff. Intercepted fractures which circumscribe the tunnel are observable from within. Many of them discharge water into the mine.

Water from these fractures as well as precipitation, surface water, and local ground water was sampled repeatedly over a 14 month period. Their chemical properties were used to link related waters that lie along flow paths. Fracture waters from the tunnel are slightly basic and primarily calcium-bicarbonate dominated. On the basis of SO_4/Cl ratios, Ca/Na ratios, and variation over time of alkalinity and silica content, waters from the west central portion of the sampled section appear influenced by Queen Creek and those from the eastern end are more similar to groundwater at Oak Flat about 3 km east (figure 4). Chemistry at an intermediate fracture is anomalous and breaks trends of increasing SO_4/Cl and Ca/Na ratios from east to west (Lyons).

The isotopic signatures of both water and solute are also being used to distinguish water source and travel time between land surface and emergence from fractures in Never Sweat Tunnel. Stable isotopes corroborate that the fracture system in the west central portion of the tunnel is most affected by recharge from intermittent flow in Queen Creek. Measured values for 25 samples indicate that the δD values (-73 to -74) are significantly lighter in this region of the tunnel than are those observed further into the tunnel, significantly removed from the effect of the valley recharge (δD = -63 to -64). The analyses of oxygen and carbon isotopes substantiate these observations; the majority of other analyses for $\delta^{18}C$ and $\delta^{11}B$ are pending (Bassett, 1991). Travel

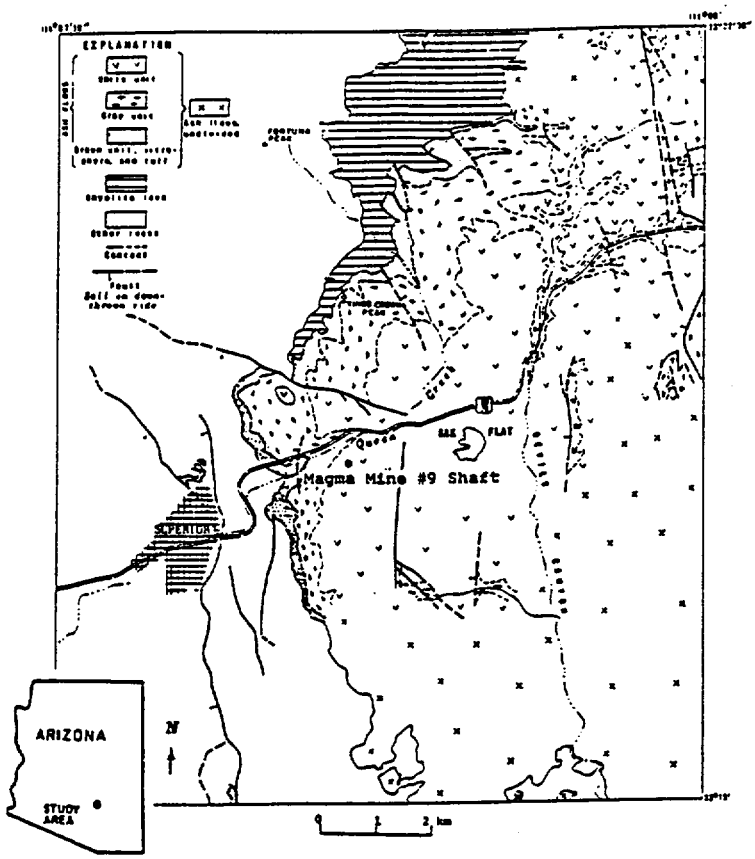


Figure 1. Generalized geologic map of the Superior quadrangle, showing the distribution of recognized field units within the ash-flow sheet (after Peterson 1968).

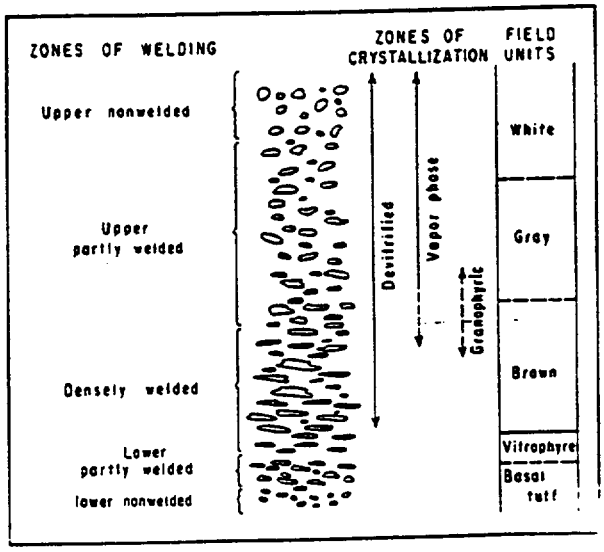


Figure 2. Physical characterists of the ash-flow sheet (Peterson, 1968).

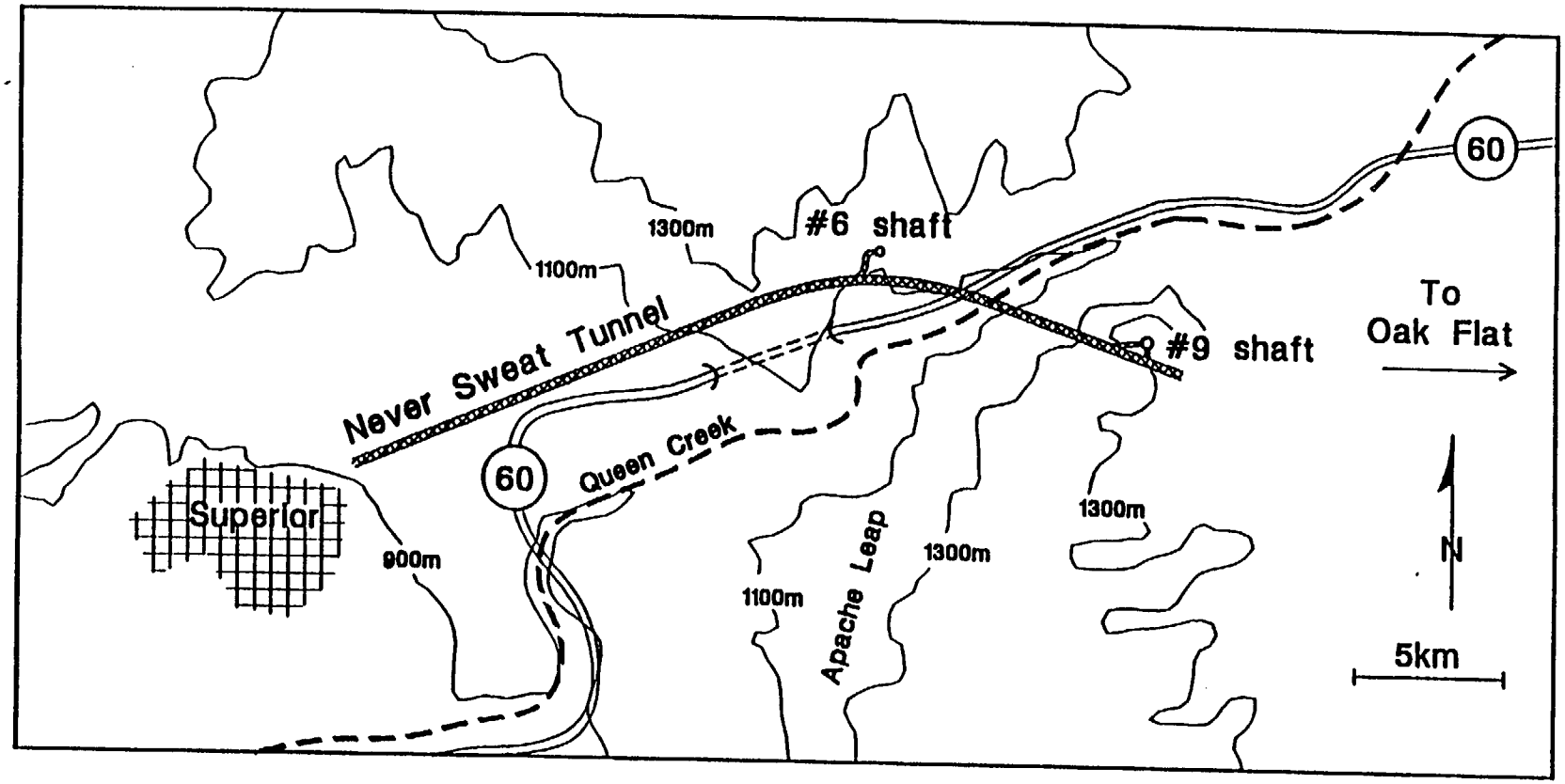


Figure 3. Map view of Never Sweat Tunnel.

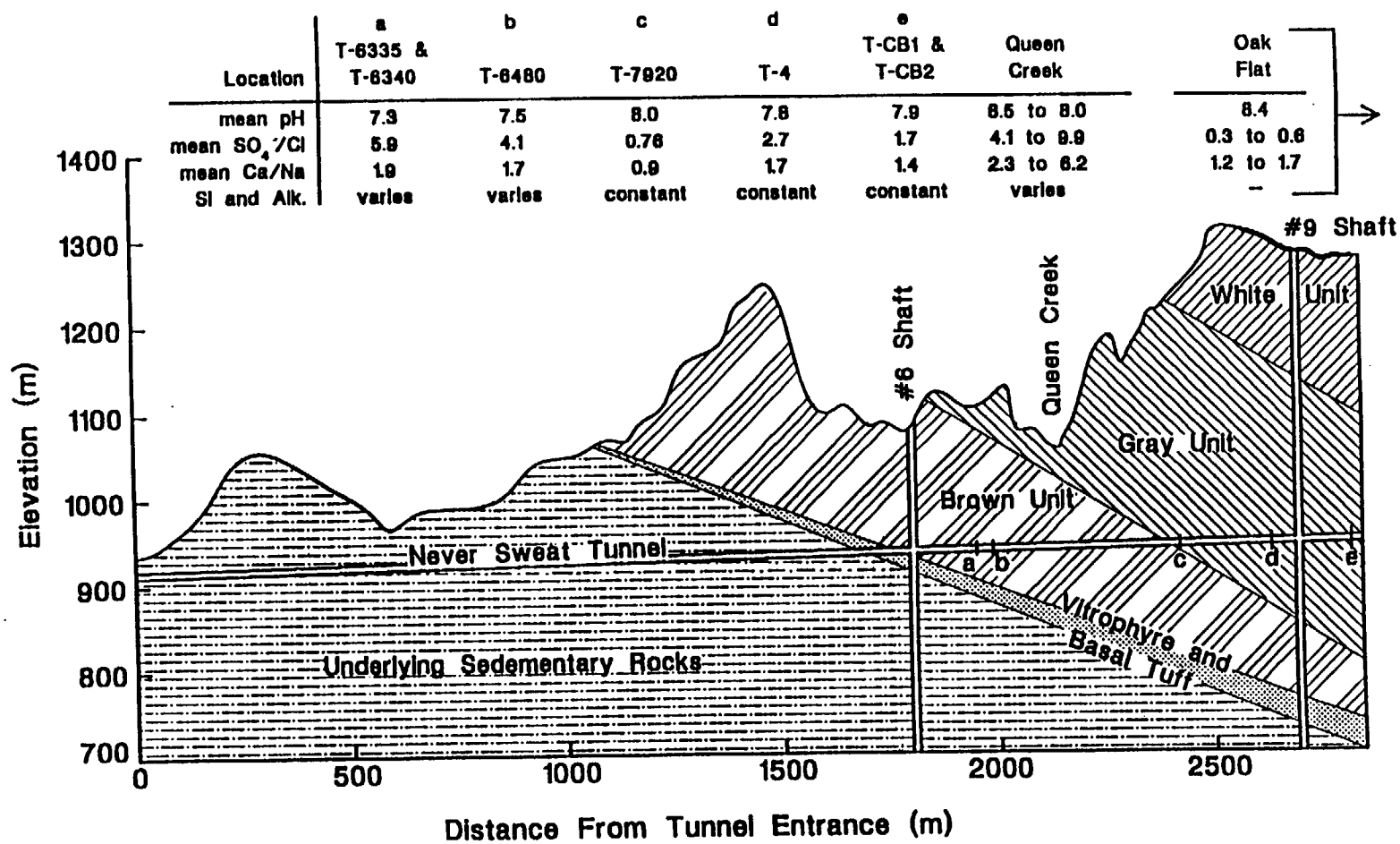


Figure 4. Linear profile of Magma Mine's Never Sweat Tunnel showing overlying topography, geology, intersecting mine shafts, sample sites, and water chemistry.

times will be evaluated by tritium and carbon-14; however no results are available at present.

A conceptual reaction path model for fracture waters is given in figure 5. At least two reaction pathways can be conceived: 1) precipitation, soil reaction and evaporation, migration through the vadose zone with reaction, then emergence in the tunnel, and 2) precipitaion, overland flow and mixing with soil water, recharge through the Queen Creek stream bed, migration through the vadose zone with additional reaction, and emergence in the tunnel. Variations in the chemistry of seeps and fracture discharge along the tunnel length suggest that these two models are valid.

Analyses of precipitation has revealed that evaporative concentration in the soil zone of between 10 and 20 fold has the most dramatic effect on water chemical compositiion. The carbon content is most impacted by soil zone silicate hydroloysis creating significant alkalinity; $\delta^{13}C$ values measured to date are typical of desert grasses (-13.6 to -15.0) and show little if any reaction with carbonate minerals (Bassett, 1991). When more analyses are available it may be possible to infer travel time from chemical variation independently; however for initial studies we are relying on the use of radioactive isotopes for this information.

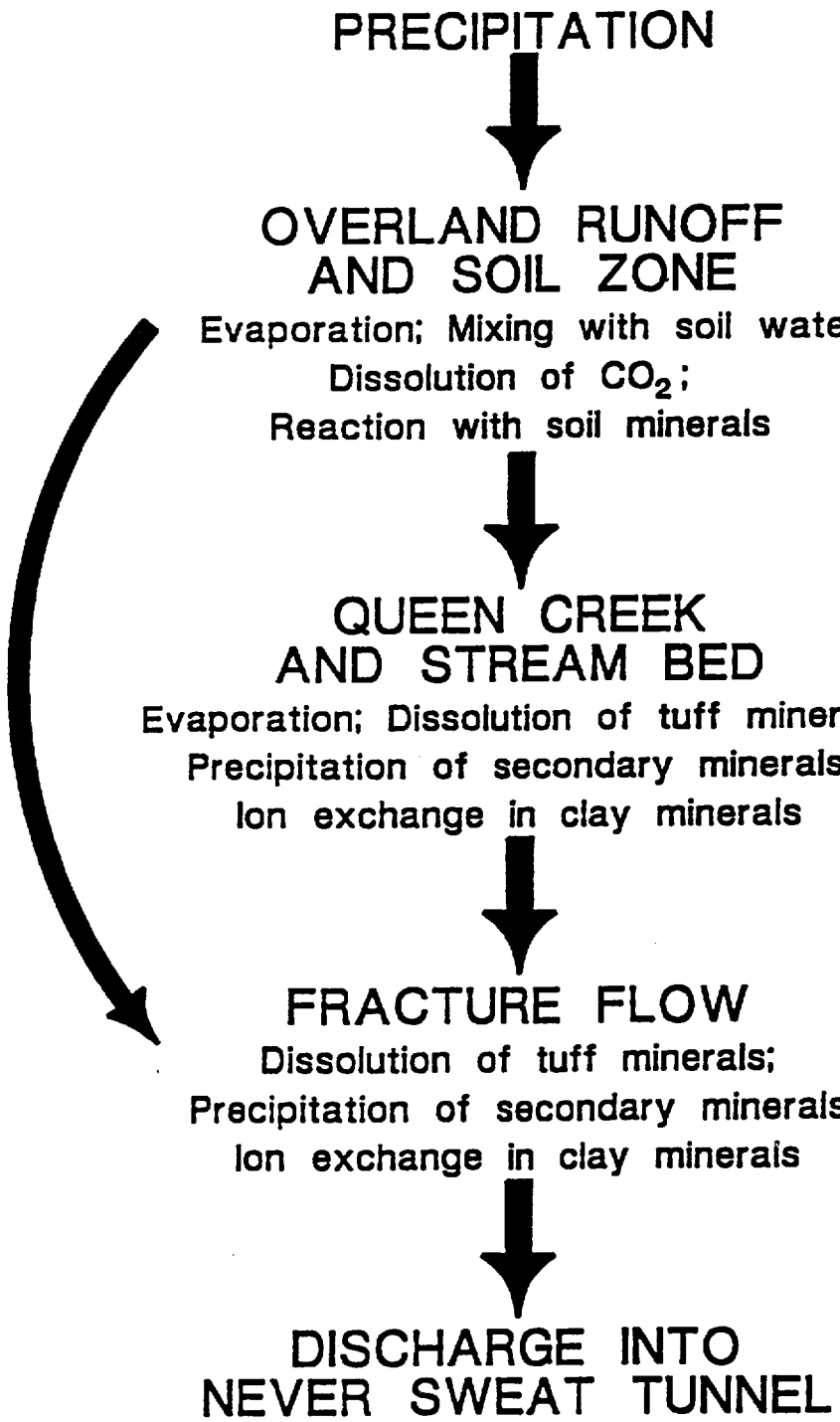


Figure 5. Conceptual reaction-path model for fracture waters flowing into Never Sweat Tunnel.

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FIELD TESTING THE EFFECTIVENESS OF PUMPING TO REMOVE SULFUR HEXAFLUORIDE TRACED DRILLING AIR FROM A PROTOTYPE BOREHOLE NEAR SUPERIOR, ARIZONA

Charles A. Peters, Peter Striffler, In Che Yang, and Janine Ferarese

U.S. Geological Survey
Water Resources Division
Nuclear Hydrology Program
Denver Federal Center, MS 421
Box 25046, Lakewood, CO 80225

INTRODUCTION

The U.S. Geological Survey (USGS), Department of the Interior is conducting studies at Yucca Mountain, Nevada, to provide hydrologic, hydrochemical, and geologic information to evaluate the suitability of Yucca Mountain for development as a high-level nuclear-waste repository. The USGS unsaturated-zone hydrochemistry study involves the collection of gas and water samples from the unsaturated zone for chemical and isotopic analyses. Results from these analyses will aid in the understanding of the movement of gas and water in the rock units at Yucca Mountain.

A prototype borehole designated USW UZP5 was drilled by the U.S. Department of Energy, Yucca Mountain Site Characterization Project Office (DOE, YMSCPO) in June 1990 in the Apache Leap Tuff of southcentral Arizona. The hole was dry drilled with air using sulfur hexafluoride (SF_6) as a tracer. This drilling method simulated that which will be used to drill boreholes for the collection of gas and water samples at Yucca Mountain. The purpose of tracing the drilling air is to quantify its removal by pumping, prior to sampling of *in situ* gases.

The objectives of our work in Arizona were to: 1) Determine the amount of time and the pumping rates required to remove the SF_6-enriched drilling air without inducing additional atmospheric contamination; 2) collect core samples for uniaxial compression to determine the amount of SF_6 gas that penetrated the core during drilling; 3) test the effectiveness of the SF_6 injection and sampling system; 4) test the installation and effectiveness of the prototype packer system; and 5) test the effectiveness of several core sealing methods.

DESCRIPTION OF FIELD WORK

An 11.2 cm diameter hole was cored using a [1]Longyear CHD-101 coring system with vacuum assist and conventional compressed air circulation to produce HQ-sized (6.1 cm) core. The hole was then reamed to a diameter of 20.3 cm with a compressed-air-cooled tungsten-carbide drag bit. The hole was completed within the unsaturated zone to a depth of 68 m. Casing was installed in the upper 7 m. Approximately 42,500 m^3 of compressed air was injected at a rate of 20.5 m^3/min during coring and reaming. About

[1]The use of brand, trade, or firm names in this report is for identification purposes only and does not constitute endorsement by the U.S. Geological Survey.

half of the air was injected during each process. Estimates of the total amount of air lost to the formation during coring range from 840 to 1,820 m^3. It is assumed that almost no air was lost to the formation during reaming because reaming is done under a vacuum.

Below a depth of 8.5 m dry nitrogen gas containing 5 percent SF_6 was added to the drilling air at rates of 1.5×10^{-4} to 6.5×10^{-4} m^3/min. Sulfur hexafluoride concentrations were analyzed on-site by gas chromatography using an electron capture detector. The drilling air was sampled for SF_6 prior to injection and after exhausting from the hole. Concentrations of gas exhausting from the hole ranged from 0.6 parts per million (ppm) to 2.2 ppm and averaged 1.33 ppm.

Continous core was collected and logged by geologists on-site. Forty -six samples of core greater than 10 cm long were selected from the interval of 11 to 68 meters. These cores were sealed by seven different methods using combinations of seven sealing materials. The core will be weighed periodically to determine the sealing method that best retains the original moisture content. The core samples will then be placed in a specially designed uniaxial compression cell to extract the gas and water for chemical and isotopic analyses.

Borehole televiewer and caliper logs were used in conjunction with the lithologic core logs to determine the smoothness of the borehole walls and the location of fractures. This information was then used to determine the locations for seating packers. Three 2.5 m long packers were lowered downhole, set at 9.3 to 11.8 m, 33 to 35.5 m, and 47.2 to 49.7 m, and inflated to 49 pounds per square inch (psi). The two zones between the packers (zones 2 and 3) and the zone below the bottom packer (zone 4) were pumped and sampled through 1.2 cm inside diameter teflon tubing. The teflon tubing was heated to 32 degrees Celsius to prevent condensation of water vapor. The upper part of the hole (zone 1) was sealed with plastic sheeting and tape and was pumped and sampled through silicon tubing.

The four sealed zones were intermittently pumped for about 2300 hours at various flow rates. A total of 3,300 m^3 of air were removed by pumping. Gas samples were collected periodically throughout the pumping period for SF_6, carbon dioxide, carbon-14, and carbon 13/12 analyses. Water vapor was also trapped on silica gel for downhole humidity calculations.

After concentrations of SF_6 were lowered to less than 0.1 ppm in all zones, about 50 cm^3 of 10 percent SF_6 in nitrogen gas were injected into zone 3. Zones 2 and 4 were then pumped at 35 liters per minute for 2 hours and samples were analyzed for SF_6. The injection test was repeated in zone 1 to test the top packer. Any detection of SF_6 would indicate poor packer seals.

RESULTS

Results of the SF_6 removal from the four zones are shown in figure 1. Background samples collected from a borehole less than one kilometer from USW UZP5 had SF_6 concentrations below 0.01 ppm. In zone 1 (0 to 9.3 m) SF_6 was completely removed (<0.01ppm) after about 1300 hours. In zones 3 and 4 (35.5 to 47.2 and 49.7 to 68 m) SF_6 was reduced to below 0.03 ppm after 1400 hours. Concentrations of SF_6 in zone 2 (11.8 to 33 m) were depleted to 0.10 ppm after 2300 hours.

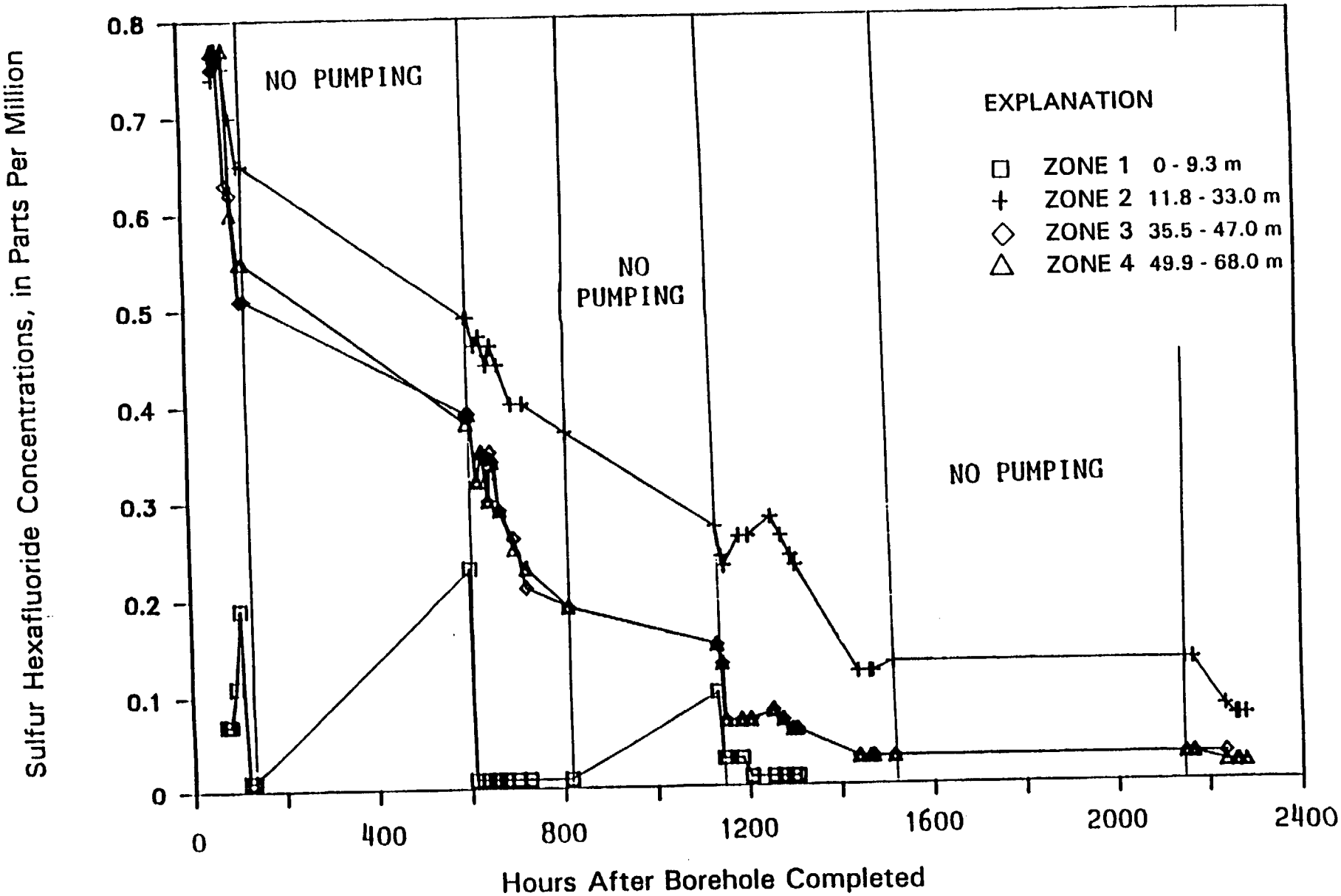

Figure 1. -- Concentrations of Sulfur Hexafluoride in each Zone after the Completion of Borehole USW UZP5.

Carbon dioxide concentrations ranged from 0.21 percent to 0.66 percent in zones 2, 3 and 4 and were 0.07 percent in zone 1 after pumping. Background carbon dioxide concentration in the atmosphere is 0.035 percent.

Carbon 14 (C-14) and Carbon 13/12 (C-13/12) samples were collected from all zones in August (1200 to 1500 hours) and September (2200 to 2300 hours). The results of these analyses (Table 1) indicate that atmospheric gas had probably been drawn into zone 2 by pumping.

Results of SF_6 injection testing indicated the packer seals were effective in isolating the various zones. The effect of heating the gas sampling tubes to 32 degrees Celsius to prevent vapor condensation inside the tubes during pumping was tested. Results indicate that when the heating system was used more than 97 percent of the water vapor was collected and when the heating tubes were not used more than 93 percent was collected.

Weights from cores collected from USW UZP5 were measured immediately after collection, and after 50, 102, 140, 161, and 190 days storage. Core weights will continue to be measured monthly. After 190 days of storage the greatest loss of water (by weight) from cores sealed by any of the methods was 6%. No water or gas chemistry results from one-dimensional compression are currently available.

DISCUSSION OF RESULTS

Results indicate that SF_6 concentrations decreased from 1.33 ppm to less than 0.10 ppm after 3,300 m^3 of air had been removed by pumping. Sulfur hexafluoride concentrations may increase or decrease during periods of no pumping due to diffusion into the borehole. At very low initial SF_6 concentrations (zone 1, figure 1) diffusion of the tracer from the formation to the borehole during periods of no pumping results in a temporary concentration increase. The rate and duration of pumping affects the rate at which concentrations decline. Pumping at a rate of more than 2.5×10^{-3} m^3/minute may cause significant decreases in SF_6 concentration in a short period of time; this is immediately followed by a period in which concentrations stabilize at a lower value. The steep decline in the concentration versus time curve represents a period during which the trace gas is removed from nearby fractures; once that gas is evacuated, gas from more distant locations in the fracture network dilutes the sample.

Significantly higher than atmospheric carbon dioxide concentrations, after 2300 hours of pumping, indicates that little atmospheric infiltration was induced by pumping. Results of Carbon-14 and Carbon-13/12 analyses (table 1), however, indicate that zone 2 probably was influenced by modern atmosphere. Fractures are about three times more prevalent (4 per meter) in zone 2 than in the other zones (1.5 per meter); it is possible that those fractures may be connected to the surface or to an open borehole 2.4 meters west of USW UZP5.

Table 1.--Results of Carbon 14 and Carbon 13/12 Analyses of gas samples from borehole USW UZP5

[USGS GD, U.S. Geological Survey, Geologic Division; USGS WRD, U.S. Geological Survey, Water Resources Division; Geochron, Krueger Enterprises, Geochron Corporation]

Zone and depth interval	Collection method	Hours after completion	Carbon 14		Delta Carbon 13/12 as per mil, PDB		
			Percent modern	Age yrs	USGS GD	Geochron	USGS WRD
Zone 1 (0 to 9.3 meters)	WG	1170	---	---	-18.21	---	-14.55
	WG	1460	---	---	-18.06	---	---
	WG	2150	---	---	-17.91	---	---
	MS	2150	---	---	-17.04	---	---
	MS	2175	89.7	875	---	-21.2	---
	MS	2275	89.4	895	---	-16.3	---
Zone 2 (11.8 to 33 meters)	WG	1170	---	---	-18.21	---	-18.09
	WG	1170	---	---	---	---	-18.24
	MS	1195	105.9	<200	---	-18.2	---
	WG	1460	---	---	-18.93	---	---
	WG	2150	---	---	-17.69	---	---
	MS	2150	---	---	-21.82	---	---
	MS	2175	106.1	<200	---	-19.6	---
	MS	2275	111.5	<200	---	-20.2	---
Zone 3 (35.5 to 47.2 meters)	WG	1170	---	---	-19.65	---	-16.73
	WG	1170	---	---	---	---	-16.66
	WG	1460	---	---	-20.54	---	---
	WG	2150	---	---	-19.85	---	---
	MS	2150	---	---	-23.22	---	---
	MS	2275	87.1	1115	---	-18.7	---
Zone 4 (49.7 to 68 meters)	WG	1170	---	---	-18.03	---	-16.81
	WG	1170	---	---	---	---	-16.78
	MS	1195	87.8	1050	---	-17.7	---
	MS	1245	86.5	1160	---	-17.4	---
	WG	2150	---	---	-18.39	---	---
	MS	2150	---	---	-22.03	---	---
	MS	2175	87.7	1060	---	-17.4	---
	MS	2275	87.1	1105	---	-18.3	---

WG-Whole Gas Sample
MS-Molecular Sieve Sample

The Behavior of Simple Fluids in Microfractures

John H. Cushman, Dennis J. Diestler
Purdue University

Martin Schoen
Universität Witten/Herdecke
Witten, Germany

The behavior of fluids in molecularly narrow (less than 100 Å) microfractures (vicinal fluids) differs from that of their bulk-phase counterparts. The differences are especially dramatic when the fractures are less than 10 fluid molecular diameters in width. The behavior of fluids in these ultrathin fractures is poorly understood. This talk presents some of our recent efforts to begin to understand these fluids on the molecular and continuum scales.

Numerical statistical mechanical techniques are used to probe the behavior of the vicinal fluid. Because typical laboratory experiments have the chemical potential, μ, as a fixed state variable, the grand-canonical is the natural choice for a statistical mechanical ensemble. That is the chemical potential, the fracture width, h, and the temperature, T, are held fixed. The Adams modification of the metropolis Monte Carlo method was used to generate realizations of a Markov chain of configurations. All equilibrium thermostatic properties were obtained as averages over the set of realized configurations.

Dynamic properties such as diffusivities and viscosities cannot be obtained from Monte Carlo simulations. These properties must be obtained using molecular dynamics techniques. We used the micro canonical ensemble molecular dynamics method in conjunction with Verlet's algorithm for integration of Newton's equations. In the micro canonical ensemble the energy, E, number of molecules, N, and h are the fixed state variables. So that the MD and MC simulations would represent the same thermodynamic state we set N in the MD method to $\langle N \rangle$ as determined from a prior MC simulation. Similarly E in the MD simulation was determined by adjusting the kinetic energy to produce the same temperature as in the prior MC simulation. Dynamic properties were determined via Kubo type formalisms as integrals of correlation functions; the correlation functions were obtained as averages over time by implementation of the ergodic hypothesis.

Fluid properties investigated included the following: diffusion, density, stress-strain, pair correlation functions, activation energies, self-part of the intermediate scattering function, hysteresis, capillary condensation and solvation force. Some of the interesting differences between the bulk phase fluid and the pore fluid included the following:

i) In microfractures less than six fluid diameters in width the fluid had a completely different phase diagram from the bulk fluid with which it was in equilibrium.

ii) For fracture widths greater than approximately 3 fluid diameters, Ficks law of diffusion is valid.

iii) In the midfracture region the coefficient of self-diffusion was larger and the activation energies lower than in the bulk phase fluid (Fig. 1).

iv) In fractures with widths less than 6 fluid diameters the fluid's state (solid, liquid, or gas) was highly dependent on the registration of the crystal structure of one surface with respect to that of the other.

v) Fluid density profiles were highly oscillatory across a given fracture.

vi) The solvation force was oscillatory as a function of fracture width (Fig. 2).

vii) As a fracture width decreases, fluid is forced out of the fracture in layers.

Acknowledgement

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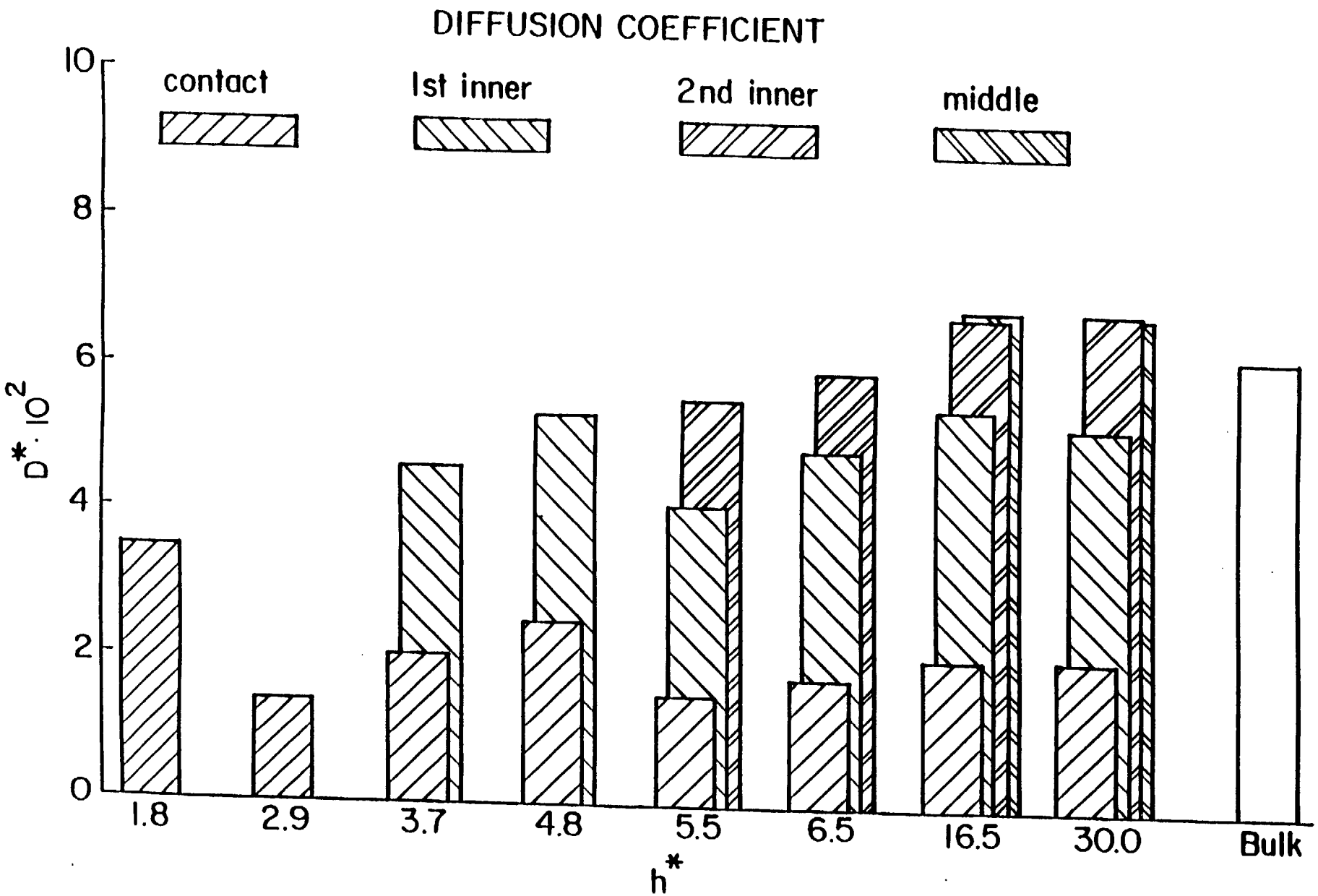

Fig. 1. Normalized self-diffusion coefficients in the slit-pore as a function of pore width.

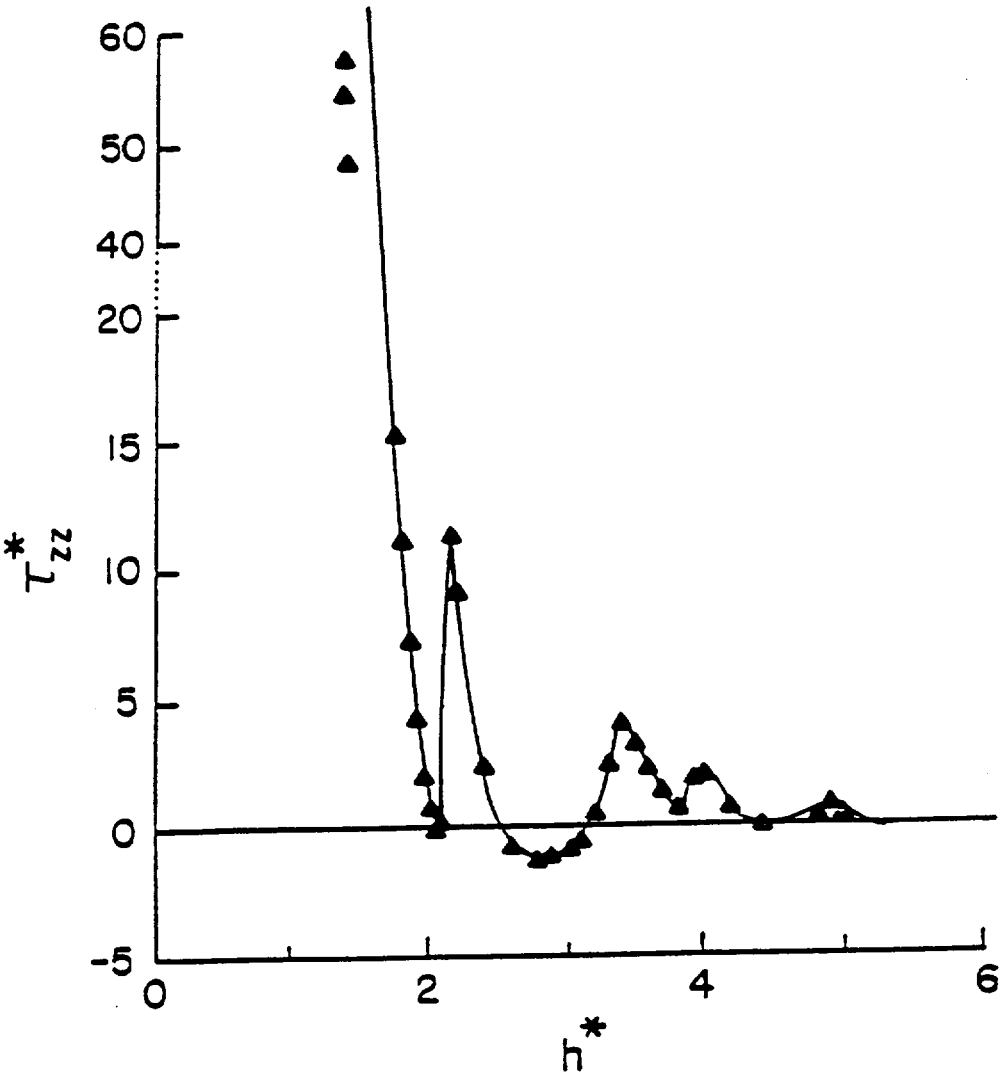

Fig. 2. Plot of normalized solvation force (normal stress) as a function of normalized pore width.

Characterization of Rock Hydrologic Properties Using Model Verification

Alan L. Flint, U.S. Geological Survey
Kenneth A. Richards, U.S. Geological Survey
Lorraine E. Flint, Raytheon Services Nevada

ABSTRACT

Model simulation of imbibition is proposed as a technique to test the adequacy of moisture characteristic and relative permeability data and the ability of the Brooks and Corey and van Genuchten equations to represent that data. The moisture characteristic data was collected using pressure plate, gas drive and submersible pressure outflow cell techniques. The relative permeability data was collected using centrifuge and gas drive techniques. The various relative permeability and moisture characteristic equations were used in a numerical flow simulator to model a laboratory imbibition experiment under two different initial conditions (5% and 46.6% saturation). For the one core tested, the sorption data from the submersible pressure outflow cell composited with the dry end of the centrifuge moisture characteristic curve and the gas drive relative permeability data using the Brooks and Corey equation proved the best fit for modeling imbibition.

INTRODUCTION

Yucca Mountain, Nevada, USA, is being considered as the nation's first potential high-level nuclear waste repository. Yucca Mountain, composed of a series of partially-saturated and fractured vitric to devitrified ash-flow and ash-fall tuffs (Montazer and Wilson, 1984), is being characterized by a series of hydrologic and geologic studies (U.S. Dept. of Energy, 1988). Characterization of the matrix hydrologic properties is an important part of those studies (U.S. Dept. of Energy, 1990). Early prototype work on matrix properties has been done by using several methods to obtain moisture characteristic and relative permeability data for nonwelded and bedded tuff samples [Flint and Flint, (1991a)].

Example datasets appear in Figure 1 and indicate that different methods can give different results. For example, at about 70 percent relative water content, relative permeability data collected using a centrifuge method is almost two orders of magnitude higher than relative permeability data using the gas drive procedure. Also, the matric potential values from the centrifuge method are about one order of magnitude lower than those from the pressure plate procedure for relative water contents between 20 and 60 percent.

In addition to the problem of identifying the most applicable measurement technique, there are several mathematical equations found in the literature used to describe these relations. It is necessary to ascertain which procedure and equation best characterizes tuff and whether or not these differences are meaningful in terms of their use in predicting unsaturated flow. This paper reports on a technique currently being developed to evaluate which methods and numerical expressions are the most suitable for characterizing the welded and nonwelded tuffs at Yucca Mountain.

Numerical expressions, which are required as input to numerical models, must

first be fit to the measured data. Although a variety of formulations are available for both moisture characteristic and relative permeability functions, this discussion will be limited to those proposed by Brooks and Corey (1964) and van Genuchten (1978). The Brooks and Corey (1964) moisture characteristic equation is

$$\Theta = \left(\frac{\psi_a}{\psi}\right)^L \tag{1}$$

in which ψ_a is the air entry water potential, ψ is the water potential, L is a fit parameter and Θ is the dimensionless water content calculated by

$$\Theta = \left(\frac{\theta-\theta_r}{\theta_s-\theta_r}\right) \tag{2}$$

where θ is relative water content (volumetric water content divided by porosity), and θ_r and θ_s are residual and saturated relative water contents, respectively. Brooks and Corey (1964) used a value of 1.0 for θ_s and used θ_r as a fit parameter. The relative permeability (k) equation they proposed is

$$k = \Theta^{\left(\frac{2}{L}+3\right)} \tag{3}$$

The moisture characteristic equation proposed by van Genuchten (1978) is

$$\Theta = \left[\frac{1}{1+(\alpha\psi)^n}\right]^m, \quad m=1-\frac{1}{n} \tag{4}$$

and the relative permeability equation is

$$k = \Theta^{1/2}\left[1-\left(1-\Theta^{1/m}\right)^m\right]^2 \tag{5}$$

where m, n and α are fit parameters. The residual and saturated relative water contents in the van Genuchten equation are generally treated as fit parameters.

The fitting of the equations to the data is not a trivial task. There are several criteria that can be used to fit data to a model, such as least squares, which is based on a specified loss function. The loss function can be specified to minimize errors in θ, Θ, ψ, log ψ, k, log k or some weighted combination. It is recognized that these "best fit" parameters are dependent on the specified loss function and each loss function may emphasize the fit to the data differently. For example, the loss function minimized on k will emphasize fit for high water contents as a result of the permeability values being several orders of magnitude higher than for low water contents. On the other hand, when the loss function is minimized on the log k the absolute magnitude of the log k values are higher for low water contents and hence influence the fit to a greater degree

than high water contents. Some models may be appropriate only for wet or dry initial conditions but not both. The most useful model would be one that adequately represents the data for a large range of water contents. This paper describes the use of easily conducted laboratory imbibition experiments to assess the accuracy of data collected using various methods and the adequacy with which different equation formulations represent that data. Peters and others (1987) reported on a similar use of imbibition data.

METHODS

Several methods were used to collect the moisture characteristic (MC) and relative permeability (k) data (Figure 1). This analysis was conducted on a single 2.5 cm diameter by 2.5 cm length core of nonwelded tuff (porosity = 0.32 cm^3/cm^3). Moisture characteristic data (which include desorption and sorption) were collected using submersible pressure outflow cells (SPOC) (Flint and Flint, 1991b). Moisture desorption curves determined on the same core using pressure plate and centrifuge methods and relative permeability data determined using the gas drive and centrifuge methods that are used in this analysis were published by Flint and Flint (1991a). Composite curves using the SPOC data from 0 to -0.5 MPa and centrifuge data for lower potentials were also evaluated.

Numerical expressions developed by Brooks and Corey (1964) and van Genuchten (1978) were used to fit moisture characteristic and relative permeability data. These were fit with the loss function minimized on θ(MC), k, log k, or θ and log k simultaneously. Parameters from the Brooks and Corey and van Genuchten moisture characteristic equations were also used to predict the relative permeability equation independent of the measured k data. Coefficients of determination (r^2) and mean squared errors (MSE) were calculated from these equations to compare equation formulations and measurement methods. (The mean squared error is defined as the experimental result minus the model result squared divided by the number of data points.)

Laboratory imbibition experiments were conducted on a single core sample at θ=46.6 percent and oven dry ($\theta \approx 0.0$ percent) to collect imbibition data and calculate sorptivity (S). Sorptivity is defined as the slope of the linear portion of a graph of water imbibed (volume of water/cross-sectional area) versus the square root of time (Philip, 1957). The imbibition data was modeled using the numerical flow simulator TOUGH (Pruess, 1987). The imbibition data for the oven dried core was compared to a simulation at θ=5.0 percent for numerical simplicity.

An additional criteria was selected to identify functions that when used gave satisfactory prediction of the measured imbibition data. This criteria was arbitrarily chosen based on the ability to detect, with a neutron moisture meter, a change in water content in a block of tuff (θ_{NB}) after simulated imbibition. The rule of thumb developed for the welded and nonwelded tuffs at Yucca Mountain is that water contents determined from neutron probe measurements are accurate to within +/- 5 percent due to random decay using a 16 second count time. For example, if the true saturation were 60 percent the neutron probe measurement could yield a saturation between 57 percent and 63 percent due to random decay. For the very dry sample (θ=5.0 percent), a +/- 10

percent rule of thumb applies and was used. The model results were evaluated by assessing if the simulated changes in water content matched the measured changes to within the estimated error of a neutron probe measurement. The hypothetical calculations were done arbitrarily assuming nine hours of imbibition from a single, saturated fracture transecting a block of tuff (equal in size to the volume of detection of the neutron probe, approximately 0.125 m^3). If the model results were within the +/- 5 percent range (+/- 10 percent for the dry sample) they were assumed to be the same as the experimental laboratory results. The neutron block relative water content (θ_{NB}) was determined for imbibition experiments into core with initial water contents of 46.6 percent and 5.0 percent and was calculated by simply multiplying S, determined from the laboratory experiment or the TOUGH simulation, by the square root of 9 hours.

RESULTS AND DISCUSSION

The van Genuchten equation, when θ_s was allowed to vary for fit, ranged from 64 to 600 percent. Values above 100 percent are physically meaningless and values less than 100 percent provide a model that is undefined for k and ψ at values of θ greater than θ_s. Consequently, TOUGH holds k equal to 1.0 and ψ equal to 0.0 for all values of $\theta > \theta_s$, which may be unrealistic. A measured value of θ_s may be very difficult to obtain for the reason that saturation is a state that is subjectively chosen, i.e. water may continue to imbibe into the matrix at low rates for a long period of time. Therefore, for further analysis θ_s was set equal to 1.0 as in the Brooks and Corey equations.

Relative permeability predicted from the Brooks and Corey (BC) and van Genuchten (VG) equations fit to the SPOC sorption MC data alone appears in Figure 2. The BC equation predicted values very close to the measured gas drive k data. Predictions from the VG equation dropped quickly and paralleled the BC values, though about one order of magnitude lower (Figure 2). When fit to the gas drive data, the BC equation predictions changed little (Figure 3). The VG equation when fit to the SPOC sorption MC data and gas drive k data simultaneously (MC, k) fit very well to the gas drive k data and then continued to decrease rapidly beyond the last measured data point (Figure 3). Both models in Figure 2 and the BC model in Figure 3 adequately predicted imbibition at θ=46.6 percent; however, neither predicted imbibition at θ=5 percent (Tables 1 and 2). The imbibition simulation with the VG equation in Figure 3 did not indicate any imbibition at all. The permeability was too low at the initial water content and numerically, no water could enter the core. This is a consequence of the residual water content being very high (θ_r=62 percent, Table 2) which halted flow.

The BC equations that were fit to the SPOC sorption/centrifuge composite data and the gas drive k data, matched imbibition at θ=5 percent and nearly matched imbibition at θ=46.6 percent (Table 1). The θ_{NB} for the imbibition at θ=46.6 percent was 58.0 percent which was higher than the range of experimental results by only 0.2 percent (Table 1). This was the only group of equations that closely simulated imbibition at both initial water contents. The moisture characteristic data is predicted using the BC equation fit to the SPOC sorption/centrifuge composite MC data and using the VG equation fit simultaneously to the MC and gas drive k data (Figure 4). The two formulations are similar in the range of water contents between 35 and 90 percent but differ by an order of magnitude or more at water contents outside of this range.

Imbibition simulations using data from all four measurement methods fit to both the BC (Figure 5) and VG (Figure 6) equations are compared to measured imbibition data. The simulation using the centrifuge data predicted the highest imbibition rate, then SPOC desorption, pressure plate and SPOC sorption data. Both formulations resulted in simulations falling in the same order. The simulations using the centrifuge data resulted in the highest imbibition values probably because the matric potential values were lowest for this method compared to other methods at θ values > 55 percent (Figures 1 and 4). Thus, the driving force for flow was greater. These results are consistent with the fact that the centrifuge, pressure plate and SPOC desorption data are all measured with desorption methods and imbibition is a sorption process.

Both equation formulations fit to SPOC sorption data closely approximated the measured imbibition at θ=46.6 percent (Figures 5 and 6). The neutron block water contents (θ_{NB}) indicated that they both were in the range of experimental results (Tables 1 and 2).

The indices of fit did not necessarily indicate the usefulness of equations for simulation of imbibition. The coefficient of determination (r^2) for the BC equation fit to SPOC sorption data was the lowest (r^2=0.69, Table 1) which fit the imbibition experimental results at θ=46.6 percent. The highest r^2 value for the BC equation (0.98) was from centrifuge data, however, it did not acceptably simulate imbibition at either water content. Both the highest (0.98) and lowest (0.78) r^2 values from the VG equations (Table 2) were from equations that when used did not simulate imbibition within the accepted range. The three lowest MSE values from BC equations for θ (0.0002, 0.0004 and 0.0014) were from procedures that did simulate imbibition at one of the initial water contents (Table 1). Even low values of MSE for k and log k indicated satisfactory simulation of imbibition (Table 1). The lowest values for MSE of k (0.0000) and log k (0.049) were from SPOC sorption MC data which fit the imbibition experimental results. All other MSE values for equations fit to MC data alone were at least an order of magnitude higher. However, when the pressure plate and SPOC sorption composite MC equations were used in combination with the equation fit to the gas drive k data (L=0.1363, MSE k=0.0000, MSE log k=0.0886) they also fit the measured imbibition data as indicated by the θ_{NB} (Table 1). The same is not true of the VG equation MSE values. The lowest values for MSE for θ (0.0005) was from the pressure plate MC data and the lowest MSE for log k (0.0038) was from SPOC desorption MC data fit simultaneously to GD k data, both of which did not fit the imbibition experimental results.

The r^2 and MSE are only an indication of how well the equation fits the data and do not reflect the accuracy of the data. Comparing r^2 and MSE values from the BC and VG equations fit to the SPOC sorption MC data alone reveals that according to the r^2 value the BC equation (r^2=0.69, Table 1) does not fit the data well while the VG equation does (r^2=0.97, Table 2). According to MSE values the opposite is true (Tables 1 and 2), but both equations fit the imbibition experimental results for 46.6 percent initial water content. These equations, when used to simulate unsaturated flow provide a better indication of the accuracy of the data. Although more data needs to be analyzed, the SPOC sorption data is the most useful in modeling imbibition which is conceptually more applicable than the other data analysed.

SUMMARY

The process of measuring moisture characteristic and relative permeability data and fitting them to mathematical functions is not straightforward. In addition, even though the Brooks and Corey and van Genuchten equations could be successfully fit, based on high r^2 values or low MSE values, it does not necessarily mean that the data are correct. Imbibition modeling was sensitive to differences in measurement methods and equation formulations and matching measured imbibition data may suggest which moisture characteristic and relative permeability data are correct.

Although, more data need to be analyzed, it appears that this simple verification technique can be useful for evaluating differences in measurement methods and equation formulations. The application of a standard comparison such as the neutron meter detection limit was also a useful technique for testing the sensitivity of the various simulations under a realistic framework, in this case, a measurable effect at the field scale.

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Table 1. Brooks and Corey equation results for modeling imbibition at two initial relative water contents (46.6 and 5 percent) compared to experimental data.

METHOD	Fit Parameters ψ_a (Pa)	L	TOUGH Results θ=46.6%† S cm/min$^{0.5}$	θ_{NB} %	θ=5.0%‡ S cm/min$^{0.5}$	θ_{NB} %	r^2	MSE MC θ	MSE GD k	MSE GD log k
Centrifuge MC	76897	0.3211	0.121	84.7	0.243	78.0	0.98	0.0019	0.0159	1.306
with GD k^*			0.073	70.3	0.136	45.9				
Pressure Plate MC	13533	0.3512	0.050	64.3	0.090	32.1	0.97	0.0004	0.0202	1.436
with GD k^*			0.029	57.1**	0.049	19.8				
SPOC desorption MC	11965	0.1794	0.057	65.5	0.107	37.2	0.82	0.0042	0.0011	0.404
with GD k^*			0.046	62.2	0.084	30.3				
SPOC sorption MC	1698	0.1275	0.023	55.3**	0.044	18.4	0.69	0.0002	0.0000	0.049
with GD k^*			0.025	55.9**	0.041	17.5				
Composite curves										
SPOC desorption MC	12919	0.1995	0.058	65.8	0.107	37.2	0.88	0.0043	0.0023	0.562
with GD k^*			0.044	61.6	0.078	28.5				
SPOC sorption MC	5857	0.1872	0.040	60.4	0.074	27.3	0.92	0.0014	0.0015	0.466
with GD k^*			0.032	58.0	0.056	22.0**				

† Experimental S = 0.022, θ_{NB} = 55.0 percent (range = 52.3 - 57.8 percent)
‡ Experimental S = 0.061, θ_{NB} = 23.4 percent (range = 21.1 - 25.8 percent)
* When k in Eq. 3 is fit directly, L=0.1363 for the gas drive data (MSE k=0.0000 MSE log k=0.0886)
** Simulation fit within range of the experimental results.

Table 2. van Genuchten equation results for modeling imbibition at two initial relative water contents (46.6 and 5.0 percent) compared to experimental data.

METHOD		Fit Parameters θ_r	α	m	TOUGH Results θ=46.6%† S cm/min$^{0.5}$	θ_{NB} %	θ=5.0%‡ S cm/min$^{0.5}$	θ_{NB} %	r^2	MSE θ	MSE log k
Centrifuge	MC	0.000	0.00001	0.2722	0.066	68.2	0.210	68.8	0.97	0.0018	0.1415
with CENT k	MC,k^*	0.245	0.00001	0.4069	0.181	102.7	0.287	91.2	0.91	0.0054	0.0277
Pressure Plate	MC	0.000	0.00007	0.2655	0.042	61.0	0.078	28.5	0.97	0.0005	0.2487
with GD k	MC,k^*	0.071	0.00013	0.2475	0.035	58.9	0.058	22.6**	0.97	0.0012	0.1813
SPOC sorption	MC	0.249	0.00031	0.1846	0.018	53.8**	0.033	15.1	0.97	0.0035	1.0866
with GD k	MC,k^*	0.619	0.00023	0.5405	–	–	–	–	0.78	0.0143	0.0120
SPOC desorption	MC	0.000	0.00002	0.2492	0.088	74.8	0.141	47.4	0.95	0.0021	0.2074
with GD k	MC,k^*	0.641	0.00003	0.5917	–	–	–	–	0.94	0.0085	0.0038
Composite curves											
SPOC desorption	MC	0.154	0.00002	0.3094	0.064	67.6	0.174	57.3	0.98	0.0014	0.2659
with GD k	MC,k^*	0.254	0.00003	0.2906	0.057	65.5	0.138	46.5	0.98	0.0035	0.1474
SPOC sorption	MC	0.000	0.00014	0.1629	0.021	54.7**	0.041	17.5	0.95	0.0033	0.7262
with GD k	MC,k^*	0.269	0.00008	0.2906	0.043	61.3	0.084	30.3	0.89	0.0035	0.1430

† Experimental S = 0.022, θ_{NB} = 55.0 percent (range = 52.3 - 57.8 percent)
‡ Experimental S = 0.061, θ_{NB} = 23.4 percent (range = 21.1 - 25.8 percent)
* MC,k indicates loss function minimized on θ & log k simultaneously
** Simulation fit within range of the experimental results.

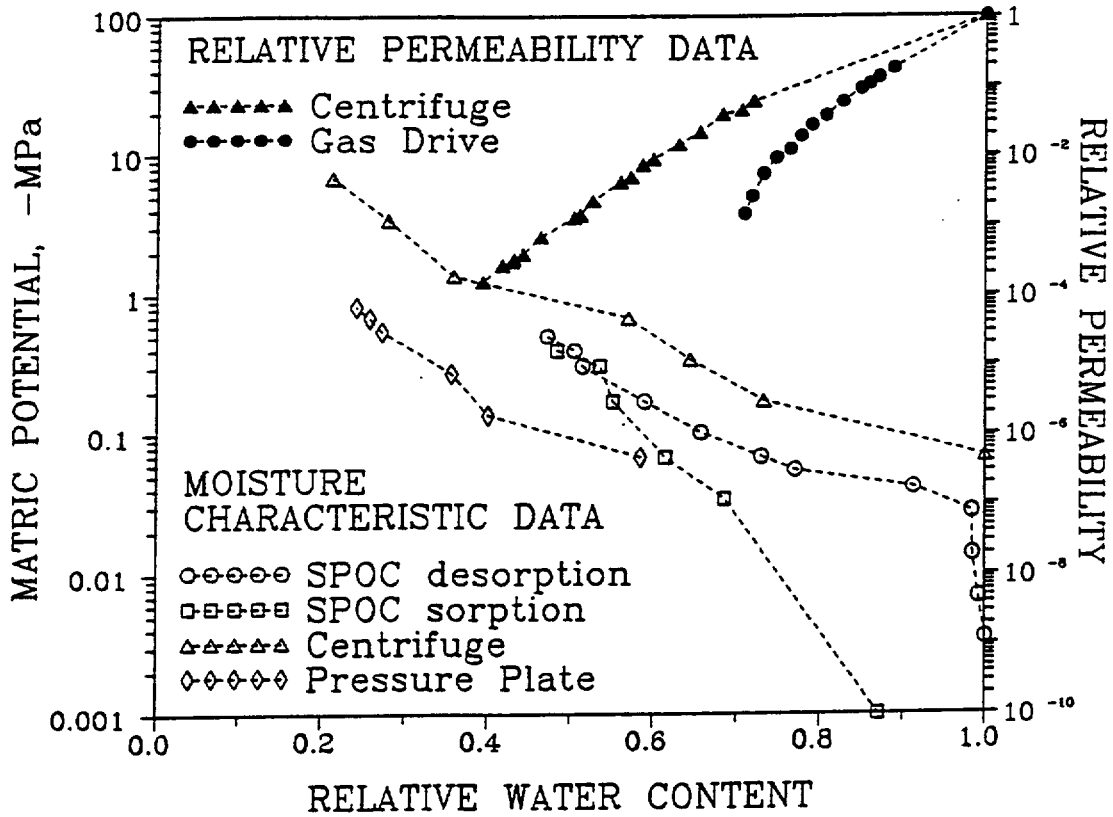

Figure 1. Datasets used for modeling imbibition. Moisture characteristic data were collected using centrifuge, pressure plate and SPOC methods. Relative permeability data were collected using centrifuge and gas drive methods.

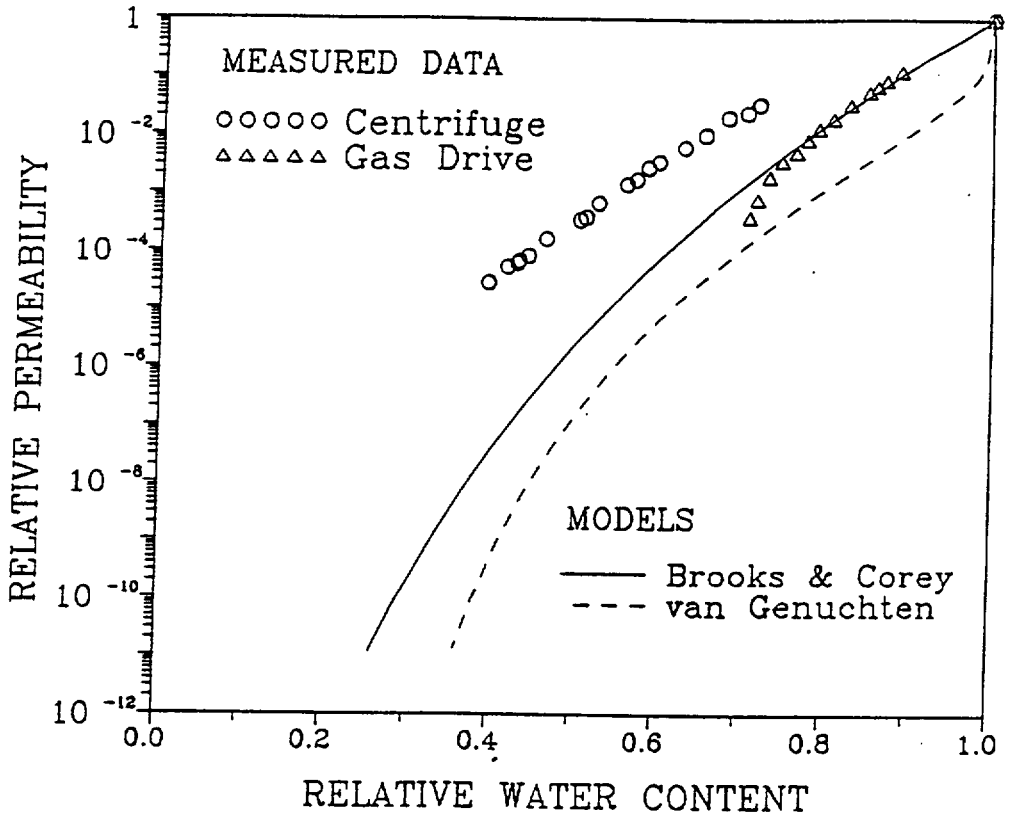

Figure 2. Brooks and Corey and van Genuchten predictions of relative permeability based on SPOC sorption moisture characteristic data.

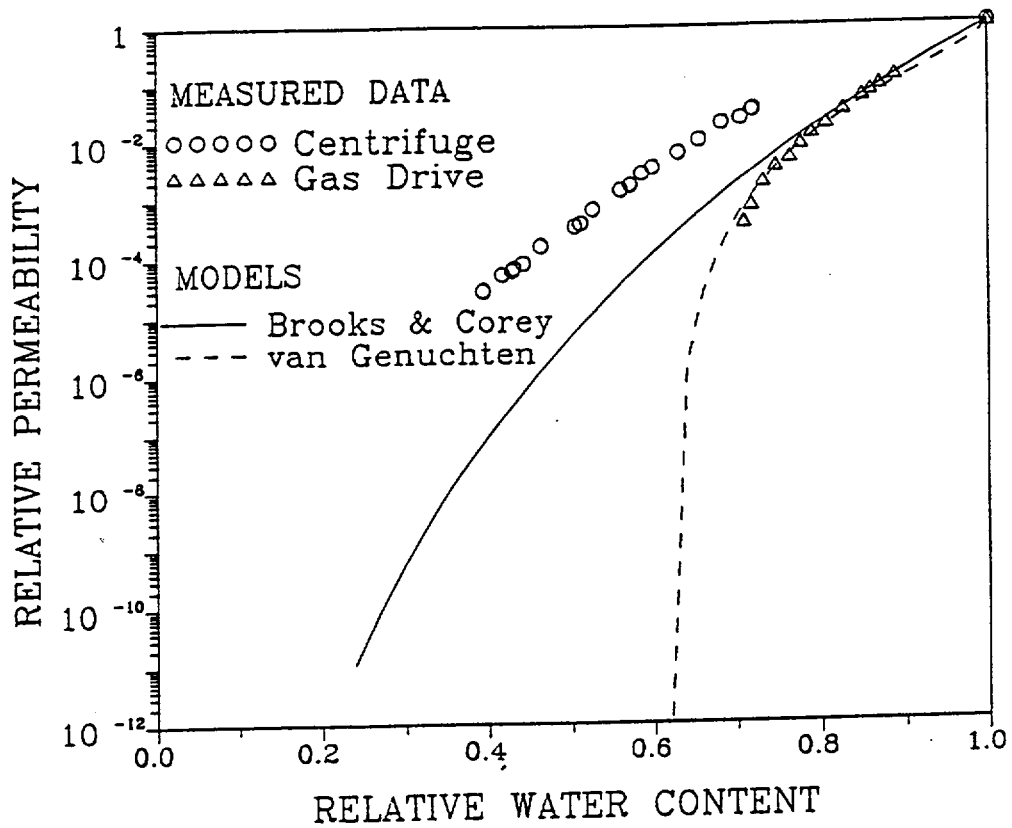

Figure 3. Relative permeability data predicted using Brooks and Corey equation fit to gas drive relative permeability data and van Genuchten equation fit to SPOC sorption moisture characteristic data simultaneously with gas drive k relative permeability data.

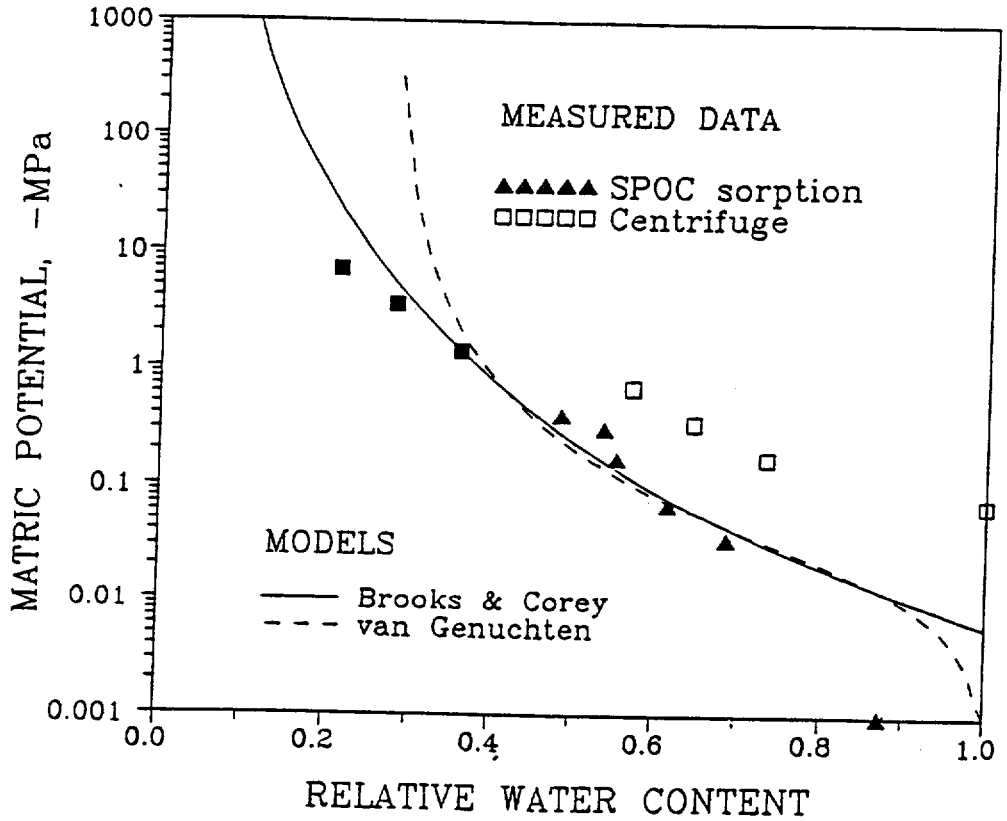

Figure 4. Moisture characteristic data predicted using the Brooks and Corey equation fit to SPOC sorption/centrifuge composite moisture characteristic data and the van Genuchten equation fit simultaneously to moisture characteristic and gas drive relative permeability data. Solid points represent moisture characteristic composite data.

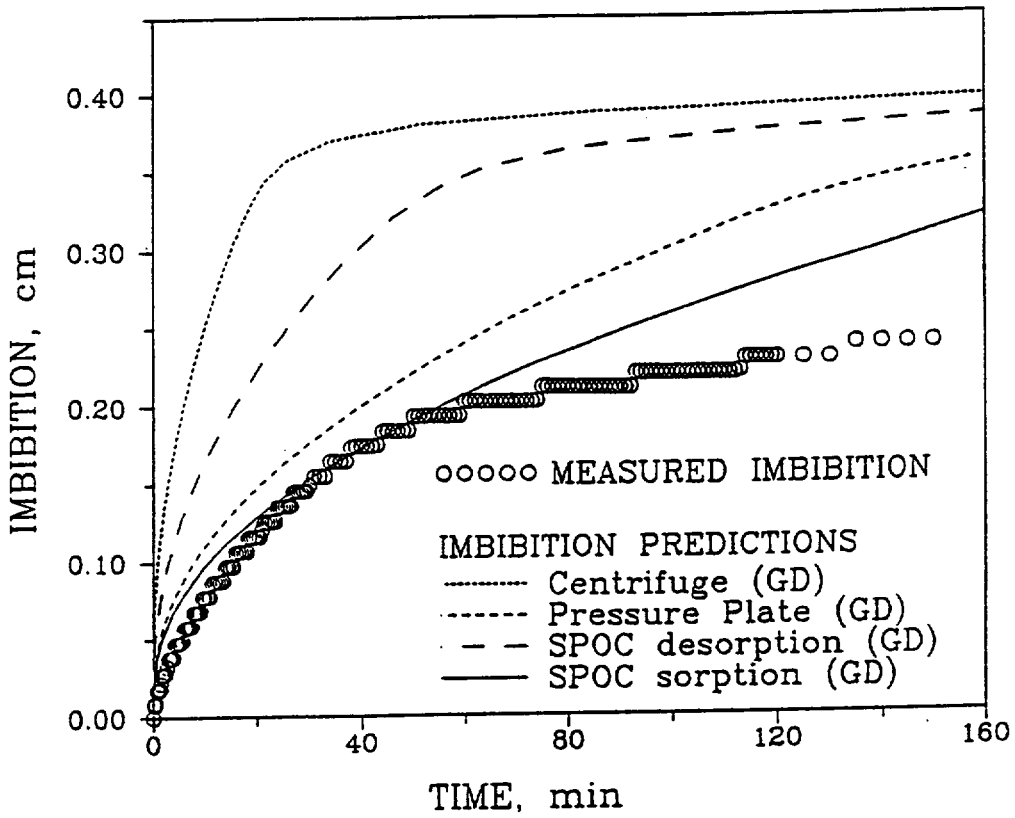

Figure 5. Measured imbibition data with imbibition simulations for nonwelded tuff at 46.6 percent initial relative water content. Model predictions are using the Brooks and Corey equation fit to centrifuge, pressure plate and SPOC moisture characteristic data, and gas drive relative permeability data.

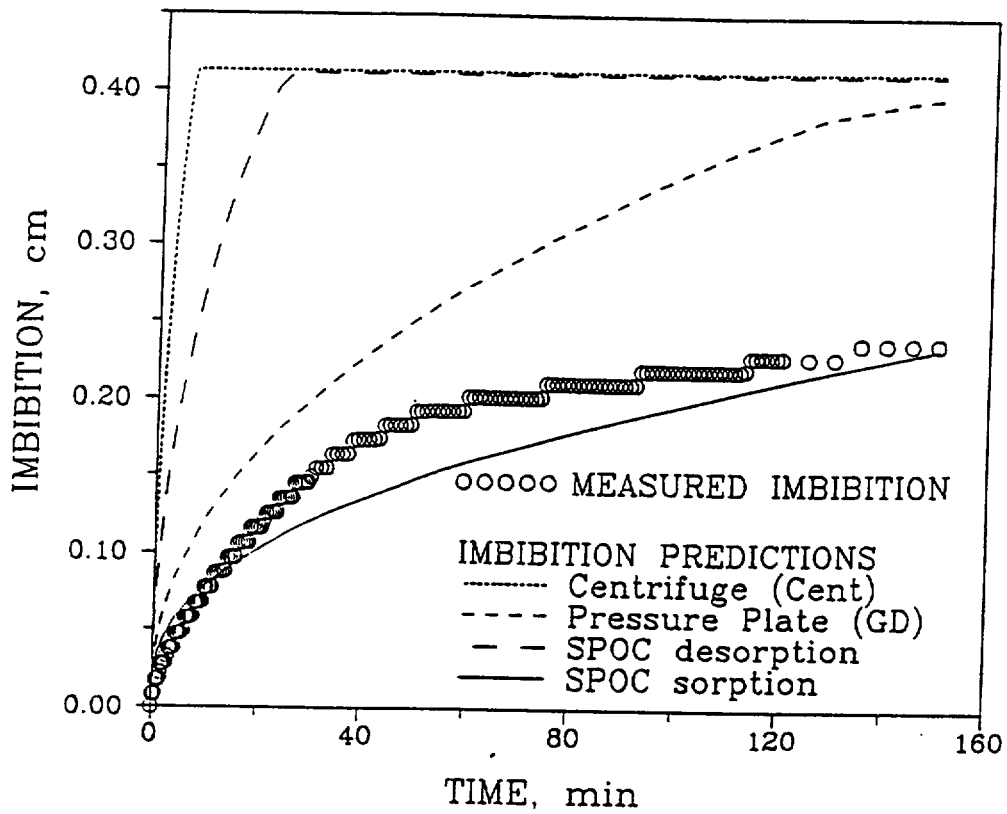

Figure 6. Measured imbibition data with imbibition simulations for nonwelded tuff at 46.6 percent initial relative water content. Model predictions are using the van Genuchten equation fit to pressure plate moisture characteristic data and gas drive relative permeability data, to centrifuge moisture characteristic data and centrifuge relative permeability data and to SPOC sorption and desorption moisture characteristic data alone.

Numerical and Laboratory Investigations of Transient and Steady-State Flow in a Fractured Core.

Edward M. Kwicklis, Falah Thamir, R. W. Healy, Carol J. Boughton,
U. S. Geological Survey, Lakewood, Colorado

and Steve Anderton, SAIC, Golden, Colorado.

1.0 Introduction

An improved understanding of the ability of fractures to transmit water at matric potentials less than zero is essential for evaluating the ability of the rocks of Yucca Mountain, Nevada, to safely isolate nuclear waste. Numerical and experimental investigations of this subject will help substantiate flux estimates of both liquid water and water vapor at Yucca Mountain, aid in assessing the effectiveness of capillary barriers at the contact between nonwelded and fractured welded units, and may provide insight as to the manner in which flow may become concentrated along specific pathways through a network of fractures under conditions of partial saturation. This paper summarizes some of the numerical and laboratory investigations that have been conducted at the U. S. Geological Survey in Denver on a core of welded tuff containing a single fracture parallel to the core axis. The objectives of these investigations were to (1) explore the possibility that the unsaturated hydrologic properties of a fracture could be estimated by applying inverse techniques to the results of transient imbibition experiments, and (2) evaluate the accuracy of estimates of unsaturated fracture hydrologic properties derived from transient tests or numerical modeling through direct steady-state measurements. The core examined in these experiments is 0.0699 m long and has a radius of 0.0208 m. It was obtained from the "columnar zone" of the Tiva Canyon member of the Paintbrush Tuff near Wren Wash on Yucca Mountain (Scott and others, 1983).

2.0 Transient Imbibition Experiment

The contribution of the fracture to water movement into the core during transient imbibition was isolated in two experiments. In both experiments the oven-dried core was placed in a beaker having a constant water depth of approximately 3.0 millimeters. In the first experiment, the core was held together by plastic bands so that in addition to water imbibed by the wetted end, water was also pulled by capillarity into the fracture. In the second experiment, the two halves of the re-dried core were separated and the cumulative water uptake into the two half-cores occurred from the wetted end alone. As shown in figure 1, the cumulative imbibition at any time was greater in the banded core than in the two half-cores. The difference between the two curves at any time represents the volume of water held by capillarity within the fracture plus the water that has entered the matrix across the fracture-matrix interface.

In order to explore the possibility that the unsaturated hydrologic characteristics of fractures can be determined by application of inverse

techniques (for example, Kool and others, 1987) to the results of transient imbibition experiments performed on fractured cores, the sensitivity of cumulative imbibition into the banded core to the fracture hydrologic properties was examined by numerical modeling. First, the cumulative imbibition data from the two half-cores was modeled to characterize the matrix properties. Then, data for the banded core was simulated by explicitly representing both the fracture and adjacent matrix in a calculational mesh and incorporating numerically generated fracture properties into the TOUGH numerical simulator (Pruess, 1987).

Cumulative imbibition into the two half-cores was simulated under the assumption that the unsaturated flow relations between matric potential, saturation, and relative permeabilities to water and air could be described by the functions presented by Luckner and others (1989). These functions are similar to those derived by van Genuchten (1980) but include additional expressions for relative permeability to air. Initial estimates for hydraulic conductivity, residual water saturation, and fitting parameters n and alpha were based upon values thought to be representative of the welded portions of the Tiva Canyon Member of the Paintbrush Tuff (Peters and others, 1984, p.61), and a residual gas saturation estimated to be 0.15. Simulations utilizing these values resulted in an underestimate of cumulative imbibition at any given time. The best fit results obtained through a trial and error approach are shown in figure 2. The fitting parameters used to generate the curve in figure 2 were n=1.75 and alpha=0.005 inverse meters. These values are within the range reported by Peters and others (1984) for welded tuffs from Yucca Moutnain. The value of saturated permeability of 7.5E-18 meters squared is approximately 7.5 times the value suggested by Peters and others (1984), but is also well within the range of measured values for welded tuff.

The porosities of the banded core and the two half-cores were determined gravimetrically as 0.082 and 0.0786, respectively. The difference between these values yielded a value for fracture porosity of 0.0038. Based on this value of fracture porosity, the surface area of the fracture and the total core volume, an average physical aperture of 123.8 microns was computed. An equivalent pneumatic aperture of 129.3 microns was estimated using air flow measurements and cubic law assumptions.

Although the mean effective fracture aperture can be readily determined, as described above, the aperture width will vary significantly over the fracture plane, ranging from zero at contact points to values substantially larger than the mean at other points. These variations in aperture width will strongly affect the ability of the fracture to transmit water under unsaturated flow conditions, because they govern the fraction of the fracture space that can transmit water. The sensitivity of unsaturated flow properties to these variations was explored by numerical simulation of hypothetical aperture distributions in a fracture having a mean aperture of 125 microns.

Hypothetical relations between relative permeabilities to air and water, saturation and matric potential were generated using a model conceptually similar to that described by Pruess and Tsang (1990). Aperture

variation within the fracture plane was approximated by discretizing the fracture into a 50 by 50 grid of spatially varying, constant aperture cells. The thicknesses of these cells follow a lognormal distribution, and are correlated spatially over a distance of 0.1 times the flow field dimensions using a spherical semivariogram. Each constant aperture cell is filled with either water or air depending upon the air-entry matric potential of that cell, the average potential prescribed for the fracture as a whole, and the presence of continuous paths of the same phase that extend to the fracture boundaries. The flux calculated at a prescribed potential is divided by the flux computed when the fracture is completely saturated by that phase to give the relative permeability. The flow equations for liquid and gas phases are formulated in the form given by Moreno and others (1988) and solved using a finite-difference and conjugate-gradient technique.

Uncertainty regarding the effects of fracture properties on unsaturated flow results from the unknown variation in aperture around the mean value of 125 microns. Therefore, the sensitivity of the unsaturated flow properties of the 125 micron fracture to the variance in aperture was examined. The computed saturation, matric potential and relative permeability relations shown in figures 3 to 5 are the averages of ten realizations. Average properties are shown for each value of variance in order to better observe general trends and minimize the significance of any single realization. Individual points on figures 4 and 5 may represent averages of only 7 to 9 realizations because for some realizations the numerical model failed to generate a convergent solution at all of the prescribed water potentials.

Figure 3 shows that at matric potentials greater than -0.118 m, the air-entry matric potential for a 125 micron parallel plate fracture, fractures with larger variances contain less water because they contain large aperture cells that drain or fill at relatively large matric potentials. Conversely, at matric potentials less than -0.118 m, fractures with large aperture variances contain more water. The same trend occurs in the relation between relative liquid permeability and matric potential (figure 4). Relative permeability to liquid becomes smaller at matric potentials larger than -0.118 m and larger at matric potentials less than -0.118 m as aperture variance increases. Relative permeability to gas drops at smaller matric potentials during wetting as aperture variance increases because small aperture cells are more numerous and these contain water at small matric potentials.

As illustrated in figure 4, only a very small range in matric potential exists over which both the liquid and gas phases have nonzero relative permeabilities. For individual realizations there was often no matric potential over which both phases had nonzero relative permeability. The range in saturations over which both phases display nonzero relative permeability may be fairly limited as well (figure 5). Residual gas saturations were typically between 0.70 and 0.80, becoming larger as the variance in the natural logarithm of aperture was increased. Residual liquid saturations became larger as aperture variance decreased, ranging from values of 0.023 to 0.056 for variances in the natural logarithm of aperture of 1.5 and 0.5, respectively. Liquid relative permeability at

these values of residual gas saturation is less than 0.02 for all aperture variances examined, suggesting that liquid water movement in a newly wetted fracture will be greatly reduced compared with liquid water movement in a completely saturated fracture. The calculations therefore indicate that hysteretic effects may be significant. Pruess and Tsang (1990) made similar observations regarding large residual gas saturations and limited ranges in saturation over which both phases display nonzero relative permeability.

Figure 6 shows the fractional area of the fracture plane that is water-filled as a function of liquid saturation for aperture variances of 0.5, 1.0 and 1.5. Following Wang and Narasimhan (1985), this relation may be interpreted as defining the relative permeability of the fracture in the direction perpendicular to the fracture plane. As such, it controls fluid movement across the fracture-matrix interface.

Imbibition into the banded core was simulated in three-dimensions using TOUGH. The fracture and adjacent matrix were explicitly represented in the computational mesh. Taking advantage of symmetry boundaries, the fracture was represented by a 0.000063 m wide column of cells at the left edge of the flow domain and the matrix by four 0.005 m wide columns of cells to the right of this. The mesh consisted of fourteen layers 0.005 m thick perpendicular to the axis of the core. Fracture properties shown in figures 3 to 6 and matrix properties deduced from the best fit analysis (Figure 2) were assigned to the appropriate cells of the computational mesh. TOUGH was modified so that the relations between liquid saturation and relative permeability to liquid and gas, fractional wetted area and capillary pressure could be entered in tabular form.

The simulated effects of an axial fracture on imbibition are shown in figure 7a for each of the assumed aperture variances. Although the numerical results predict the enhanced imbibition rates in a qualitative sense, agreement with the experimental data for the banded core is poor, significantly overestimating the measured cumulative imbibition in each case. The curves relating simulated cumulative imbibition to time are slightly sensitive to the fracture properties employed, with imbibition rates becoming larger as the variance in the natural logarithm of aperture decreases. This may be due to the calculated increase in saturated permeability of the fracture and the decrease in entrapped air with decreasing aperture variance. The experimental data for the banded core indicate that water movement into the core is enhanced relative to the separated core because water moves into the intact matrix across the wetted area along the fracture-matrix interface as well as from the bottom of the core. The rock surfaces along the fracture-matrix interface increase the surface area potentially available for imbibition by a factor of approximately 5.3. The model results overestimated the rate of fluid exhange between the fracture and intact matrix. Simulations of imbibition into the banded core were repeated under the assumption that the relative permeability of the fracture in the direction perpendicular to the fracture plane was equal to the relative permeability parallel to the fracture plane (figure 7b). Although the physical basis for this assumption is lacking and agreement with the experimental data is still

not satisfactory, the results indicate (figures 7a and 7b) that the simulated imbibition rates are relatively sensitive to the manner in which transverse relative permeability for the fracture is defined. However, it is clear that the model again overestimated the rate of fluid exchange between the fracture and intact matrix. Three possible causes are that: (1) The rock matrix is anisotropic, with permeability perpendicular to the axis of the core less than the permeability parallel to the axis of the core; (2) fracture coatings not accounted for in the model are impeding fluid exchange in the experiment; or (3) the rock immediately adjacent to the fracture has been altered, either during the process of fracturing or by subsequent mineralization, so that it is now denser and less permeable than the matrix as a whole. The sensitivity of imbibition rates to fracture characteristics alone does not appear sufficient to explain the discrepency between measured and simulated imbibition rates.

Further examination of the core revealed that lithic fragments within the matrix were highly flattened parallel to the fracture plane, supporting the hypothesis that anisotropy in matrix permeability is the cause of the discrepency between predicted and measured imbibition rates. Further numerical modeling using fracture properties derived for an assumed aperture variance of 1.0 found that good agreement between the simulated and experimental results was obtained when the saturated matrix permeability perpendicular to the fracture plane was set at 0.01 times the saturated matrix permeability parallel to the core axis (figure 7c). However, this anisotropy ratio may be unrealistically small and no quantitative information on the degree of anisotropy is available for the core at this time.

3.0 Steady-State Experiment

To evaluate the accuracy of estimates of the unsaturated fracture properties derived from other methods, the permeability of the fractured core at different matric potentials was measured using steady-state methods. The core was first placed in the assembly shown in figure 8. Porous polymer plates 0.0064 m thick with an air-entry matric potential of approximately -0.35 m of water were hydraulically connected to the ends of the core by 0.0032 m thick layers of coarse sand. Sand was included between the plates and the core to ensure good hydraulic contact and to minimize the possiblity that the plates might impede flow though the fracture at matric potentials close to zero. Aquarium sealant held the core in place against the plexiglass endcaps and sealed the fracture traces along the sides of the core to keep water from leaving the fractures when positive water pressures were applied to the upper and lower plates. The core was housed in plexiglass and sealed with o-rings to minimize evaporation. Inflowing water had a concentration of 2000 parts per million formaldahyde to inhibit bacterial growth. Figure 9 shows the overall test design. The matric potential at the outer boundary of the upper plate in the sample assembly is controlled by the difference in height between the water level in the upper intermediate reservoir and the upper polymer plate. Similarly, the difference in height between the air-water interface in the tube leading to the lower intermediate reservoir and the lower porous plate controls the matric

potential in the lower porous plate. The water level in the upper intermediate reservoir and the air-water interface in the sample assembly outflow tube are separated by a distance equal to the height of the sample assembly so that raising or lowering the entire sample assembly changes the matric potential in the end plates equally and an average unit hydraulic gradient through the core is maintained. When the water level in the upper intermediate reservoir falls below the level of the upper sensing electrode, the solenoid valve opens and water flows from the upper reservoir until the upper sensing electrode is again submerged. Both water inflow and outflow are recorded. Steady flow was assumed when inflow equalled outflow and both were relatively constant in time.

Initially the core was saturated. Matric potential at the plate boundaries was held constant at each level until steady flow was attained. Matric potential at the boundaries was initially 0.0 m and was sequentially reduced in approximately 0.025 m increments. As shown in figure 10, flow rates on the initial drying curve were several hundreds of cubic centimeters per hour until the matric potential was reduced from -0.0776 m to -0.1333 m, at which point flow rates dropped below 1.0 cubic centimeter per hour. Steady flow rates at larger matric potentials did not appear to show a systematic trend. Flow rates appeared to be sensitive to both barometric pressure and temperature fluctuations. This sensitivity may be due to the expansion of air bubbles in the plates and sand as barometric pressure dropped or air temperature increased, and the contraction of air bubbles as barometric pressure rose or air temperature dropped. A pronounced hysteresis in flow rates was then observed as matric potentials at the boundaries were increased until positive pressures were attained. Flow rates did not increase until unequal positive pressures were applied to the upper and lower boundaries.

Flow rates measured during the first drying and wetting cycles, as well as those predicted for a 125.0 micron fracture and different values of aperture variance are shown in figure 11. Predicted flows are calculated on the assumption that because of the extremely small permeability of the matrix, all flow from the core occurs through the fracture. Although none of the predicted flow rates match the data very well, measured flow rates are most closely matched by flow rates predicted for a 125.0 micron parallel plate fracture. Flow rates for the parallel plate fracture most closely approximate the abrupt decline in measured flow rates at matric potential between -0.0776 and -0.1333 m.

4.0 Discussion

The motivation for performing the imbibition experiments and the accompanying simulations was to test if the cumulative imbibition curve for the banded core is sensitive to the properties estimated for the fracture. If not, it can be reasoned that inverse techniques will have little success in determining the unsaturated properties of the fracture from experiments of this type, and that cumulative imbibition data collected from fractured cores will provide a poor database for evaluating the accuracy of unsaturated fracture properties generated by other

means. Sensitivity of the numerical results to fracture characteristics alone did not appear to be sufficient to explain the discrepency in imbibition rates between the experimental data and the model simulations. For these simulations, uncertainty in the unsaturated flow properties of the fracture is apparently minor in comparison with the uncertainty concerning matrix anisotropy, fracture coatings, alteration rinds, etc.

The agreement between the equivalent parallel plate pneumatic aperture and the average physical aperture indicates that aperture variance within the fracture is small. Furthermore, during the steady flow experiment, flow dropped precipitously as matric potential approached the air entry value for a 125 micron parallel plate fracture. However, contradictary evidence exists in that a parallel plate fracture should not have displayed the hysteretic effects that were observed.

Numerical experiments in which the flux through a variable aperture fracture composed of spatially-correlated, constant-aperture cells was calculated have indicated that the parallel-plate hydraulic aperture deviates more from the average physical aperture as the variance in the natural logarithm of aperture increases (figure 12), presumably because there are more small aperture cells to create constrictions to flow. Because compressive stresses were minimal in this particular experiment, contact area between the opposing walls of the fracture was probably also minimal. Large contact area within the fracture plane would have the effect of increasing tortuousity for flow and thus causing further deviation between the pneumatic parallel plate aperture and the average physical aperture (Pyrak-Nolte and others, 1987).

It is proposed that because hydraulic aperture and physical aperture are relatively simple to measure in comparison with relative permeability, that these data be used in conjunction with relations such as that shown in figure 12 to estimate the appropriate variance to be employed when generating permeability-matric potential and saturation-matric potential relationships numerically. A partial test of this hypothesis was made using data from what appears to have been a parallel plate fracture. Future tests of the hypothesis require that the fractures tested be subjected to larger compressive stresses.

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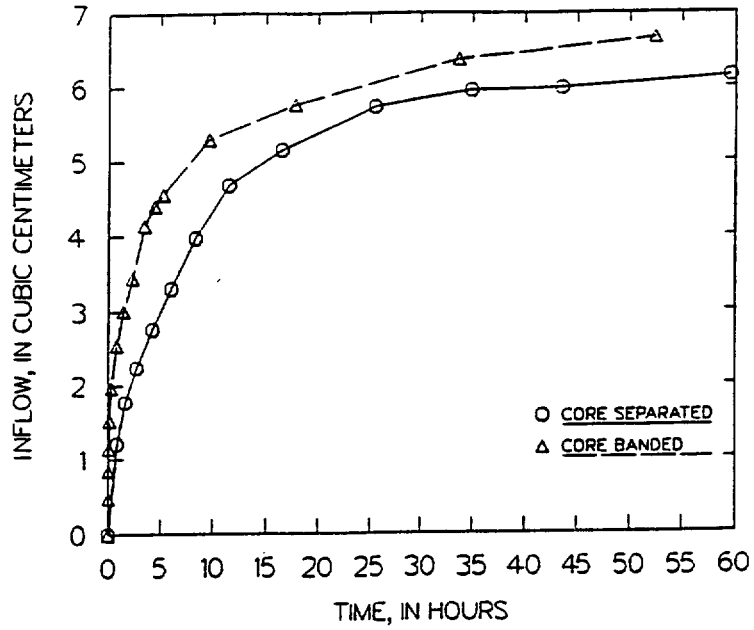

Figure 1. Graph showing cumulative imbibition as a function of time for the separated and banded cores.

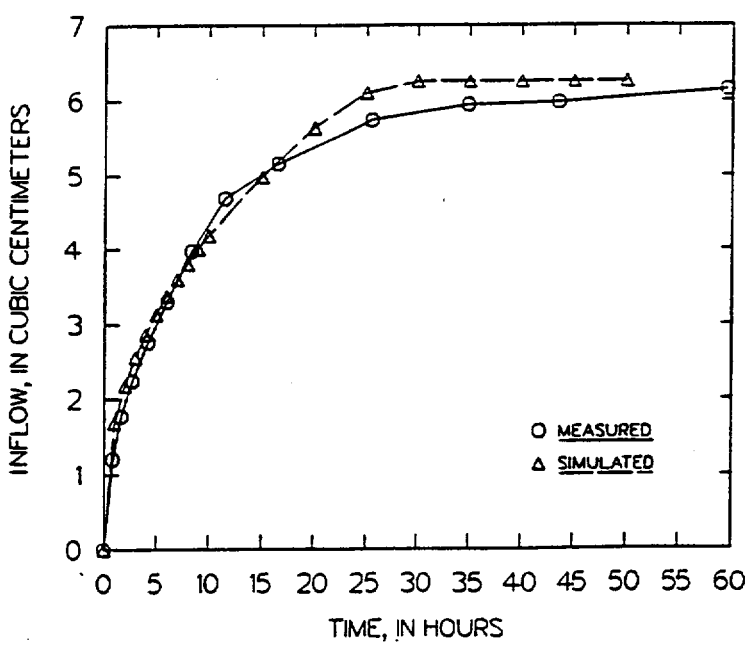

Figure 2. Graph showing measured and simulated cumulative imbibition as a function of time for the separated core.

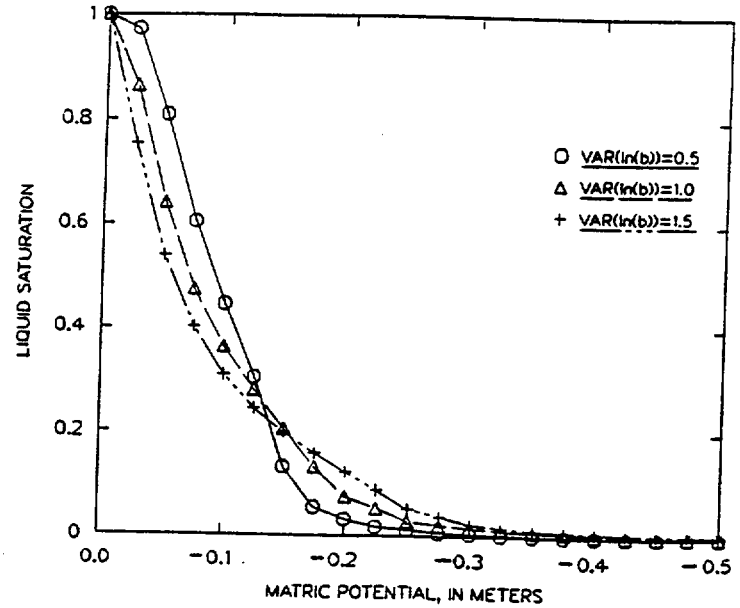

Figure 3. Graph showing the sensitivity of the computed liquid saturation-matric potential relations to assumed aperture variance.

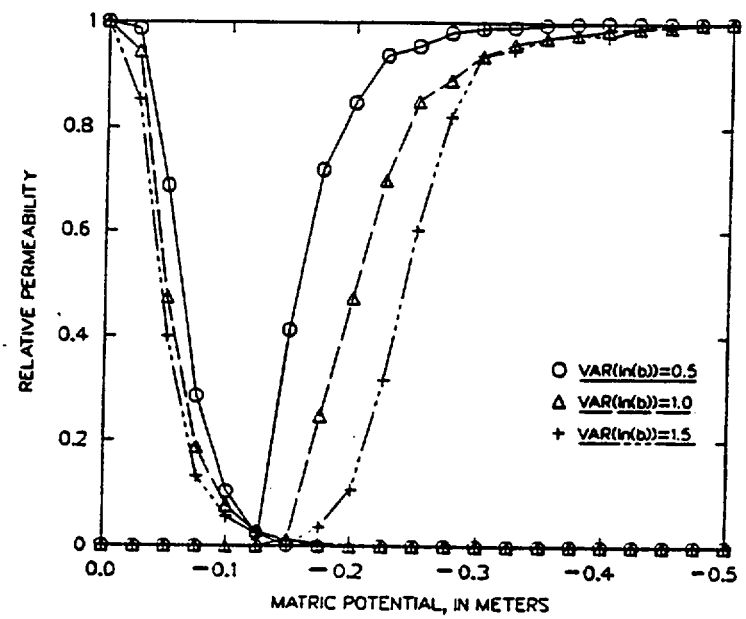

Figure 4. Graph showing the sensitivity of the computed relative air permeability-matric potential and relative water permeability-matric potential relations to assumed aperture variance.

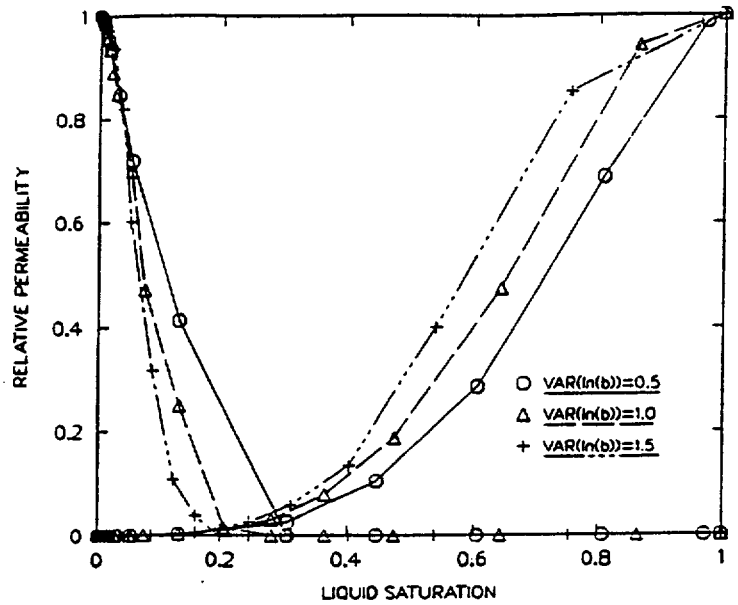

Figure 5. Graph showing the sensitivity of the computed relative air permeability-liquid saturation and relative water permeability-liquid saturation relations to assumed aperture variance.

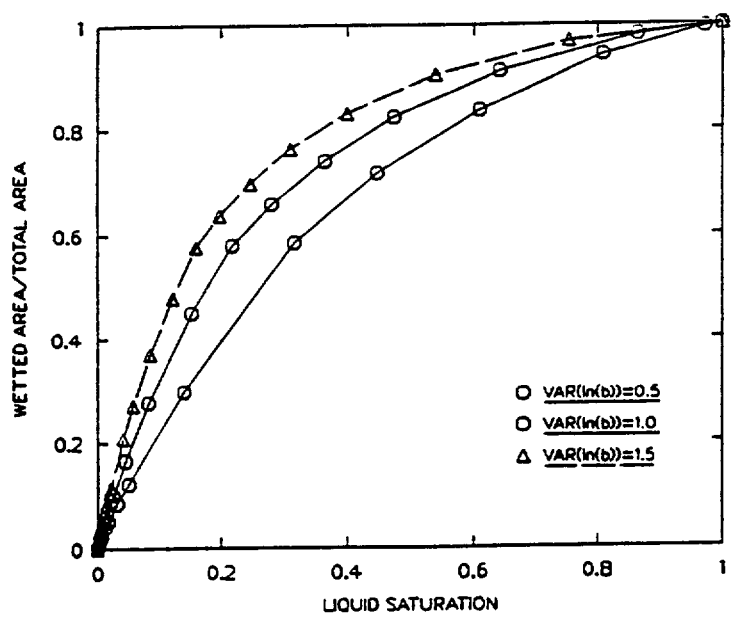

Figure 6. Graph showing the sensitivity of the computed fractional wetted area-liquid saturation relations to assumed aperture variance.

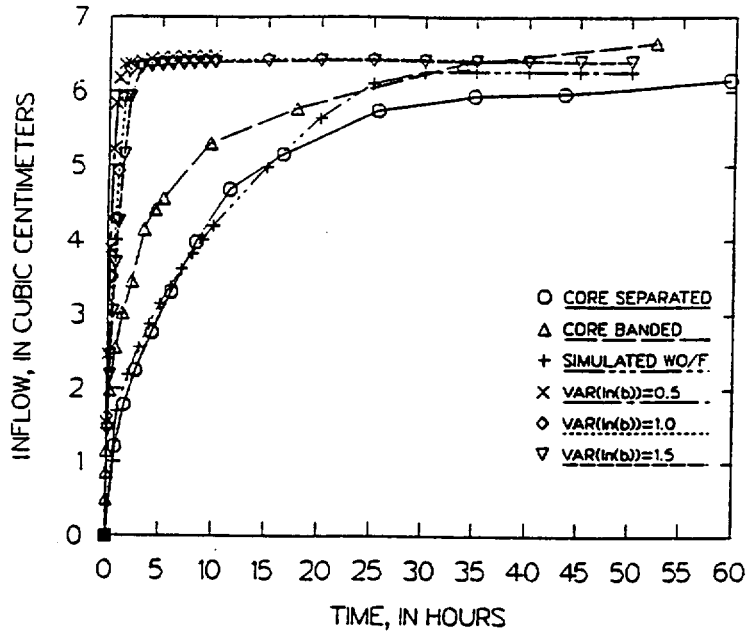

Figure 7a. Graph showing the simulated effects of the fracture on cumulative imbibition assuming transverse relative permeability of the fracture equals fractional wetted area.

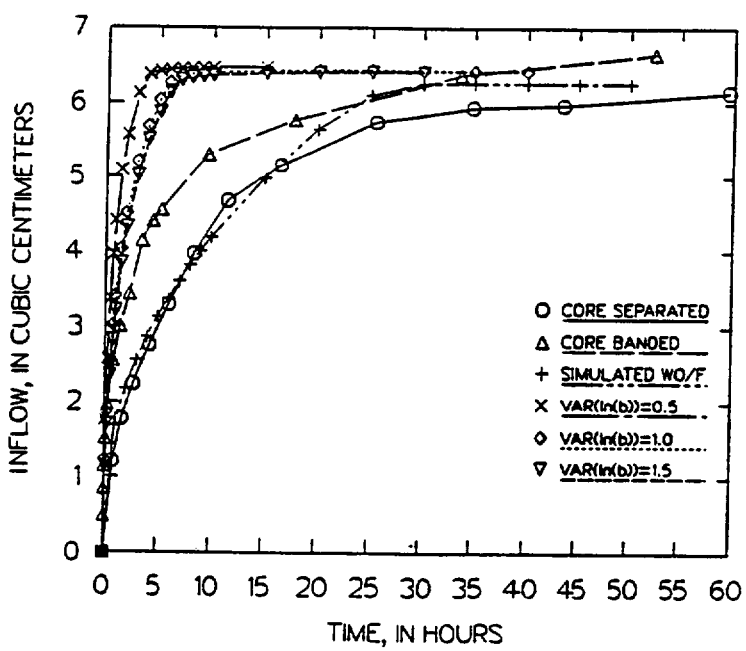

Figure 7b. Graph showing the simulated effects of the fracture on cumulative imbibition assuming transverse relative permeability of the fracture equals longitudinal relative permeability.

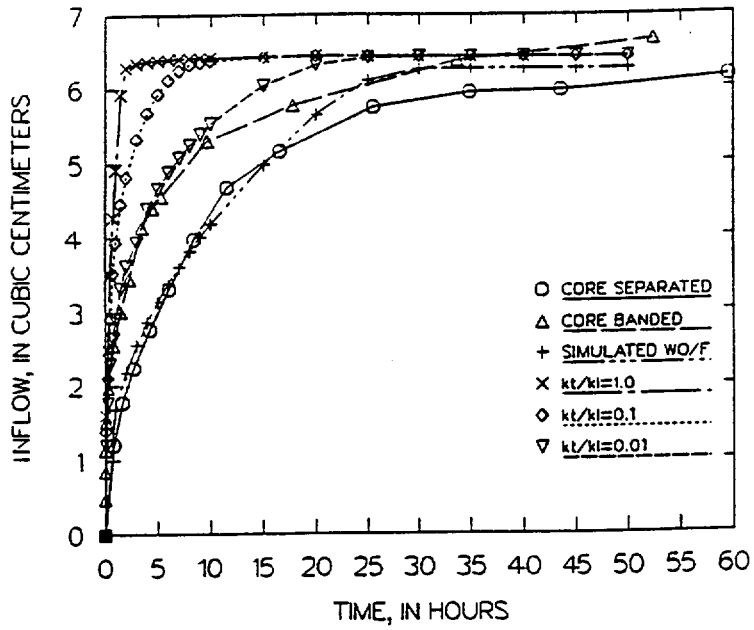

Figure 7c. Graph showing the simulated effects of the fracture on cumulative imbibition assuming transverse relative permeability of the fracture equals fractional wetted area, but the saturated matrix permeability is anisotropic to varying degrees.

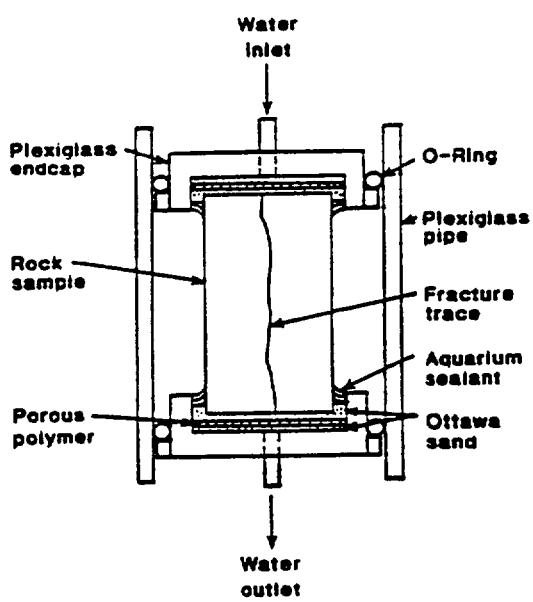

Figure 8. Diagram showing the experimental design of the core assembly.

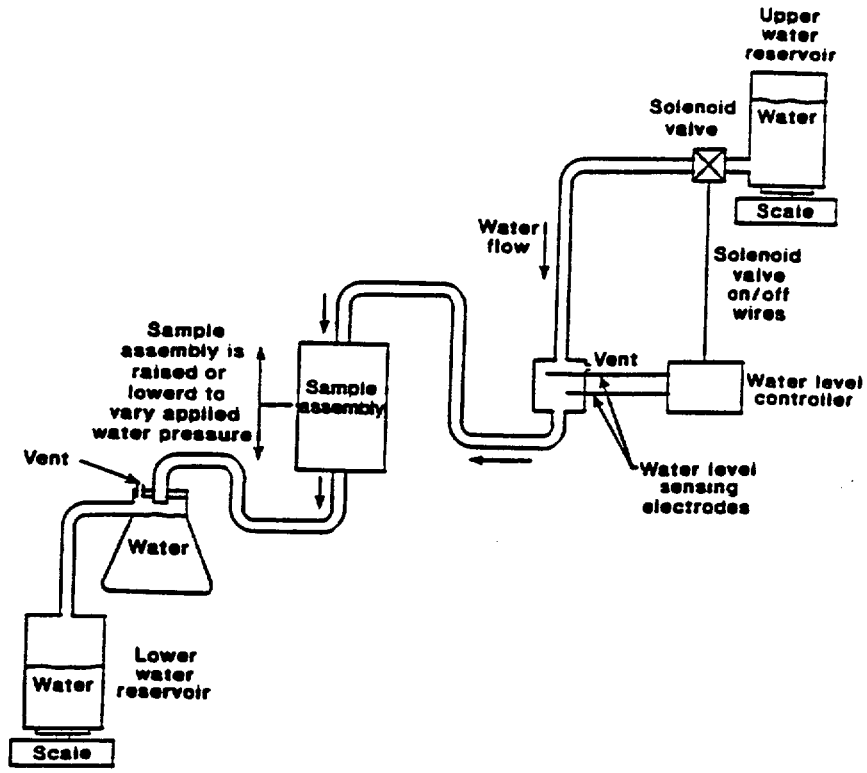

Figure 9. Diagram showing the overall experimental design used to control the matric potential at the upper and lower boundaries of the core.

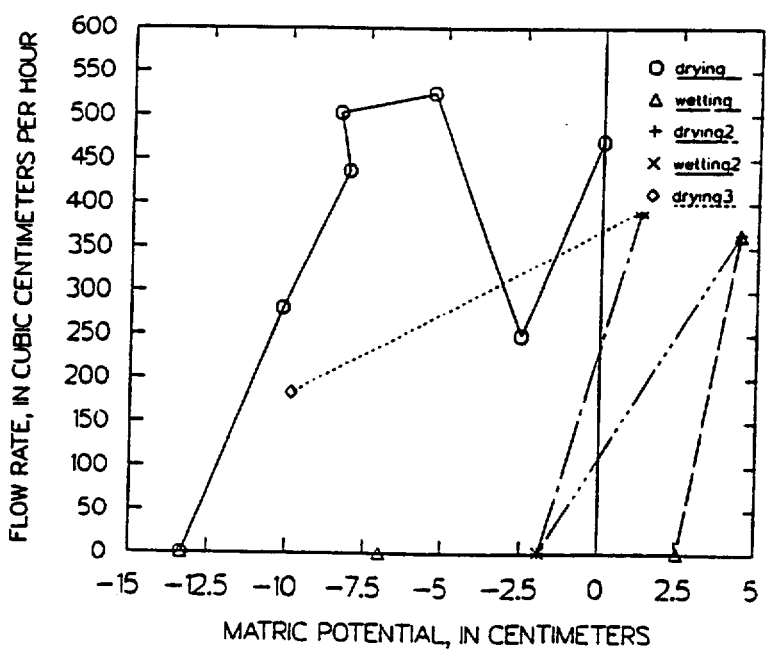

Figure 10. Graph showing the relation between volumetric flow rate and average matric potential within the core for various wetting and drying cycles.

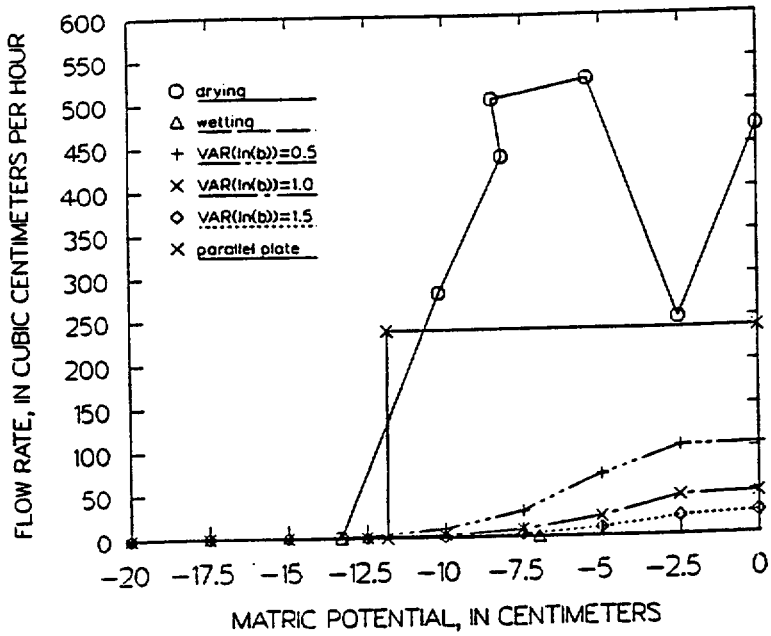

Figure 11. Graph showing a comparison between the measured volumetric flow rates and those predicted for different aperture variances assuming there is no air-entrapment within the fractures.

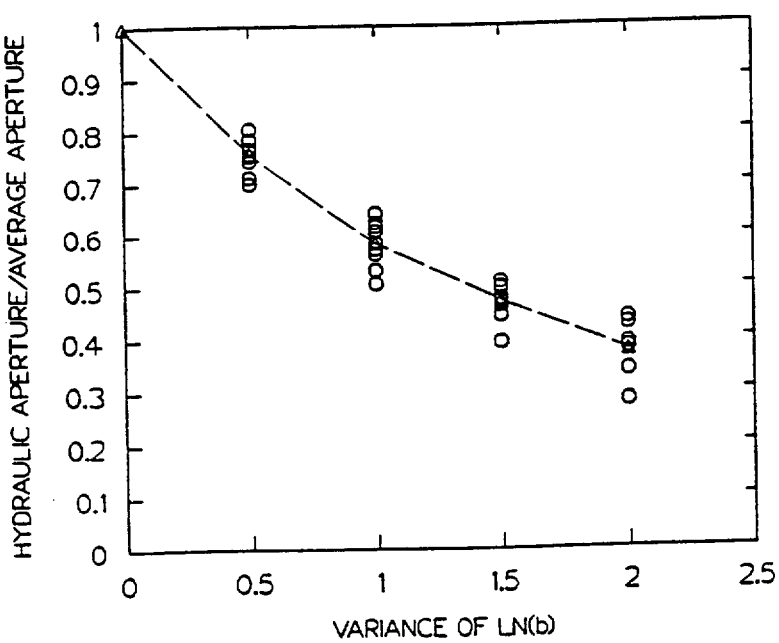

Figure 12. Graph showing the calculated dependence of the ratio of hydraulic to average physical aperture on the variance of the natural logarithm of aperture.

GROUND WATER FLOW THROUGH UNSATURATED FRACTURED ROCK[1] RESEARCH NEEDS

William Ford
U.S. Nuclear Regulatory Commission

ABSTRACT

This report presents: (1) a discussion of unsaturated fractured rock flow concepts; (2) a summary of unsaturated fractured rock flow modeling methods; and (3) a discussion of scientific investigations that may be needed to build confidence in the numerical modeling of ground water flow through unsaturated fractured rock. At the present time few experiments have been identified that test the concepts of unsaturated flow in fractured rock. Further, neither the continuum, discrete fracture network, nor the stochastic analytic modeling approaches to modeling ground water flow through unsaturated rock have been tested against either laboratory or field experiments.

INTRODUCTION

Characterization of the proposed Yucca Mountain high level nuclear waste repository will require the modeling of ground water flow through unsaturated fractured rock. Because applied modeling is usually a simplification of basic scientific concepts, the scientific community should be confident in its understanding of the basic physics of ground water flow through unsaturated fractured rock. If a sound scientific understanding of basic concepts has been established, modelers can be more confident in applying them. However, even if the basic concepts have been scientifically established modelers may need additional scientific input. These needs may arise in a variety of ways: (1) models may contain unique parameters for which new data collection and interpretation techniques must be developed; (2) the model may need to be tested against experiments to improve confidence in its application; and (3) different model input approaches may have to be evaluated, developed, and tested. Therefore scientific investigations may be required by the scientific community to confirm and develop a sound understanding of unsaturated ground water flow concepts through fractured rock and to apply and build confidence in their application in numerical models. This paper attempts to identify scientific investigations that may be needed to build confidence in the numerical modeling of ground water flow through unsaturated fractured rock.

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[1] This paper was prepared by an employee of the United States Nuclear Regulatory Commission. It presents information that does not currently represent an agreed-upon staff position. The Nuclear Regulatory Commission has neither approved nor disapproved its technical content.

UNSATURATED FRACTURED ROCK FLOW CONCEPTS

Concepts of ground water flow in unsaturated fractured rock have evolved from theories of unsaturated ground water flow through soil. In the Site Characterization Plan, Yucca Mountain Site, (U.S. DOE, 1988), the conceptualization of unsaturated flow in a fractured-porous medium is "based on capillary bundle theory (e.g., Wang and Narasimhan (1985)) which states that there is a relationship between pore size and equilibrium pressure head. Thus, the saturation of a material containing pores of many different sizes is related to the equilibrium pressure head in the material..." (Klavetter, 1986a, p. 6). Further, as water is added to a rock or soil; water will fill small pores in preference to large pore spaces, because of the higher capillary suction (tension) forces exerted by small pores. For the same reason, when a rock matrix is at low saturation, a fracture with a larger average aperture than the average matrix pore diameter will be essentially dry. Under these conditions water flow will be confined to the matrix with little or no flow across or down fractures. For most fractures it is assumed that the pore spaces caused by matrix grain to grain contacts across the fracture (asperities) are smaller across the fracture than longitudinally within the fracture. Therefore, as saturation increases and the water occupies larger pore spaces, water movement across a fracture will tend to occur, while little or no water flows down a fracture. At slightly higher saturations the fracture conductivity in the plane of the fracture should become nonzero allowing water to flow longitudinally in sinuous channels in the fracture. Finally, when the matrix and the fracture are almost completely saturated the fractures become efficient contributors to water flow (Klavetter, 1986).

This concept indicates that fracture flow is a function of saturation and aperture size. For unsaturated conditions, this relationship implies that, because fractures are generally irregular in shape and have irregular apertures it is possible to have water flow in regions of the fracture with small aperture and not have flow in other areas of the fracture with larger apertures (Klavetter, 1986). Similarly, it is also possible to have water flow in fractures with small average apertures while little or no flow is occurring in fractures with larger average apertures. When a rock is completely saturated, the situation is reversed. "The majority of the flow in the fracture occurs in those regions where the fracture aperture is large, with little flow occurring where the fracture aperture is small because the flow rate is proportional to the cube of the aperture" (Klavetter, 1986, p. 13).

To summarize this concept, "the average fracture conductivity for water movement in the plane of the fracture is a highly nonlinear function of fracture saturation or pressure head. If the flux is less than the saturated conductivity of the matrix, then the water will tend to flow only in the matrix as it moves downward. If the flux is greater than the saturated conductivity of the matrix, then the matrix will saturate, and the fractures will carry water also" (Klavetter, 1986, p. 15)

This concept is subject to the following constraints:

1. The system is changing very slowly with time, so that pressures heads in the fracture and matrix are in equilibrium with each

other. For example, equilibrium may not exist if a large pulse of water preferentially enters fractures (perhaps at the ground surface) fast enough to cause saturated flow in the fractures. Water would then rapidly flow down through fractures surrounded by unsaturated matrix. This situation would persist until the water in the fracture flowed into the matrix or until it reached a zone of positive pressure such as a water table or perched zone.

2. Darcy's law and the Richard's equation are valid. This assumption may not be true for large aperture fractures where the sides of the fracture have very little contact. In this situation as the saturation of the matrix increased, water could not cross the fracture laterally, but may tend to form droplets on the sides of the fracture. These droplets could then run down the sides of the fracture (non-darcian flow). Alternatively a large aperture fracture could receive a large pulse of water which would rapidly flow down the fracture under non-darcian (similar to stream channel) flow conditions.

3. "The manner in which the water flows in a hydrologic unit depends on other boundary conditions besides the flux. For example, in the capillary fringe area near the water table, the matrix is always saturated because of the capillary forces of the small pores in the matrix: thus, in this capillary fringe area some water will be in the highly conductive fractures no matter how small the downward flux is" (Klavetter, 1986, p. 15).

APPLICABILITY OF UNSATURATED FLOW CONCEPTS TO YUCCA MOUNTAIN

Modelers have applied this concept to presumed unsaturated ground water flow conditions at Yucca Mountain and reached some conclusions about it's applicability. Wang and Narasimhan (1985) concluded that for the tuffs at Yucca Mountain, the conductivity for flow across the fractures is estimated to be high compared with the conductivity within the matrix. Klavetter (1986a), concluded that because the fracture conductivity for water movement across the fractures is probably much larger than the adjacent matrix conductivity, flow across the fracture is controlled by the adjacent matrix conductivity. Therefore, the conductivity across the fractures can be replaced by the matrix conductivity in flow calculations. This suggests that lateral flow across fractures does not have to be included in modeling the unsaturated flow regime at Yucca Mountain.

Modeling that evaluated water infiltration pulses at Yucca Mountain has been done by Travis et al. (1984) and by Martinez (1988). Martinez simulated a surface completely saturated for one hour, while Travis simulated a slug of water on the order 2 m tall injected into a 100-micrometer fracture. "Both Travis and Martinez seem to indicate that episodic pulses of water at the surface will not penetrate significant distances into Yucca Mountain if the fracture aperture is less than 100 micrometers (an approximate upper value suggested by Sinnock et al. (1984). The water injected into the fracture moves quickly into the matrix because of two complementary effects:

1) At the front end of the pulse, a large pressure-head difference exists between the saturated fracture and the partially saturated matrix (this difference may be of the order of 100 m).

2) Because the fracture conductivity ahead of the water pulse is very low (the fracture may be near its residual saturation), flow in the fracture is retarded and the pulse diverted into the matrix. Wang and Narasimhan (1985) indicate that the fracture conductivity for flow within the plane of the fracture may be zero until the nearby matrix material is nearly saturated" (Klavetter, 1986a, p. 14).

These calculations indicate that the penetration distance into fractures contained in low-conductivity, densely welded tuffs similar to those that form a caprock of Yucca Mountain (unit TCw) is of the order of 10 m or less if the fracture aperture is 100 micrometers or less" (Klavetter, 1986a, p. 15). "Thus, at depth, where the results of both Travis and Martinez indicate that the water flux is a slowly varying function of time, it is likely (according to the work of Wang and Narasimhan, 1985) that the matrix and fracture pressure heads are identical" (Klavetter, 1986a, p. 15).

These modeling studies support the assumption that the Yucca Mountain unsaturated ground water system is changing very slowly with time. However, it is pointed out in Klavetter (1986a, p. 15) "that episodic pulses of water may penetrate to great depth in regions near large structural features, such as fault zones, or where the fracture apertures are very large so that capillary bundle theory is not applicable." Simulations of these situations have not, to Klavetter's knowledge, been completed.

UNSATURATED FRACTURED ROCK MODELING METHODS

There are numerous methods of modeling unsaturated fractured rock flow. The following is not a complete list of methods, but it represents some of the major methods that have been identified to date.

EQUIVALENT POROUS MEDIA APPROACH

In modeling unsaturated flow conditions in soil, the hydrologic properties are represented by characteristic curves which describe moisture content and conductivity as a function of pressure head. "Procedures have been developed for soils by which to infer closed-form analytic representations for this dependence from the corresponding moisture retention curve (Brooks and Corey, 1964; Mualem, 1976; van Genuchten, 1980)....That this approach is appropriate to describe the rock-matrix properties is supported indirectly in that moisture-retention curves measured on individual samples of tuff can be fitted" to an analytic representation developed for soils by van Genuchten (1980)..." (U.S. DOE, 1988, p. 3-143).

One result of the assumption of the validity of Darcy's law for unsaturated flow in fractures is that, like the rock matrix, flow in the fractures can be modeled as an equivalent porous medium. Under unsaturated flow conditions, the hydrologic properties of the fracture can then be

represented by characteristic curves which describe moisture content and conductivity as a function of pressure head. However, the staff does not know if anyone has experimentally determined these relationships for a fracture, or if it is currently possible to conduct such an experiment. The importance of experimentally determining these relationships is that it "would make it possible to model the flow characteristics in a macroscopic sense using current code capabilities..." (Klavetter, 1989, p. 4). Most of the presently available codes use this approach, and if the characteristic curves of the fracture cannot be measured in the laboratory or field, it is not clear how these relationships can be established for use in the models.

One approach is to determine characteristic curves for a fracture is to derive them theoretically. "Wang and Narasimhan (1985) used a single heterogeneous continuum approach to simulate flow in a hypothetical, unsaturated fractured rock. A formula for calculating fracture conductivity under partially saturated conditions was developed. The effects of distortion of flow paths by the air pockets were taken into account by a phase-separation constriction factor in a generalized cubic law for fracture flow under a partially saturated condition. The reduction of matrix-fracture flow area was taken into account by summing the aperture distribution function to a saturation cutoff aperture, which is inversely proportional to the suction head as prescribed by capillary theory. Based on the statistical theory, they generated fracture hydraulic conductivity curves as a function of saturation, saturation-suction curves, and matrix hydraulic characteristics curves for the densely welded tuff of the Topopah Spring Member at Yucca Mountain, southern Nevada..." (Yeh, 1988, p. 6).

CONTINUUM APPROACHES

Using computer models to explicitly model individual fractures at the scale of Yucca Mountain at this time may not be possible or necessary. For example in the Yucca Mountain Site Characterization Plan (U.S. DOE, 1988, p. 3-173), it is stated that "no way is known to generate a complete set of fracture location and geometry data. Secondly, if the Topopah Spring welded unit has a mean fracture density of 20 fractures/m^3 and has a mean thickness of 300 m over the approximately 7×10^6 m^2 area of the central Yucca Mountain block, then one would have to consider flow in approximately 4×10^{10} discrete fractures". This amount of detail would be too large to model at this time.

A proposed method of representing coupled matrix and fracture flow is to regard the "matrix and fractures as constituting either separate but overlapping continuum systems or as a single composite continuum system. These approaches assume that the matrix and fracture properties can be represented as spatial averages over rock mass volumes whose linear dimensions are very much smaller than the thickness of the hydrogeologic unit but sufficiently large to include a representative, statistical sample of hydraulically connected fractures. The rock mass volume over which the averaging is performed is commonly designated as a representative elementary volume (REV)..." (U.S. DOE, 1988, p. 3-173).

COMPOSITE-POROSITY APPROACH

Klavetter and Peters (1986) developed a "composite-porosity" model which describes fluid movement in a single continuum composed of both matrix material and fractures. Using this approach characteristic curves are developed to represent the combined hydrologic properties of the matrix and fractures. A problem with using the composite curve is that it may have a complex shape, which is difficult to represent mathematically. This problem may cause computer code stability problems when the composite characteristic curve contains a sharp transition from matrix only flow, to matrix and fracture flow. Again these are curves that at this time cannot be experimentally derived and have to be derived theoretically. "Peters et al. (1986) and Wang and Narasimhan (1986) attempted to solve this problem by deriving the effective permeability of a fractured-porous medium as the sum of the fracture and matrix permeability weighted by the cross-sectional areas of the flow channels" (Yeh, 1988, p. 6).

DUAL OR DOUBLE CONTINUUM APPROACH

Another approach to modeling a site at the scale of Yucca Mountain, may be to use a dual or double continuum approach. Double continuum models consist of two interconnected continua. In the case of fractured rock one continuum is the porous medium and the other continuum is the fractures. The continuum are connected by a fracture-matrix transfer term that simulates flow between the fracture and the matrix. "For saturated ground water flow, the transfer term between the matrix and the fractures depends on the hydraulic conductivity of the porous medium. If this concept is extended to unsaturated flow then the transfer term would depend on the degree of saturation of the matrix..." (Updegraff, 1990, p. 3). If the degree of saturation of the porous media becomes small, the transfer term also becomes small; restricting water flow between the fracture and the matrix.

One of the advantages of the double continuum approach is that the fracture-matrix transfer term can simulate other phenomena; such as mineral coatings on fracture walls, which can influence water flow between the matrix and fractures. The approach also may not have the disadvantage of code instabilities which can occur in a single continuum approach when the characteristic curve of the fracture-matrix continuum has a complex shape (previously described).

The difference in scales between matrix pores and fractures may cause problems in the dual continuum approach. "In general, fractures operate on a larger scale than pores. In a porous matrix, flow occurs only through the pore space, while in fractures, flow occurs in the aperture or region between fracture walls. If the scales of the pores and the fracture are nearly equivalent, then a double porosity model is applicable. If the fracture scale is much larger than the pore scale, then the double porosity approach is probably not valid" (Updegraff, 1990, p. 4). Again as with all the equivalent porous media approaches, characteristic curves for the fracture continuum must be generated that at this time cannot be experimentally derived and other methods of deriving them must be found. Furthermore, the fracture-matrix term is another parameter that cannot be

measured in the field and at this time other methods of deriving this term must be found.

The single continuum and the double continuum approaches are based on the concept of a representative elementary volume. A representative elementary volume is a volume above which average properties can be used to describe fluid flow through a rock. Below this volume average properties can no longer be used to describe the flow of fluid through a rock and the complex distribution of pore channels at the microscopic level must be considered. For Darcy's law a representative elementary volume is a size corresponding to a large number of pores. Because the pore size is usually small, the representative elementary volume is usually small compared to most modeling problems. However, "in fractured rocks the size of fractures is much larger than the size of pores. Also, the density of fractures at the macroscopic level is much lower than the density of pores. As a result, one has to enlarge the size of the representative elementary volume in order to visualize the fractured rocks as an equivalent porous continua at large-scale. The implication of this assumption is that the detailed spatial distribution of individual fractures within the representative elementary volume is ignored" (Yeh, 1988, p. 3). To date the staff is not aware of any experimental studies that have demonstrated a representative volume for unsaturated fractured rock allowing the fractured rock to be modeled as an equivalent porous continua at large-scale.

DISCRETE FRACTURE NETWORK APPROACH

Discrete fracture network models are another approach. This approach treats fractures as distinct flow channels embedded within a porous medium. The size of the representative elementary volume for fractures is not the same as that for the rock matrix. Individual fractures are then visualized as a continuum with a smaller representative elementary volume which ignores much smaller scale discontinued flow channels within the fracture. An example of a discrete fracture network approach is a model proposed by Huang and Evans (1985) to simulate flow and transport processes in three-dimensional fractured media. "The model was developed to provide estimates of global hydraulic conductivity within a rock mass for specified distributions of fracture orientations, apertures, and densities. The model is also able to calculate solute travel times and breakthrough curves. However, the model assumes steady, saturated flow conditions, and uses a piston flow approximation for simulating mass transport. The model later was extended with some simplified assumptions by Rasmussen (1987) for applications to variably-saturated fractured media. This is accomplished by defining a characteristic curve which relates the total head within the fracture to a capillary aperture using capillary theory. Also, an integrated air/water flow formulation is developed to explain hysteretic effects within the fracture rock network as the fluid potential changes. Finally, the capacity to account for matrix diffusion of solutes into the walls of the fractures has been added" (Yeh, 1988, p. 7).

STOCHASTIC APPROACH

Both discrete fracture network network models and continuum models can be further modified to incorporate stochastic methods. "The stochastic approach uses estimates of spatial auto-correlation functions of hydraulic

properties over local scales to determine hydraulic properties at larger scales" (Yeh, 1988, p. 7). This approach may prove to be useful, but at this time these methods require large amounts of data to establish the statistical parameters used in the code.

EXPERIMENTAL SUPPORT

At the present time few experiments have been identified that test the concepts of unsaturated flow in fractured rock. This is supported by the Site Characterization Plan for Yucca Mountain, which states that "Theoretical models for liquid-water flow in single fractures have been developed (Montazer and Harrold, 1985; Wang and Narasimhan, 1985) but have not been field and laboratory tested" (U.S. DOE, 1988, p. 3-171).

Only one study has been identified which investigated unsaturated flow in fractured tuff in a physical experiment. Russo and Reda (1988, p. 1) studied the "drying of an initially saturated welded tuffaceous rock experimentally. Gamma-beam densitometry was used to measure the material's effective porosity distribution prior to the drying experiment. It was then used to measure liquid saturation distributions during a 1400 hour drying period. The core selected for study was taken from the Busted Butte outcrop at the Nevada Test Site, part of the Topopah Spring Member of Paintbrush tuff. This specimen contained several microfractures transversely oriented to the direction of the water or vapor migration. These fractures were found to be regions of rapid dry out or low saturation even though they were displaced from the drying surface. An imbibition experiment was performed earlier on the same core. In the imbibition experiment the presence of most of these microfractures was detected by discontinuities in the measured saturation curves, which indicated a delay in liquid transport past the microfractures." It was concluded that "During the isothermal drying process in small-pore tuffaceous rocks, the presence of microfractures and high porosity regions significantly affect the saturation distribution within the rock. These high-porosity regions appear to dry first even though they are internal to the core volume" (Russo and Reda, 1988, p. 1 and 6).

It is important to note that "neither the continuum, discrete fracture network, nor the stochastic analytic models have been verified with either laboratory or field experiments" (Yeh, 1988, p. 7).

DISCUSSION AND RECOMMENDATIONS

To date few experiments have been identified that test the concepts of unsaturated flow in fractured rock. Further neither the continuum, discrete fracture network, nor the stochastic analytic modeling approaches to modeling ground water flow through unsaturated fractured rock have been verified with either laboratory or field experiments.

Modeling approaches such as the single heterogeneous continuum approach, the composite-porosity approach, and the dual or double continuum approach assume that like the rock matrix, flow in fractures can be modeled as an equivalent porous medium. Under unsaturated flow conditions, the hydrologic properties of the fracture can be represented by characteristic curves which describe moisture content and conductivity as a function of

pressure head. However, it is not known how these curves can be experimentally determined or what is the appropriate method to derive them for use in models.

Dual or Double Continuum Approaches to modeling unsaturated ground water flow consist of two interconnected continua. In the case of fractured rock one continuum is the porous medium and the other continuum is the fractures. The continuum are connected by a fracture matrix transfer term that simulates flow between the fracture and the matrix. However, the fracture-matrix transfer term is a parameter that cannot be measured in the field at this time and other methods of deriving this term must be found.

The single continuum and the double continuum approaches are based on the concept of a representative elementary volume. A representative elementary volume is a volume above which average properties can be used to describe fluid flow through a rock. Below this volume average properties can no longer be used to describe the flow of fluid through a rock and the complex distribution of pore channels at the microscopic level must be considered. In order to visualize the fractured rocks as an equivalent porous continua at large-scale for use in single continuum and double continuum simulations the representative elementary volume has to be enlarged. To date the staff is not aware of any experimental studies that have demonstrated a representative volume for unsaturated fractured rock allowing the fractured rock to be modeled as an equivalent porous continua at large-scale.

In applying unsaturated flow concepts to Yucca Mountain, Klavetter (1986a), concluded that because the fracture conductivity for water movement across the fractures is probably much larger than the adjacent matrix conductivity, flow across the fracture is controlled by the adjacent matrix conductivity. Therefore, the conductivity across the fractures can be replaced by the matrix conductivity in flow calculations. This suggests that lateral flow across fractures does not have to be included in modeling the unsaturated flow regime at Yucca Mountain. However, to date the staff has not found any experimental data that tests this assumption.

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Modeling Heterogeneous Unsaturated Flow Systems

Rachid Ababou

Southwest Research Institute
Center for Nuclear Waste Regulatory Analyses

INTRODUCTION

To adequately model large–scale flow and radionuclide transport in naturally heterogeneous unsaturated rock formations, the inherently three–dimensional spatial variability, stratification, and fracturation of porous geologic media must be accounted for. In particular, it is now increasingly recognized [1] that accurate modeling of radionuclide transport over large space–time scales depends on an adequate representation, in the simulated flow system, of a hierarchy of natural heterogeneities and/or fractures of many sizes and shapes. Moreover, in the case of unsaturated flow, the spatial features of geologic media must be represented through nonlinear matrix/fracture hydrodynamic properties. In what follows, some possible approaches towards realistic large–scale unsaturated flow modeling will be discussed, and some initial results and analyses will be presented. We focus here on the solution of the flow problem as a prerequisite to reliable solute transport simulation.

To summarize, one of the main difficulties in large–scale subsurface modeling of flow and transport is the existence of a complex three–dimensional hierarchy of natural geologic heterogeneities. Moreover, in the case of partially saturated or unsaturated flow, this difficulty is compounded by the nonlinear nature of the governing equations owing to the nonlinear pressure–dependence of water retention and hydraulic conductivity.

HIGH–RESOLUTION MODELS OF UNSATURATED FLOW

One possible modeling approach is to take into account the detailed geologic features, explicitly and directly, in the governing flow equations. These must then be solved numerically. One such approach, based on a continuum random field representation of heterogeneity, was developed for saturated as well as unsaturated groundwater flow systems [2]. Even in the absence of explicit fractures, the spatially random unsaturated flow model attains a high level of complexity, and tends to behave like a complex nonlinear system. Typically, the simulation results require a good deal of auxiliary analysis, both experimental and theoretical, in order to be properly understood and interpreted [2,3]. If more complex types of processes were included, e.g. multiphase and coupled hydro–thermo–mechanical processes, the overall model could become even more intricate. Although we are concerned here only with the case of partially saturated flow, note that the latter can be viewed as a special case of immiscible two–phase flow.

In an initial effort to evaluate certain aspects of the unsaturated flow modeling problem from a numerical viewpoint, a study was recently developed to examine the effects of nonlinearity on the stability and accuracy of numerical solutions, the interplay between capillary–driven and gravity–driven flow, and the convergence of nonlinear solution schemes in the case of homogeneous media [4]. The findings of this study outline the role of gravitational flow, which is expressed through a dimensionless Peclet number proportional to the slope a of the log–conductivity/pressure curve. The parameter $\lambda_c=1/a$ is essentially a capillary diffusivity length scale. The mesh size of a numerical flow model should be no larger than λ_c, which typically lies in the range 10–100 cm for sandy to clayey soils, but could be smaller for a fractured rock mass, and larger for the tight porous matrix of an intact rock mass.

Let us now consider the case where the unsaturated flow model explicitly incorporates detailed three–dimensional features of the heterogeneous geologic medium [2,3]. In the case of a continuum porous matrix with random heterogenity, previous theoretical analyses and high–resolution numerical experiments, reported in References 2 and 3, indicate that the effects of nonlinearity and heterogeneity are inextricably intertwined. This makes it difficult to analyze, not only the simulated flow processes, but also the numerical solution schemes themselves. Nevertheless, the accuracy of solutions can be evaluated ex–post using mass balance checks. Also, the large datasets generated by the numerical model can be processed graphically and confronted to other informations from field observations and/or theoretical studies. A specific application is discussed below.

A high–resolution, three–dimensional finite difference model based on a mixed variable formulation of partially saturated/unsaturated flow was used to model strip source infiltration and drainage in a randomly heterogeneous and imperfectly stratified soil [2,3]. The flow regime, soil properties, and boundary conditions, were selected to mimick (albeit some differences) the first Las Cruces strip source experiment, one of the test cases of INTRAVAL [5]. The nonlinear behavior and statistical properties of the soil were inferred, in part, from preliminary hydrodynamic data collected at the trench site. The 15 m x 15 m x 5 m computational domain was discretized into 300,000 cells, each with its own distinct unsaturated conductivity curve.

The transient moisture plume simulation is visualized with the aid of three–dimensional iso–surface and volumetric color graphics techniques. This approach provides direct evidence of moisture–dependent horizontal spreading, which lends credence to a previous theoretical finding based on linearized spectral perturbation solutions of stochastic unsaturated flow [6]. Moisture–dependent anisotropy is due to the imperfect, random layering of hydraulic soil properties. Such imperfect stratification is a pervasive feature of both consolidated and unconsolidated geologic media.

EFFECTIVE AND SUBSCALE MODELS OF UNSATURATED FLOW

While spatial variations of groundwater velocity are known to play a significant role in radionuclide transport and dispersion [1], there are obvious limits to how extensively and explicitly the broad spectrum of geologic heterogeneities can be represented in a flow model. In the first place, site–specific data are not likely to be available with the required degree of detail, so that much work must be put in auxiliary analyses — e.g. statistical interpolation and conditioning, use of soft information, auxiliary hydrodynamic models, hydrogeologic analogs, and so on. Secondly, the computational demands are likely to be high, which requires an informed evaluation of computational feasibility and a careful selection of advanced solution methods and supercomputer resources. The computational demands in the case of fractured porous media, with both continuum and discontinuum–type heterogeneity, are likely to be even higher owing to the extreme disparity of active fluctuation scales — from fracture aperture up to the largest identifiable geologic feature.

Alternative modeling approaches based on submodels may alleviate part of the above–mentioned demands. The main idea is to simplify the detailed flow model by subsuming some of its features in a black–box model. For instance, only macroscale features would be explicitly represented, while microscale to mesoscale heterogeneities and fractures would be subsumed in various subscale models, or submodels. The simplest types of submodels merely serve to express certain effective constitutive relationships, matrix/fracture transfer relationships, etc, in a quasi–analytical fashion.

Part of the modeling effort is thus transferred from the global model to the submodel(s). However, many questions regarding the conceptual/empirical basis of the submodels, their consistency with the global model, their intrinsic range of validity, and the identifiability of their internal parameters, must be fully answered before such submodels can be used with confidence.

A continuum submodel for the effective hydrodynamic properties of heterogeneous unsaturated media with anisotropic and/or fracture–like features is being developed. Briefly, the submodel starts with a general two–parameter random field model of unsaturated conductivity. Besides anisotropy due to stratification and/or preferred fracture orientation, the model also takes into account statistical cross–correlation between saturated conductivity and capillary diffusivity (λ_c – defined above). The statistical properties of the family of unsaturated curves are investigated analytically. This analysis reveals the existence of an upper envelope and of a dense crossing point. The latter occurs at a certain critical pressure which corresponds, roughly, to a local minimum of the effective conductivity anisotropy ratio as a function of pressure. Both the upper envelope and the crossing point of unsaturated conductivities depend significantly on the cross–correlation coefficient. These preliminary findings need to be further confirmed using simulations and field data analyses. Refinements of these and other similar concepts are being explored, with a view to applications to unsaturated flow in fractured/porous rocks.

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Use of a Submersible Pressure Outflow Cell for Determination of Moisture Characteristic Curves on Rock Core

Lorraine E. Flint, Raytheon Services Nevada
Alan L. Flint, U. S. Geological Survey

ABSTRACT

A simple device for developing moisture characteristic data curves, the submersible pressure outflow cell, was modified for application to rock core at matric potentials of 0 to -0.5 megapascals (MPa) and possibly to -1.0 Mpa. An automated system was developed to continuously and simultaneously collect data from many cells, obtain sorption and desorption characteristic curves to provide hysteretic information, and data from multi-step outflow experiments. The latter can be used to estimate unsaturated hydraulic conductivity. The system has resolved many of the problems inherent in standard measurement techniques. Model simulations of imbibition using the hysteretic data collected are in close agreement with laboratory measurements of imbibition, suggesting the moisture characteristic data correctly describes the core properties.

INTRODUCTION

Moisture characteristic curves are critical to the hydrologic characterization of unsaturated porous media. This paper describes the development of a method to obtain data needed to construct moisture characteristic curves for the unsaturated tuffaceous rocks at Yucca Mountain, Nevada, a potential site for the nation's first high-level nuclear waste repository. To understand and predict the magnitude and direction of the flow of water in the unsaturated zone, it is necessary to determine the unsaturated hydraulic conductivity of each rock type for a wide range of moisture potentials and saturations. The measurement of unsaturated hydraulic conductivity of low permeability materials is difficult, expensive and time consuming, but may be predicted from moisture characteristic curves (Brooks and Corey, 1964; van Genuchten, 1980; Flint and others, 1991). In addition, when curves are produced for sorption and desorption conditions it may be possible to glean understanding regarding wetting and drying histories of the rock if the moisture conditions of the rock were preserved when it was collected. Sorption curves are useful to relate hydrologic characteristics of the rock to natural conditions in the field such as infiltration (imbibition). It is also possible to calculate unsaturated hydraulic conductivity from multi-step outflow data if it is recorded with time and at known potentials (Stonestrom, 1987).

Many methods have been developed for the determination of moisture characteristic curves for soils, and some have been successfully adapted for use on rocks. There are advantages and disadvantages to each of the commonly used methods. For example, the centrifuge method is fairly rapid and has been found to provide sorption and desorption curves (Skuse, 1984), but often performs poorly at potentials above -0.1 megapascals (Mpa). Mercury porosimetry, which is also rapid, is destructive, and introduces errors due to differences between the contact angles of mercury and water with the porous media (Amyx and others, 1960). The vacuum cell or hanging water column is

simple and nondestructive but is limited to potentials above -0.1 Mpa. The psychrometer method can be used fairly quickly (Riggle and Slack, 1980), depending on the time required for moisture to become evenly distributed within the particular porous media, but is not very accurate at potentials above -0.2 MPa. In addition, measurements and calibrations must be performed under precisely controlled (+/- 0.01 C) temperature conditions.

The pressure plate method is useful at matric potentials above 0.5 MPa and has had several configurations developed for both sorption and desorption measurements (e.g. Tanner and Elrick, 1958). A common problem with these configurations is the accumulation of air bubbles in the water reservoir. This method has been shown to yield artificially high water contents (Madsen and others, 1986; Riggle and Slack, 1980) due to as nucleation of air bubbles during depressurization of the apparatus (Chahal and Yong, 1965), and hysteresis (Bouma and Dekker, 1984). The bubbles also may form in the water columns connecting the sample and the plate, causing the sample to stop draining. Peck (1969) provides a discussion of air entrapment in soil water. This method typically utilizes gravimetric measurements for water content determination, which require depressurization of the sample, or volumetric measurements, which need to be configured to control evaporation and can introduce uncertainty if there are bubbles under the plate.

The submersible pressure outflow cell (SPOC), a modification of the original Tempe pressure cell (Reginato and van Bavel, 1962), was developed to measure soil moisture characteristics and soil water diffusivity at a range of temperatures while the cell is suspended in a temperature controlled water bath (Constantz and Herkelrath, 1984). This method is being applied to rock core and has been modified to permit operation at lower matric potentials, while attempting to solve some of the above disadvantages of standard techniques. The SPOC method enables direct, simultaneous measurement of gravimetric water content and matric potential without disturbance of the core sample or the necessity to depressurize the vessel for water content determination.

During measurements, the SPOC is submersed in water, keeping the porous plate in contact with the water reservoir. This permits sorption and desorption measurements, which, using small pressure intervals between 0 and -0.3 MPa reduces the effect of nucleation of air bubbles, and allows for bubble equilibration (Peck, 1969) before the weight measurement.

MATERIALS AND METHODS

The developed SPOC measurement system is shown in Figure 1. The SPOC is constructed to be as light as possible for the best possible weight resolution, while still accommodating a 2.5-cm diameter core sample, which is the core diameter used by the petroleum industry for permeability measurements. The saturated core sample is placed on a slurry of diatomaceous earth on top of a saturated porous ceramic plate. A spring at the top of the cell presses the core sample against the porous plate. The cell is suspended in the water bath on its side at a slight angle to ensure the escape of any air bubbles that dissolve through the porous plate and also to allow any water collected during SPOC assembly to drain through the plate.

In the original design, quick disconnect fittings were used to detach the cell from the air supply and suspend it from a balance to record weight changes. This technique allows a slight pressure drop inside the SPOC and may cause hysteresis. The developed system can record the weight of each SPOC automatically without depressurization. The weight of each SPOC is measured using load cells, calibrated at different temperatures, and a datalogger. Laboratory temperature is measured and used to correct for any temperature sensitivity in the load cell calibrations. The weight of each SPOC is measured with a resolution of <0.1 g. The data from this modification is, however, not yet available.

Core samples from tuffaceous rocks at Yucca Mountain were used for measurements of moisture characterization curves (desorption only) (Flint and Flint, 1991) using the standard methodology of centrifugation and pressure plate. Measurements of sorption and desorption were made for comparison on the identical samples, using the SPOC. To illustrate the importance of hysteretic information and verify that the SPOC system gave realistic data, Flint and others (1991) used the numerical flow simulator TOUGH (Pruess, 1987) to predict imbibition from the moisture characteristic data collected using the SPOC system and a core sample from the Yucca Mountain Member and a gas drive relative permeability curve (Flint and Flint, 1991). The imbibition experiment (described in Flint and others, 1990) was conducted at a core saturation of 46.6 percent (approximately -0.4 MPa) which is in the data range of the SPOC, hence, the composite curve was not utilized in the simulation.

RESULTS AND DISCUSSION

Sorption and desorption measurements on selected nonwelded tuffs are shown in Figures 2a, b, and c. Figure 2a is from the Yucca Mountain Member of the Paintbrush Tuff nonwelded unit (Yucca Mountain Member) with a porosity of 42 percent. It shows a defined air entry potential at about 98 percent saturation, a hysteretic effect up to just less than -0.4 MPa, and a difference of 19 percent saturation in sorption and desorption values at zero potential. The sample in Figure 2b, from the tuffaceous beds of Calico Hills (Calico Hills) is devitrified and zeolitized and has a porosity of 34 percent. Air entry occurred at about 95 percent saturation, but it is not clear that all hysteretic effects are described within the -0.5 MPa range of measurement. Figure 2c is also a sample from the Calico Hills. It is zeolitized and has a porosity of 28 percent. Smaller pore sizes are evident as the air only just began to enter the rock within the measured range.

One limitation of this system is the inability to achieve potentials below -0.5 or -1.0 MPa. Potentials lower than this require a porous plate with such a small conductivity that it greatly extends the equilibration times between pressure steps. A possible solution for this is currently being tested which uses a porous cellulose membrane in place of the ceramic plate. The membrane has a saturated conductivity higher than that of the core. This enables the collection of useful outflow data during the pressure step increases as the moisture characteristic data is collected. This may reduce the time required for equilibration at each pressure step change, while extending the range. The extent of the potential measurement range is not yet determined but is at least -1.0 MPa.

Repeatability of the developed SPOC system is illustrated using two desorption/-sorption experiments on a single core sample from the Pah Canyon Member of the

Paintbrush nonwelded tuff unit (Pah Canyon Member) (Figure 3). The two sets of curves match each other very well. Figure 4 shows a comparison of data collected from the SPOC system with that collected on the same core sample using the standard pressure plate method (Klute, 1986) and the centrifuge method (Slobod and others, 1951). As often occurs, the core, when measured with the standard pressure plate method, was wetter at any given potential than the SPOC or centrifuge methods. The centrifuge data matches the desorption curve from the SPOC. Methods better describing moisture characteristics at lower potentials may be used in conjunction with the SPOC data to construct composite curves. This could be done with data collected using the centrifuge or psychrometer. The centrifuge method occasionally fails at very high potentials, however it may be reliable at potentials as low as -7.0 MPa. An example of a composite curve is shown in Figure 5 for a sample from the Yucca Mountain Member. The SPOC data describes the hysteretic characteristics to -0.6 MPa and the centrifuge extends the dataset where hysteresis is no longer apparent.

Another possible use for hysteretic information is in the determination of the wetting and drying history of a core sample taken from depth. The water content and matric potential of the sample are determined as received (indicating *in situ* conditions); then the sample is saturated and sorption and desorption curves are developed for the sample. The location of the measurement point of water content and potential as received, whether on a wetting or drying curve, or between them, may indicate if the sample was in a drying or wetting phase when *in situ*, or has been repeatedly wetting and drying.

Verification of the moisture characteristic data collected with the SPOC system was obtained by modeling imbibition (Figure 6) and resulted in predictions that closely matches the measured imbibition data. Data are fit to equations using the Brooks and Corey method (Brooks and Corey, 1964). The use of the sorption curve from the moisture characteristic data correctly reflects the reduced saturation at a given potential which then corresponds to a reduced conductivity and allows the model simulation to be more realistic. For more details on the analysis see Flint and others (1991), this volume.

SUMMARY AND CONCLUSIONS

The submersible pressure outflow cell (SPOC) was adapted for use on rock core, and an automated system was developed. It was shown to be successful in inexpensively collecting reliable, repeatable moisture characteristic data for nonwelded tuff samples. It is accurate at very high potentials allowing for determination of air entry values, but has only been used successfully thus far to approximately -1.0 MPa. Automation has allowed for a better determination of equilibrium and reduces operator time. If hysteresis appears to be less pronounced below the SPOC limits, a composite curve can be constructed using SPOC data at high potentials and data obtained by another method, such as the centrifuge method, could be used to extend the curve to lower potentials. It was shown that SPOC sorption data could be used successfully to model another hydrologic characteristic such as imbibition. Additional testing is currently underway to optimize the use of the SPOC for multi-step outflow experiments to calculate unsaturated hydraulic conductivity on rock core during the collection of moisture characteristic data.

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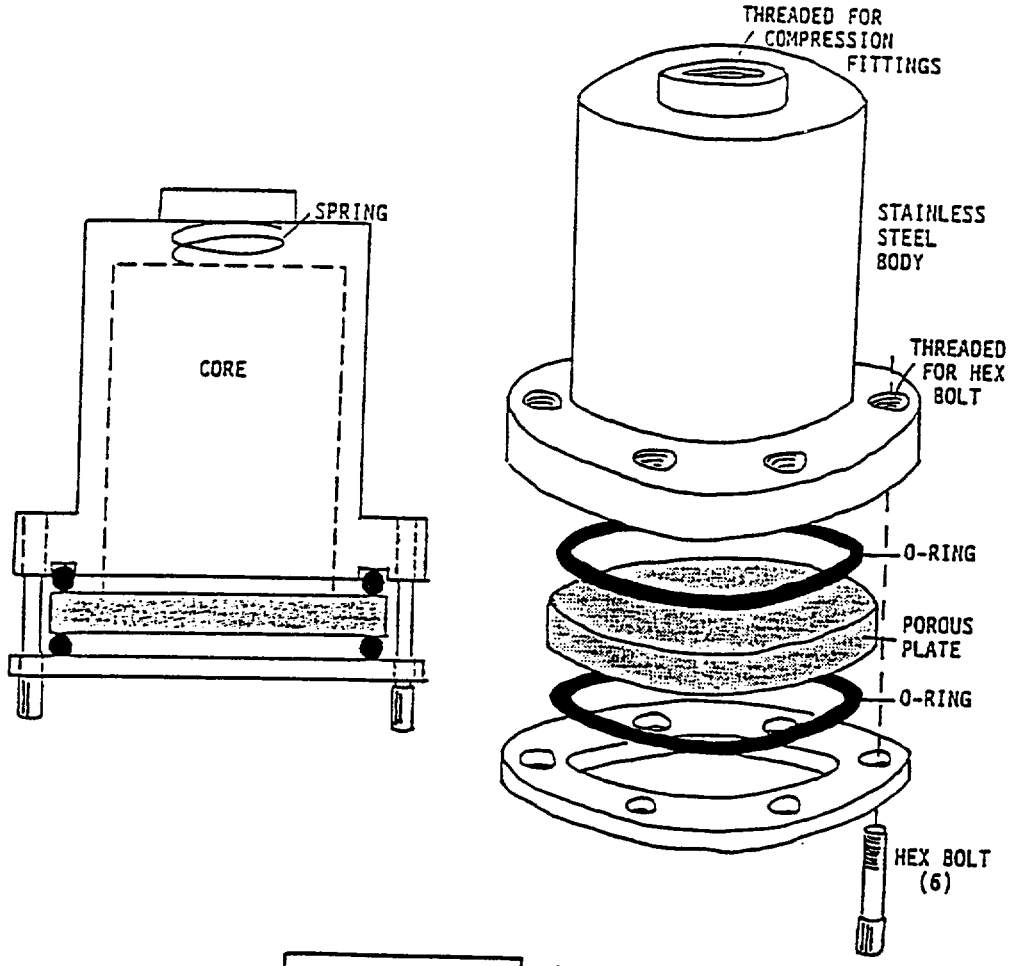
a)



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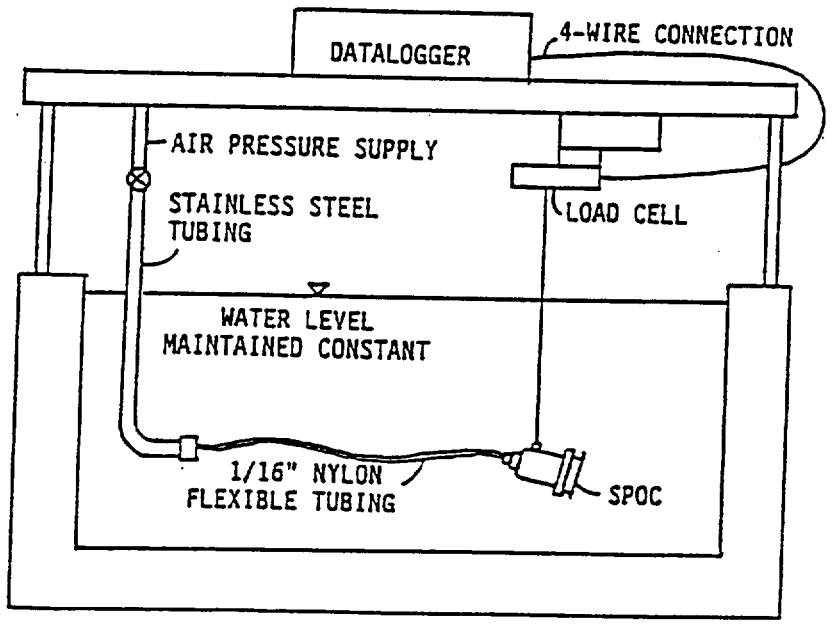

Figure 1- a) SPOC unit design, and b) design of automated measurement system.

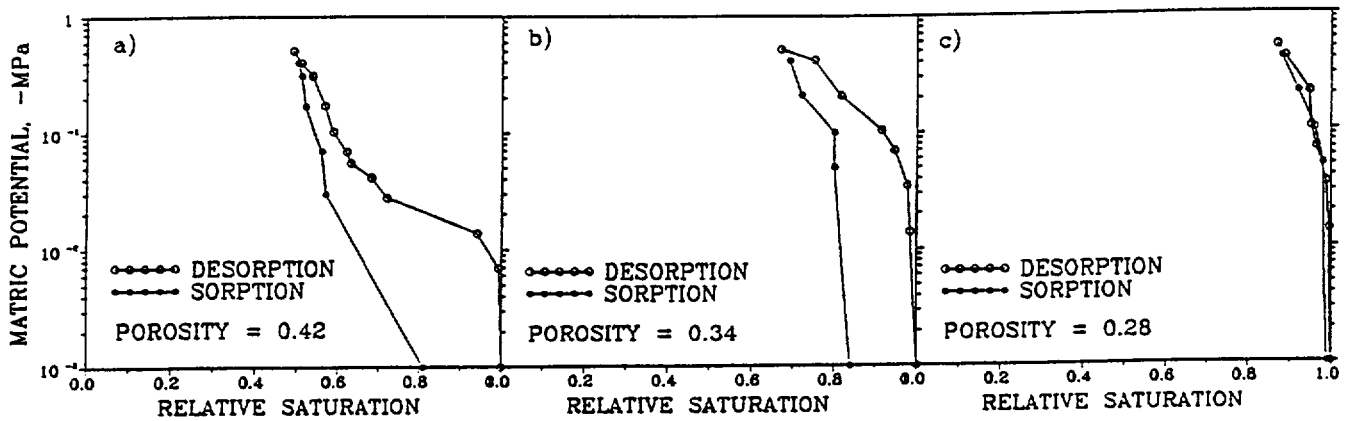

Figure 2- Moisture characteristic curves (desorption and sorption) using the SPOC for nonwelded cores from a) the Yucca Mountain member of the Paintbrush Tuff with a porosity of 0.42 cm^3/cm^3, b) Calico Hills, zeolitized, with a porosity of 0.34 cm^3/cm^3, and c) Calico Hills, zeolitized with a porosity of 0.28 cm^3/cm^3.

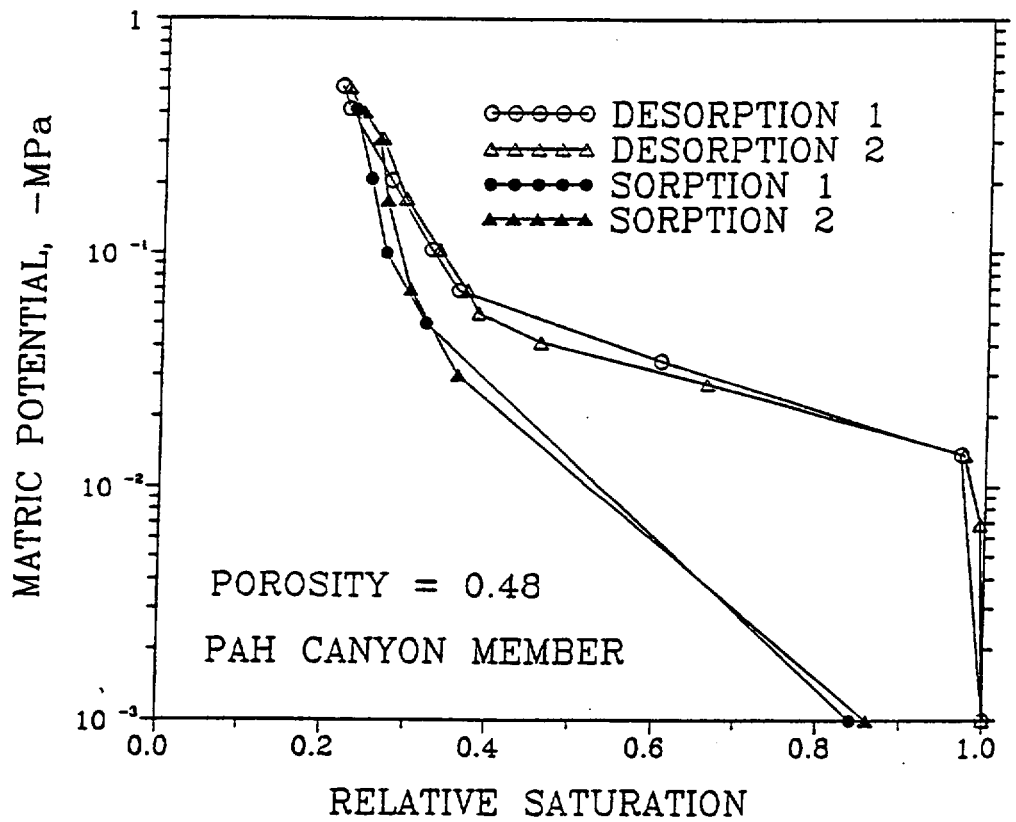

Figure 3- Repeatability shown from two determinations of desorption and sorption using one core from the Pah Canyon member of the Paintbrush Tuff with a porosity of 0.48 cm^3/cm^3.

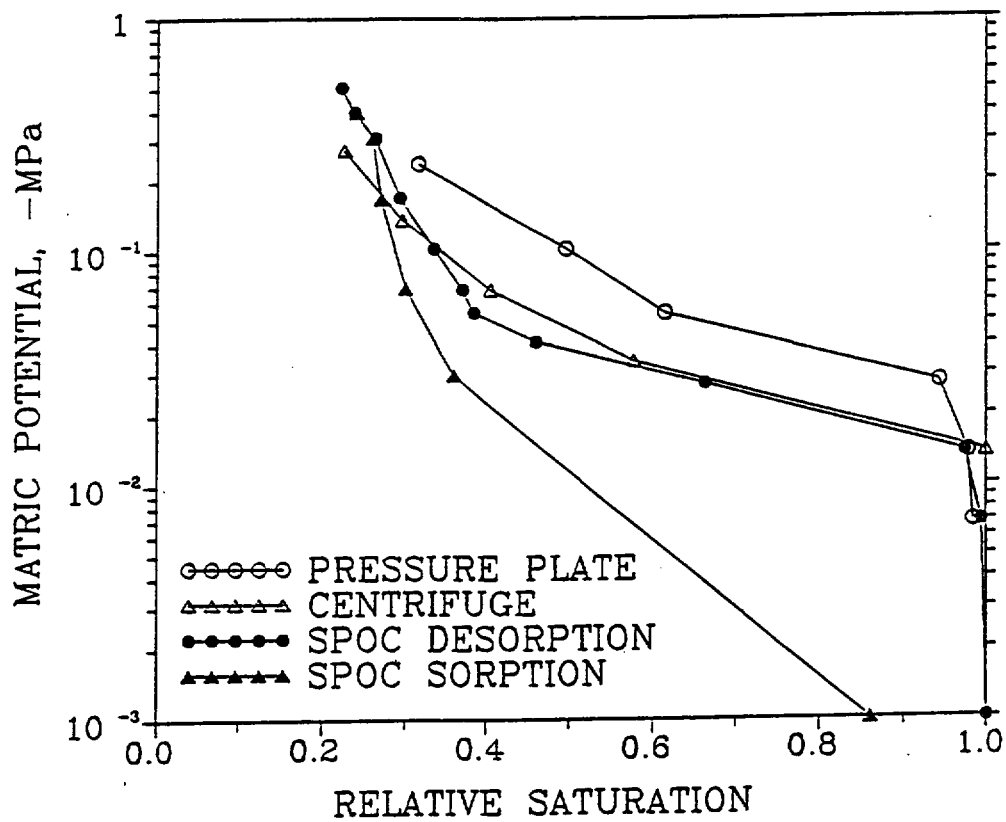

Figure 4- Comparison of SPOC desorption and sorption curves with desorption data collected on the same core (Pah Canyon, porosity 0.48 cm^3/cm^3) using centrifuge and standard pressure plate methods.

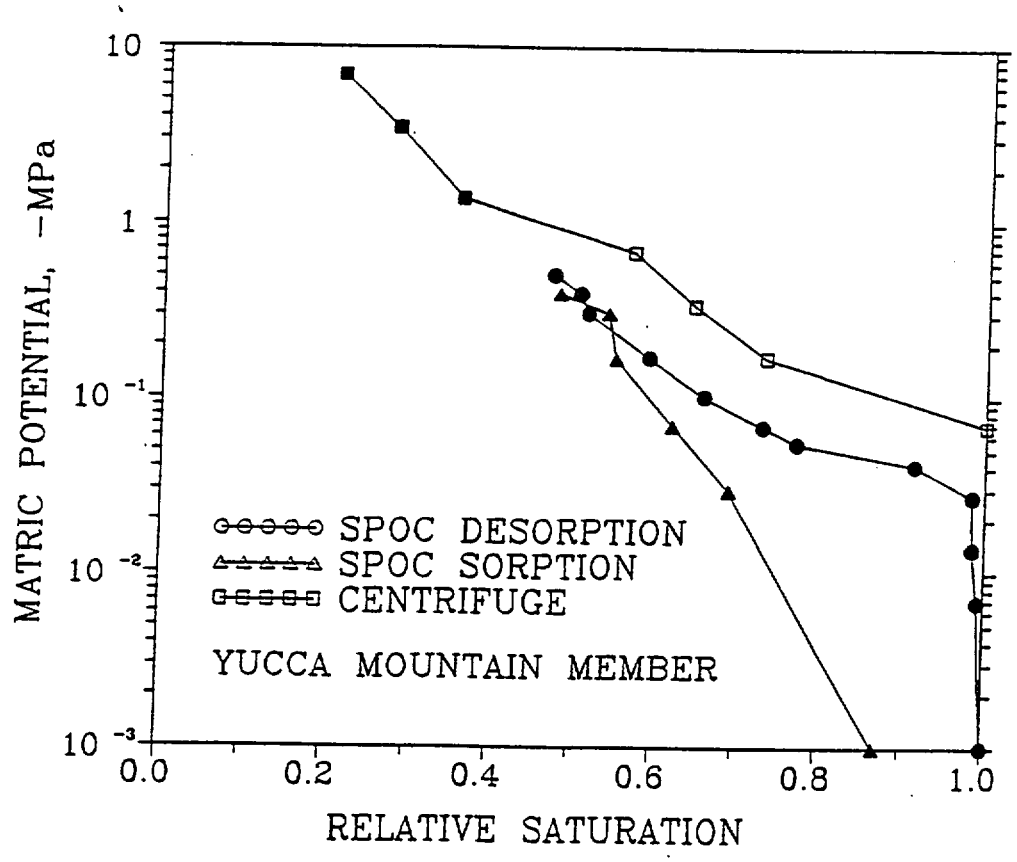

Figure 5- An example of a composite curve using centrifuge and SPOC data (Yucca Mountain member, porosity 0.31 cm^3/cm^3). Solid points are data used in the desorption and sorption composite.

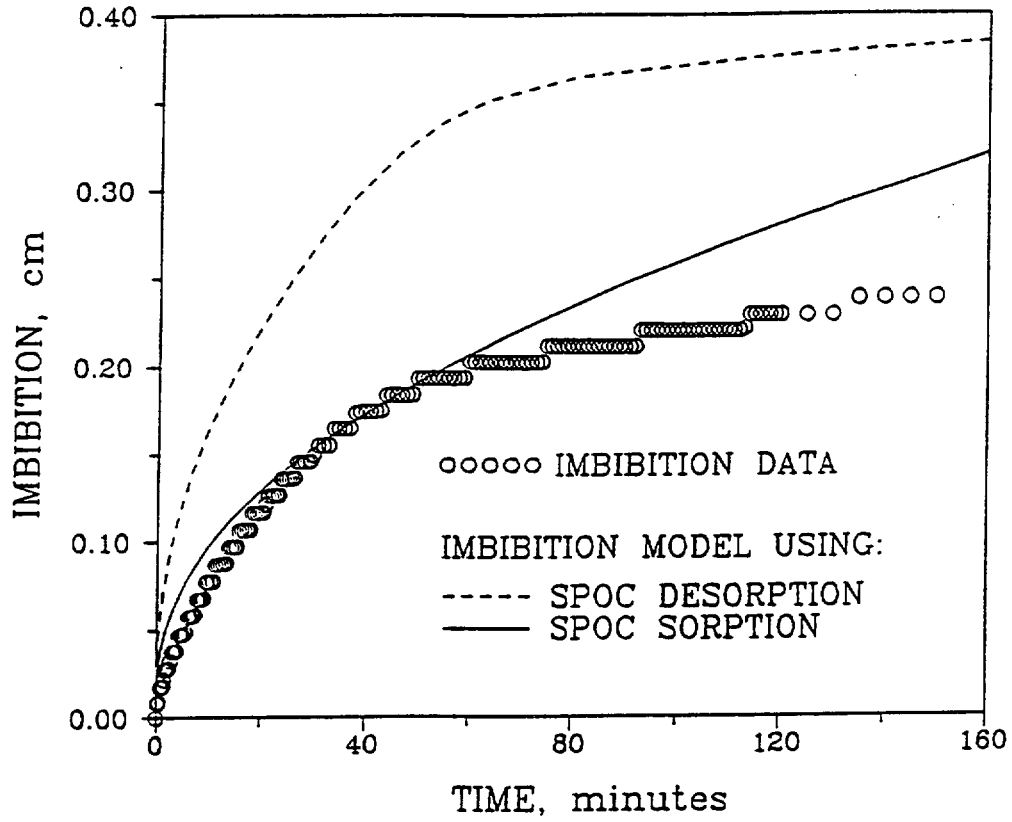

Figure 6- Imbibition modeled with curves fit using Brooks and Corey equation to sorption and desorption data in Figure 5 from SPOC only. Imbibition data is collected on same core sample.

Coupled Processes

Chin-Fu Tsang
Lawrence Berkeley Laboratory

Introduction

A nuclear waste repository emplaced in a geologic formation is a major perturbation to the system, inducing various hydrological, chemical, mechanical and thermal processes. Hydrological processes (H) include fluid flow and tracer transport through a rock joint and transient pore fluid pressure changes caused by changes of system conditions (such as those occurring during the operation of an injection or pumping well, or the construction of underground space). Chemical processes (C) include dissolution or precipitation of solutes in the fluid, interaction of the solutes with each other forming complexes or colloids, and interaction of the solutes with joint surfaces and joint infill materials. Mechanical processes (M) include dilation, shear, joint propagation, and fracturing at joint tips. Finally thermal processes (T) include changes of temperature and presence of transient temperature gradients.

These four different kinds of processes may be one-way coupled, i.e., the progress of one process affecting the progress of another, or fully coupled, i.e., the progress of one process affecting the progress of another and vice versa simultaneously. The coupled processes that result from such coupling may have significant impact on the performance of a nuclear waste geologic repository (Tsang, 1987), and on a more basic, local scale, are important for the understanding of the behavior of rock fractures (Tsang, 1990).

Coupled Behavior of Rock Fractures

If the rock medium in which a repository is constructed is homogeneous and of low permeability, it would be relatively straightforward to evaluate its suitability as a repository site. However, the rock medium is marked by fractures, which may form expedient flow paths for the leakage of radionuclides from the repository. Thus it is important to evaluate the role of fractures under the coupled processes of thermal output of the nuclear waste repository, hydrological flow around the repository, geochemical reactions of waste chemical with the medium and the induced mechanical stresses that may increase or decrease the fracture aperture.

Considerable theoretical and experimental work have been done on stress-flow relationship in single fractures in recent years (Gangi, 1978; Tsang and Witherspoon, 1981, 1983; Walsh, 1981; Barton, 1986; Gale, 1987; Pyrak-Nolte et al., 1987; Makurat et al., 1990). Many of these studies emphasized the variable-aperture nature of the rock joints in models of stress calculations. At the same time the observation of the so-called channeling effect for flow and transport observed in a series of field experiments by Neretnieks (1985, 1987) and Abelin et al., (1987) brought out the importance of incorporating the effect of variable apertures of rock joints in calculating flow and

solution transport. This has stimulated many hydrologic studies (Tsang, 1984; Tsang and Tsang, 1987, 1989, 1990; Brown, 1987; Moreno et al., 1988; Tsang et al., 1988; Pyrak-Nolte et al., 1988).

The picture that emerges from these studies may be briefly described as follows. Rock joints are considered to be two rock surfaces in the rock mass separated by the aperture, b(x,y) = 0. These are the contact areas or contact points. To determine the normal stress-flow relationship of the rock joint, one needs to calculate the flow rate through the joint under different mechanical stresses. First, mechanical stress-displacement relationship is calculated as the mechanical pressure averaged over the points of contact between the two surfaces that is needed to compress the asperities (Gangi, 1978) or deform the void spaces (Tsang and Witherspoon, 1981). Here asperities are the rock grains that protrude from the mean rock surface and come into contact with the opposite rock surface, and void spaces are aperture spaces between contact points. Then, the fluid flow and effective permeability are calculated for the two-dimensional aperture void space defined by b(x,y). Often detailed information of b(x,y) is not available and stochastic method has to be used (Moreno et al., 1988). Within this method one estimates the probability density function of aperture values, defined usually by two parameters, the mean and standard deviation of b values, and the spatial correlation length which describes the two-dimensional spatial structure of the apertures.

Because of the variable aperture nature of the rock joints, permeability to fluid flow is strongly controlled by regions where b is small (aperture constrictions), and flow has to seek paths of least resistance. Tsang and Tsang (1987) pointed out that flow channeling is very sensitive to normal stress, because an increase of stress with accompanying compression of the joint surfaces will proportionally reduce the b values much more at regions of aperture constrictions and in some instances completely close them off (b=0). Thus the flow channeling pattern in the joint place will be drastically changed. Evidence of such behavior is found in the highly stress-sensitive break-through curves of non-reactive tracers that have traveled with fluid through fractures under normal stresses.

Shear stress and fluid flow relationships are investigated by Makurat (1985), Barton (1986) and Makurat et al. (1990). Here the situation is much more complicated. Under low normal stress, shear strain may allow the asperities from the two rock surfaces to "climb on top of" each other, thus opening up the fracture aperture. This is the shear dilation of joints. Permeability increases of orders of magnitudes under shear were measured (Makurat, 1985). On the other hand, under high normal stresses or for relatively soft materials, shear force may deform and damage the asperities and the aperture distribution b(x,y) will be drastically changed. Hysteresis effects during cyclic loading may be a result of this phenomenon. Further laboratory and modeling work is needed to establish empirical relationships for different materials and different normal stress conditions (Makurat et al., 1990).

The above discussions are summarized in Figure 1 which shows schematically a two-dimensional rock fracture with variable apertures. The coupling between hydraulic and mechanical processes can be studied through the function b(x,y). In general the fracture

plane may be curved in the three-dimensional space, so that x and y are measured on that curved surface. Thus one has to relate b(x,y) to the conventional measure of joint roughness and joint matedness, and to study the modification of b(x,y) under normal or shear stresses. On the other hand the impact of such modifications on fluid flow has to be evaluated. Recent studies have shown that the impact can be very large on a local scale. Larger scale studies involving a statistical treatment of the local scale events may be a fruitful direction of research.

Thermal coupling may by added to the hydromechanical effects discussed above in a straightforward way. The usual practice is to assume that the quantity of water in the fracture is small so that it carries negligible thermal energy. Thus the calculation reduces to the simpler coupled thermo-mechanical rock behavior in the presence of fractures. The result of such a calculation will be changes in the principal stresses across the fracture, which in turn will affect the aperture b(x,y).

The hydromechanical processes related to variable-aperture fractures may also be found in situations where chemical reactions occur. If dissolution takes place, asperities may be reduced and the aperture distribution b(x,y) will be modified. On the other hand, if precipitation occurs because of chemical reactions, the precipitates may accumulate at aperture constrictions (small b regions) and clog up flow paths. New flow paths will develop. In the extreme case flow may be stopped and local fluid pressure will build up. Dissolution may occur because of the higher pressures and open up the flow paths again. However, the pressure buildup may also cause local fracturing dependent on local stress conditions and joint properties.

The channeled flow paths in the rock joints and the possible changes in flow paths due to stress variations or clogging effects may be significant factors in determining the degree of surface sorption and matrix diffusion of solutes. The limited flow paths imply that rock surface areas available for surface sorption and matrix diffusion may be only 10% or 20% of the total fracture surface area. Changing flow paths during the transport will allow new joint surface areas to be available for these processes.

Conclusion

The above discussion illustrates the inter-relationships of the T, H, M, C precesses and how the coupled processes may affect the flow and transport through fractures. To approach the study of rock fracture behavior from the view of coupled processes enables one to identify and focus on some of them which may be easily overlooked. Much work, both theoretical and experimental, still remains to be done in this area of research.

Acknowledgements

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Modeling Hydrothermal Flow in Variably Saturated, Fractured, Welded Tuff During the Prototype Engineered Barrier System Field Test of the Yucca Mountain Project

Thomas A. Buscheck and John J. Nitao

Earth Science Department

Lawrence Livermore National Laboratory

1. Introduction

The Yucca Mountain Project (YMP) of the U.S. Department of Energy (DOE) is investigating the suitability of the tuffaceous rocks occurring in the unsaturated zone at Yucca Mountain, Nevada for nuclear waste storage. The Engineered Barrier System Field Tests (EBSFT) will be conducted within the Topopah Spring member of the Paintbrush Tuff at Yucca Mountain, primarily to examine the thermohydrological response of the repository environment to thermal loading from waste packages (Yow, 1985). The Prototype Engineered Barrier System Field Test (PEBSFT) was carried out by Ramirez and others (1989, 1990) in G-Tunnel complex of the Nevada Test Site to test and evaluate components of the geophysical instrumentation network and to support the validation of thermohydrological models. This report describes the modeling of the PEBSFT carried out by Buscheck and Nitao (1990) with the V-TOUGH code (Nitao, 1989) which is a modified version of the TOUGH code (Pruess, 1987).

2. Discussion of Numerical Models, Physical Data and Assumptions

The Grouse Canyon member of the Belted Range tuff found in G-Tunnel consists of a highly fractured, densely welded tuff. In situ permeability testing found fractures to be major conduits for fluid flow (Ramirez and others, 1990) which are discretely accounted for in our fracture-matrix model (FMM). As such, we utilize distinct fracture and matrix properties considered to be applicable to Grouse Canyon tuff, including data obtained by Peters and others (1984) for Topopah Springs sample G4-6. Based on Zimmerman and Blanford (1986) we assumed an initial matrix saturation of 65 percent and a matrix porosity, ϕ_m of 20 percent. Based on permeability measurements and fracture surveys conducted by Ramirez and others (1989 and 1990), we assumed a fracture aperture, b of 100 μm and a fracture spacing, B of 0.3 m and determined the fracture permeability on the basis of the cubic law.

The FMM assumes an infinitely long, horizontal heater, orthogonally intersected by uniformly spaced fractures, with periodic boundaries along the symmetry planes down the center of the fracture and matrix, respectively, (Figure 1). With gravity neglected, the model is radially symmetric about the heater axis. Table 1 lists the numerical grid spacing. The heater is a 0.25-m-diameter heat generation cell with a three-stage heating schedule: (1) full-power at 1 kw/m ($0 < t < 4$ months), (2) a linear "rampdown" from full power to zero ($4 < t < 6$ months), and (3) no heating ($6 < t < 12$ months).

A comparison with the temperatures measured during the PEBSFT found the infinite heater assumption results in the FMM overpredicting temperatures. It is necessary to account for the finite heater length because heat flow around the heater is spherical (rather than radial as is assumed in the FMM). Due to the impracticality of discretely accounting for all of the fractures along the entire heater length, it was necessary to account for fractures with an equivalent continuum model (ECM). For situations in which the matrix and fractures are effectively in equilibrium, fracture and matrix properties may be volume-averaged with the bulk porosity, ϕ_b, bulk saturation, S_b, and bulk conductivity, K_b (either thermal or hydraulic) of the equivalent medium given by:

$$\phi_b = \phi_f + (1-\phi_f)\phi_m$$

$$S_b = \frac{S_f\phi_f + S_m(1-\phi_f)\phi_m}{\phi_f + (1-\phi_f)\phi_m}$$

$$K_b = K_m(1-\phi_f) + K_f\phi_f$$

where ϕ_m, S_m, ϕ_f, and S_f are the porosity and saturation of the matrix and fractures, respectively. In general, the ECM is appropriate for situations where the fracture spacing is small enough to result in a

negligible lag in the hydrothermal response in the matrix relative to that of the fractures. For the ECM we applied the actual PEBSFT heating schedule: (1) full-power at 1.12 kw/m ($0 < t < 128$ days), (2) a linear "rampdown" to zero power ($128 < t < 195$ days), and no heating ($t > 195$ days). Note that this only deviates slightly from the schedule used in the FMM. With gravity neglected, the model is radially symmetric about the heater axis and, due to the remoteness of the constant property boundaries, is axially symmetric about the midpoint of the heater. Table 2 lists the numerical grid spacing.

3. Discussion of Results

3.1 Fracture-Matrix Model

In addition to simulating the reference case, a parameter sensitivity study was carried out, investigating the following matrix properties: porosity, permeability, and initial saturation; and fracture properties: aperture, permeability, and spacing. The impact of vapor venting through the heater borehole to the access drift was investigated as well as the functional dependency of the rate of drying-out of the rock on the heating rate. For all cases, heat flow was found to be conduction-dominated, accounting for 86.9 percent of the total heat flow during the full-power stage in the reference case.

Drying of the matrix is seen to preferentially occur along the heater borehole wall and the fracture face (Figure 2). As in Figure 1, axial distance is with respect to the fracture midplane and radial distance is with respect to the heater axis. Due to the low matrix permeability, high gas-phase pressures are required to drive water vapor to the free faces (Figure 3). Upon reaching the fractures, most of the vapor is driven radially away from the boiling zone to the condensation zone where, due to the high suction potential, it is imbibed by the matrix. In cases where borehole venting was allowed, some vapor flows radially towards the heater and out to the access drift. During the full-power stage of the reference case, venting removed 38.5 percent of the moisture driven from the dried-out zone, thereby removing 5.0 percent of the cumulative thermal input. The volume of the dried-out zone was found to be proportional to $\sqrt{k_m}/B$ and $Q_h^{5/2}$ where Q_h is the heat generation rate per unit length of heater. For $b > 20\ \mu m$ the volume of the dried-out zone is insensitive to b. Therefore, for most of the fractures observed in G-Tunnel, flow resistance in the fractures is unlikely to throttle the rate of drying.

As the rock cools below boiling conditions, vapor flow, particularly along fractures, dominates re-wetting of the dried-out zone. Due to the large increase in vapor pressure, nearly all of the air has been driven away from the boiling zone. Condensation results in gas-phase pressures dropping below atmospheric, pulling vapor in towards the dried-out zone. In addition to the bulk flow of vapor, saturation gradients and the corresponding relative humidity gradients result in binary diffusion-driven vapor flow from wetter to drier regions, particularly along fractures. Upon reaching drier rock, this vapor condenses along fracture faces and is imbibed by the matrix. Because re-wetting is dominated by binary gas diffusion and capillary condensation along fractures, re-wetting is strongly dependent on the fracture distribution and connectivity, and is much less sensitive to fracture aperture and permeability.

3.2 Equivalent Continuum Model

In the rock the agreement between the ECM-predicted and the measured temperatures is outstanding (Figure 4). At the borehole wall, the ECM overpredicts temperatures (with a 7°C discrepancy at the end of full-power heating). This discrepancy is at least partly due to heat source itself. Both during the PEBSFT and benchtop testing of the heater, the top of the heater was observed to be approximately 40°C hotter than the bottom of the heater. The borehole temperatures in Figure 4 were measured at the bottom of the heater borehole. Had temperatures been measured on the upper borehole wall, it is likely that the predicted temperatures would be bracketed by the measured temperatures. The outstanding agreement between the predicted and measured temperatures is at least partly attributed to heat flow around the PEBSFT being dominated by conduction. Consequently, even though certain aspects (notably wetting behavior) of the fluid flow field are not well represented by the ECM, the temperature field is relatively insensitive to discrepancies between the predicted and actual heat convection behavior.

Figure 5 is a comparison of the predicted and measured radial saturation profile at the midpoint of the heater at the end of full-power heating. The measured profiles were obtained by neutron logging along two observation boreholes, ne2a (located above the heater) and ne6 (located below the heater).

For the dried-out zone, the agreement between the ECM and the measured data is quite good. Apparently, the assumption that flow resistance in the matrix is negligible holds reasonably well for drying. Conversely, this assumption (along with the assumption that gravity is negligible) results in a significant discrepancy between the predicted and observed wetting behavior. Because matrix imbibition is very slow relative to the time-scale of the PEBSFT, neglecting the time it takes for the matrix to imbibe the condensate, results in the ECM confining the saturation "halo" to a very tight interval. Saturation measurements showed a negligible increase in saturation beyond the boiling front. Moreover, temperatures measured along one side of the boiling zone indicated a region where two-phase conditions persisted, probably caused by gravity drainage of condensate from above. Figure 5 also indicates the impact of gravity drainage on drying behavior. Although temperatures above the heater were hotter than below, drying above the heater lagged behind drying below the heater. Above the heater, condensate drainage causes refluxing, thereby retarding the drying rate, while below the heater, condensate constantly drains away from the boiling front.

4. Conclusions

Using the V-TOUGH code the PEBSFT was modeled using two different conceptual models: (1) discretely representing the fracture and matrix properties (FMM) and (2) volume-averaging their properties through the use of an equivalent continuum model (ECM). Using the FMM, the distinct hydrothermal response of the fracture and matrix could be observed, along with some of the functional dependencies of drying and wetting behavior to various parameters, including heating rate. Heat flow was found to be dominated by conduction, with the explicit representation of the finite heater length (in the ECM) being crucial to obtaining a good match with the observed temperatures. While the ECM was found to adequately represent drying behavior, neglecting flow resistance in the matrix to imbibition and the effect of gravity on condensate drainage were found to result in significant discrepancies between predicted and observed wetting behavior.

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Table 1
Numerical Grid Spacing for the
45x26 R-Z Fracture/Matrix Model Mesh

Radial Direction, ΔR (m)							
0.125	0.025	0.05	18*0.1	10*0.2	2*0.3	0.4	4*0.5
1.0	2*2.0	2*4.0	10.	1.0×10^{-30}			
Vertical Direction, ΔZ (m)							
0.00005	0.0001	0.00015	0.00023	0.00034	0.00051	0.00076	0.00114
0.00171	0.00257	0.00386	0.00578	0.00867	12*0.01	0.00413	

Table 2
Numerical Grid Spacing for the
34x17 R-Z Equivalent Continuum Model Mesh

Radial Direction, ΔR (m)							
0.125	0.025	0.05	13*0.1	5*0.2	6*0.3	0.4	0.8
1.6	3.2	6.4	12.8	1.0×10^{-30}			
Vertical Direction, ΔZ (m)							
0.02	4*0.325	0.18	0.20	4*0.325	0.65	1.3	2.6
5.2	10.4	1.0×10^{-30}					

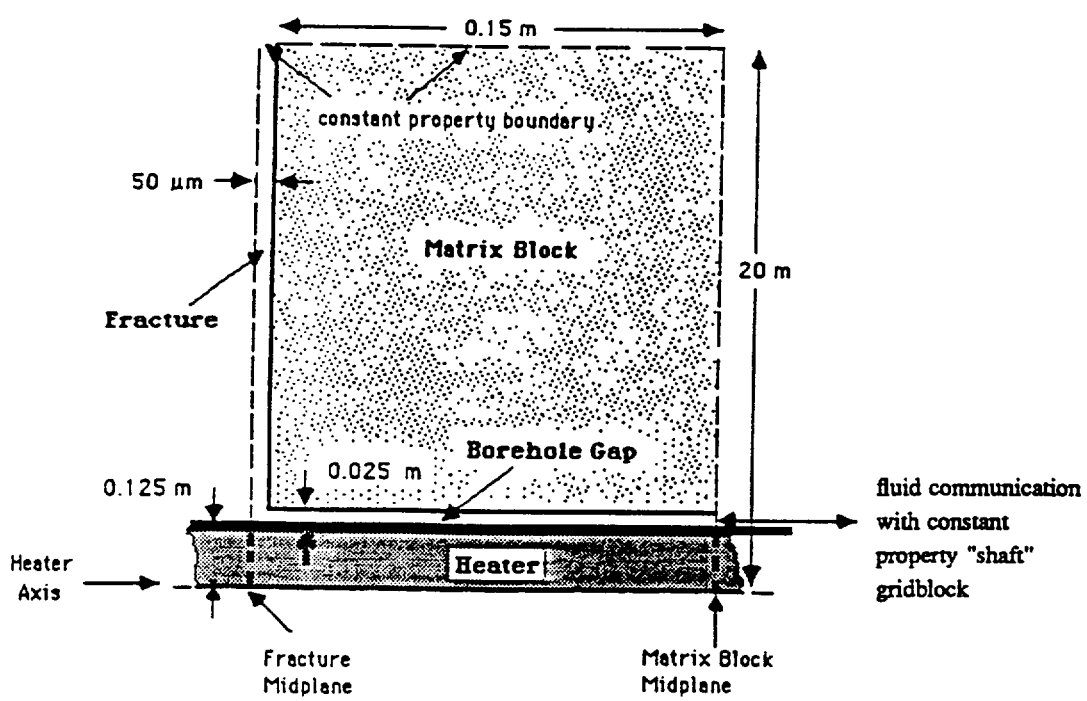

Figure 1. Schematic of the conceptual model used in the F/M model. Figure is not to scale.

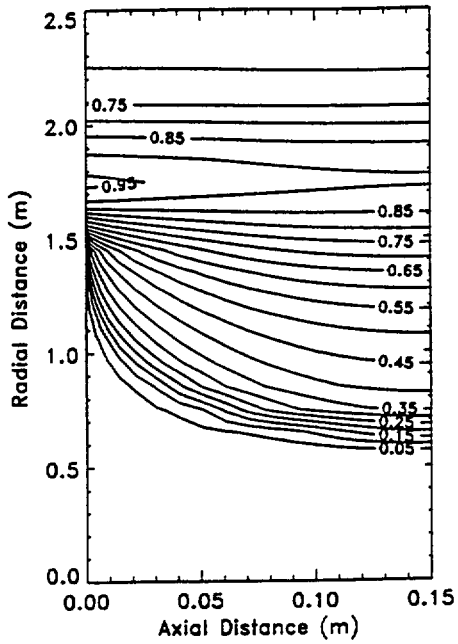

Figure 2. Contour plot of saturation at the end of full-power heating (t = 4 months) for the FMM. Axial distances are exaggerated by a factor of 10.

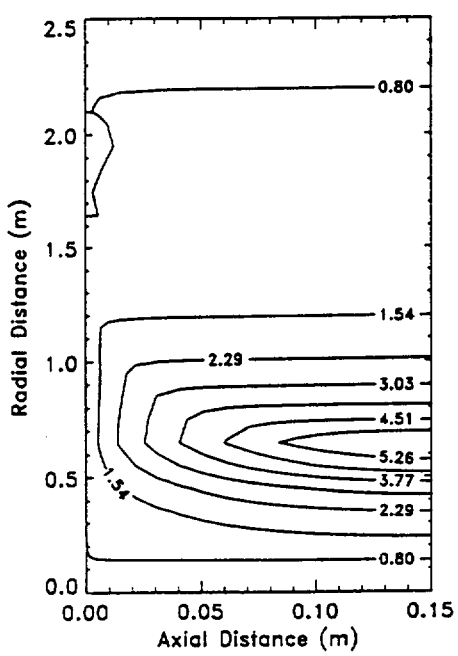

Figure 3. Contour plot of gas-phase pressure (*atm*) at the end of full-power heating (t = 4 months) for the FMM. Axial distances are exaggerated by a factor of 10.

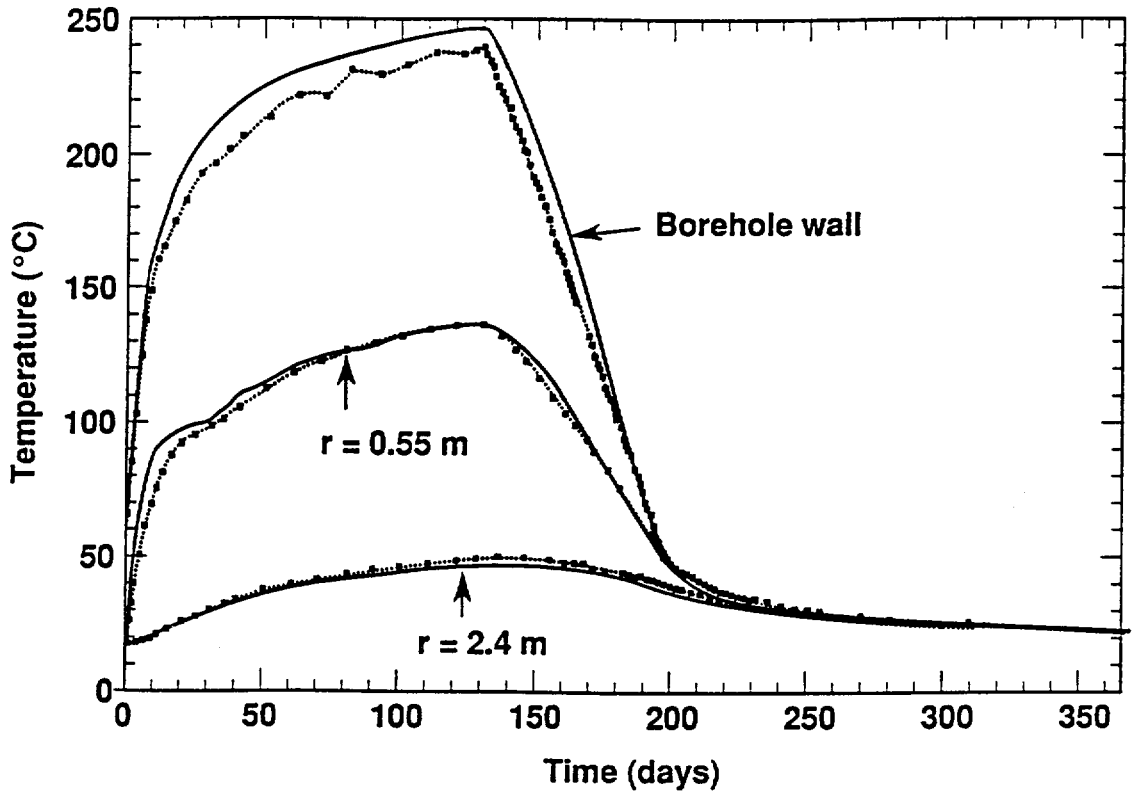

Figure 4. A comparison of the ECM-predicted (solid lines) and measured temperature history at three radial distances, located at the midpoint of the heater.

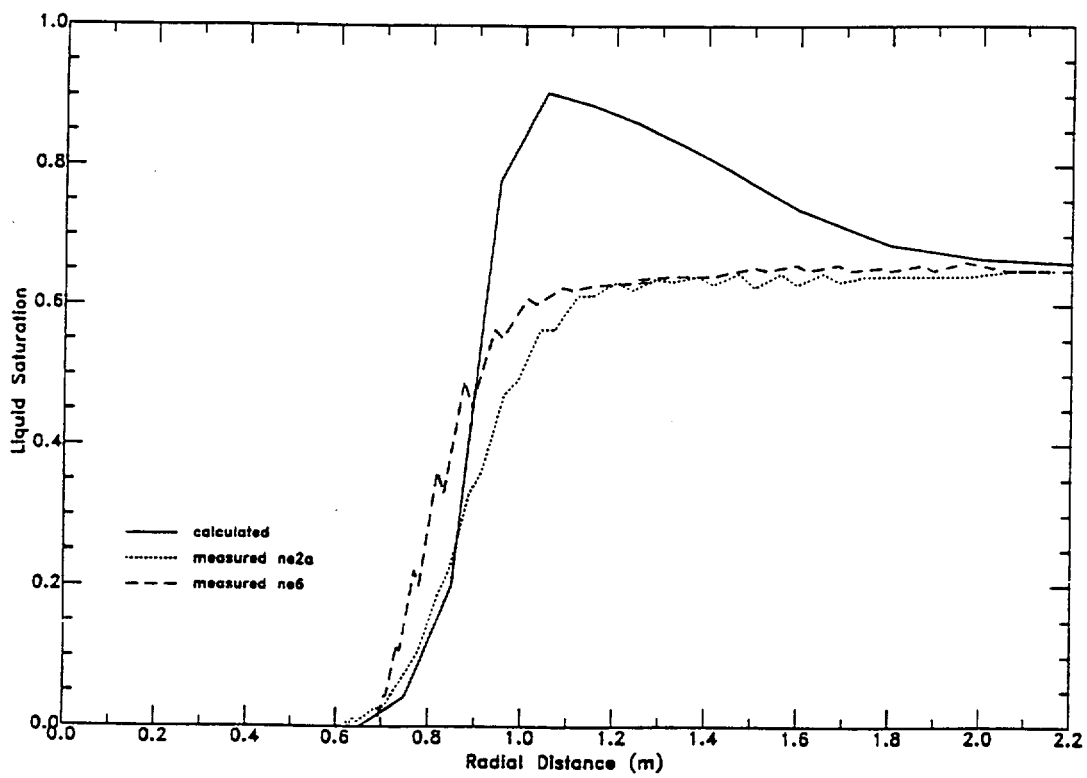

Figure 5. A comparison of the ECM-predicted and measured radial saturation profiles at the end of full-power heating (t = 128 days) at the midpoint of the heater.

A SURVEY OF HYDROTHERMAL MODELING RELATED TO YUCCA MOUNTAIN[1]

Rex G. Wescott
U.S. Nuclear Regulatory Commission

INTRODUCTION

Present design requirements call for the emplacement of approximately 62,000 metric tons of commercial reactor spent fuel and 8,000 metric tons of Defense and West Valley vitrified high level waste in a geologic repository (USDOE, 1988). The proposed underground repository at Yucca Mountain will cover an area of over two square miles and will have a design areal thermal power density of 57 kilo-watts per acre. Most of the initial decay heat is due to fission products, however long lived actinides and daughter elements will provide significant thermal output after the fission products have decayed to a steady but much lower thermal output level (USNRC, 1983). Depending on the container loadings and emplacement configuration, temperatures in excess of 100 deg. C can occur in the emplacement media and significantly higher temperatures can occur in the waste package. In that the host rock is partially saturated, water can significantly affect heat transfer near the waste package and possibly beyond the repository as well.

The purpose of this paper is to present a survey of various efforts involving hydrothermal modeling for the high-level waste repository at Yucca Mountain. These efforts are discussed according to the size or distance scale of modeling supported. The conclusion section presents the author's views as to how these various efforts may be used. Data and information needs are also outlined.

NEAR FIELD (WASTE PACKAGE SCALE)

Most waste package scale analyses which were performed to determine maximum package and emplacement hole temperatures used conventional heat transfer models. Heat transfer by conduction in the host rock and by natural convection and thermal radiation in the air gap surrounding the canister were generally assumed. Often, convection and thermal radiation through spaces are modeled using an equivalent thermal conductivity. Examples of conventional analyses include an analysis by O'Neil et al.

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[1]This paper was prepared by an employee of the United States Nuclear Regulatory Commission. It presents information that does not currently represent an agreed-upon staff position. The Nuclear Regulatory Commission has neither approved nor disapproved its technical content.

(1984), an analysis by St. John (1984), and the G-Tunnel small diameter heater experiments described by Blanford and Osnes (1987) and Zimmerman et al. (1986).

Modeling projects on the waste package scale designed to investigate multiphase heat transfer include the prototype engineered barrier system field test which was recently carried out in G-Tunnel (Buscheck and Nitao, 1990). In making the evaluations, a modified version of TOUGH (Pruess, 1987) was used to compare observed temperatures with both a discrete fracture matrix model and a equivalent continuum model.

Nuclear Regulatory Commission (NRC) sponsored research which may be applied to saturated flow at the waste package scale includes work carried out at the University of Delaware and later at Colorado State University by F.A. Kulacki. Examples of this research include papers by Prasad et al. (1986), Muralidhar and Kulacki (1986), and Muralidhar et al. (1986). Ongoing NRC sponsored research includes a thermohydrology project presently being conducted by the Center for Nuclear Waste Regulatory Analysis in San Antonio, Texas. This laboratory experiment simulates temperature driven unsaturated flow using plexiglass chambers and glass beads. Computer modeling work associated with this study includes simulations using a modified version of the TOUGH code (Green et al., 1990).

Moisture movement in a tuff core as a result of a temperature gradient was investigated by Bill Davies (1987) at the University of Arizona. A sensitivity analysis of saturation and temperature distribution in a drill core used by Davies was performed by NRC staff (McCartin et al., 1990) for the purpose of assessing the UAZ experiments and to assist in further experimental design.

NEAR FIELD (REPOSITORY SCALE)

Repository scale research includes those studies which were designed to investigate heat and moisture movement in and around the compartments and drifts of the repository.

Mondy et al. (1983) and Hopkins and Eaton (1987), separate SNL studies, investigated the effect of ventilation on repository temperatures and moisture removal from the host rock. In these studies, equations for conductive and convective heat transfer were coupled with equations for unsaturated flow.

Some of the previously cited NRC sponsored research under F.A. Kulacki at Colorado State University are considered in this paper as examples of repository scale hydrothermal modeling. These studies, Lai et al. (1988) and Prasad et al. (1986) used numerical modeling to calculate overall Nusselt Numbers and vertical velocities for various heater configurations and

Rayleigh Numbers.

There have been a number of publications regarding calculation of multiphase heat transfer on the repository scale using the TOUGH code. Some very recent publications by researchers at Lawrence Berkeley Laboratory describe and compare calculations made using the discrete fracture approach and the effective continuum approach (Pruess et al. 1990a, 1990b). Differing assumptions regarding liquid mobility in fractures are described and are found to greatly affect near field heat transfer. Some experimental work used to form the basis for mathematical models of the "heat-pipe" effect in geologic media has been described by Udell (1985).

FAR FIELD (REGIONAL SCALE)

Modeling of the far field effects of thermal influences is necessary to define the disturbed zone and to determine possible thermal effects on flow and radionuclide transport. Such influences may include vapor movement and thermal convection.

Studies of repository induced thermal convection in unsaturated media have been performed by Tsang and Pruess (1987) and by Pollock (1986). Tsang and Pruess used TOUGH (two-dimensions) and Pollock used a one-dimensional model. Results from both models were found to be dependent on the assumed downward moisture flux as well as other variables which have not yet been determined or bounded with certainty.

Calculations were also made by Richard Codell of NRC for a staff evaluation of the relative importance of heat transfer by moving groundwater in high-level nuclear waste repositories. These calculations considered heat transfer by forced convection and by natural convection in saturated media. The analysis concluded that heat transfer by convection is likely to be very small provided that vapor transport is neglected. Codell (1984) also constructed an analytical three dimensional model of far field temperature distribution based on a Green's function solution of the conduction problem and a convolution integration over time.

An NRC funded study by the Itasca Consulting Group, Inc. (Mark et al., 1989) investigated rock mass modifications around the repository due to thermal stresses. The results of this study included two-dimensional cross section figures showing areas of fracture aperture increase and decrease at different post closure times.

Studies have also been made on the effect of waste heat on geochemical processes. These studies include work by Braithwaite and Nimick (1984), Verma and Pruess (1986), and the Nuclear Regulatory Commission (USNRC, 1986). The Nuclear

Regulatory Commission also sponsored formation of a board of consultants chaired by Dr. Paul Witherspoon of the University of California, Berkeley. The board prepared two reports by Chin-Fu Tsang and Donald Mangold (1984, 1985) which discussed the present state of knowledge regarding coupled processes related to repository performance and also provided comments from board members.

COMPARISON OF MULTIPHASE HYDROTHERMAL MODELS

Detailed comparisons of multiphase hydrothermal codes have been made using problems with exact or numerical solutions or with experimental results. These include a study by Sandia National Laboratory (Updegraff, 1989) and an NRC in-house study (Codell and Ornstein, 1984). A comparison of hydrothermal codes developed or being developed prior to 1983 is presented by J.S.Y. Wang et al. (1983). A more recent review is presented by K. Pruess and J.S.Y. Wang (1987).

CONCLUSIONS

In the area of waste package scale modeling, a variety of models with varying sophistication have been used, often for specific purposes, such as comparison of emplacement schemes or configurations. Conventional heat transfer models may be expected to provide near field upper limit temperatures for a given configuration of disposal. Multiphase models, on the other hand, should be able to provide more realistic scenarios in regard to combined moisture and temperature effects on a waste package.

In regard to repository scale modeling, limits on release from the engineered barrier system (10 CFR 60.113) may require a reasonably sophisticated determination of radionuclide transport within the repository drifts and compartments. Any scenario which may result in both increased moisture flow into the repository and waste package failure during the initial period of high temperatures could require a significant modeling and research effort for accurate performance assessment. Models and approaches which may be applicable to this problem include results from laboratory scale model tests (to determine velocity fields under saturated conditions), as well as coupled multiphase flow and transport models. Simpler models without complete coupling may be useful to determine some boundary or initial conditions such as the extent of initial drying due to ventilation, for example.

Hydrothermal modeling on the regional scale will still require a better understanding of moisture flow paths below Yucca Mountain. Until these are understood, the travel times and pathways of any heat driven liquid or vapor flow will be uncertain. While maximum temperatures and temperature gradients

may be established with conventional heat conduction codes, the actual effects of heat induced mechanical and chemical changes on hydrologic parameters (such as hydraulic conductivity) may be considerably more difficult to predict and may require more sophisticated heat transfer modeling.

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NONISOTHERMAL LABORATORY AND NUMERICAL EXPERIMENT RESULTS

by
Ronald T. Green, Steve J. Svedeman, Ronald H. Martin
and Franklin T. Dodge
Center for Nuclear Waste Regulatory Analyses
Southwest Research Institute

I. Introduction

Thermohydrological processes as related to a high-level waste repository are investigated by performing non-isothermal experiments and analyses of partially-saturated media. The objective is to better understand the processes that contribute to the complex flow phenomena expected to be present near high-level waste emplaced in a geologic medium.

The preliminary results of two recent laboratory experiments have been analyzed. The laboratory experiments are vertically-oriented, two-dimensional chambers with a vertically-oriented simulated fracture. The experiment is non-isothermal with the vertical end plates maintained at different temperatures. Numerical simulations have been performed using a modified version of the TOUGH code. The intention of performing the simulation is to assist in investigating the thermohydrologic processes and to evaluate the theory incorporated into the TOUGH code.

II. Experimental Setup

A laboratory experiment, referred to as Test 5, was recently conducted. The apparatus consisted of a planar-shaped chamber with plexiglass side walls and aluminum ends of which the two opposing vertical ends were heat exchangers. The media consisted of a 50\50 mix of 40-micron and 80-micron diameter silica glass beads with pre-determined levels of water saturation. Located midway between the two heat exchangers and oriented vertically was a fracture simulated using a thin layer of 160-micron diameter glass beads. The test chamber used for Test 5 container had dimensions of 14.6 cm x 20.7 cm x 1.8 cm. The side walls of the container were insulated with 1.9 cm thick styrofoam to minimize heat loss and attendant fluctuations in temperature.

Moisture content, moisture movement and temperature were monitored during Test 5. A densitometer with a gamma-ray emitting ^{137}Cs source was used to detect differences in density as a measure of moisture content. Colored dyes were periodically injected into the medium through access ports in the side walls during the experiment. The movement of dye (and presumably moisture) was observed and recorded with photographs. Thermistors were installed in each of the heat exchangers to monitor the edge temperatures of the test chamber. The ambient temperature and pressure were monitored throughout the duration of the experiment. Although all ports into the test chambers

were closed so as to ensure a closed system, water in the form of vapor may have escaped from the test chamber.

The two vertically-oriented end plates contained heat exchangers whose temperatures were adjusted to impose a horizontal temperature gradient across the test chamber. The temperature differential between the end plates was 40°C (with the end plates at 20 and 60°C) for a temperature gradient of 2.7°C/cm. This imposed temperature gradient was reversed during the early stages of Test 5.

III. Experimental Results

The porosities of the bead media were calculated to be approximately 35%. The hydraulic characteristics of the test medium were measured by conducting a positive-pressure, porous-plate experiment (ASTM Method D 2325) on the glass beads. The van Genuchten parameters were determined by regression of the observed laboratory data (van Genuchten, 1978). Van Genuchten parameters were calculated for both the glass bead mix used in the matrix and for the larger-sized glass beads used to simulate the fracture. The calculated van Genuchten parameters for the bead mix and the larger-sized beads were similar: alpha = 0.7586 m^{-1} and n = 7.38 for the bead mix and alpha = 0.7405 m^{-1} and n = 7.42 for the larger sized beads in the fracture.

Although densitometer measurements correlated positively with moisture movement observed in the test chamber during the experiment, moisture content levels in the test chamber measured with the densitometer had insufficient resolution to be used quantitatively. Information that proved to be useful was photographs of the locations of the dyes injected into the medium in order to visibly track the movement of water.

Test 5 produced results of interest in two areas, both of which were associated with the nature of flow of water through porous media with a simulated fracture. The initial direction of dye flow next to the heated end plate was downward to the bottom of the container then toward the interior of the chamber until the simulated fracture was encountered. As evidenced by the dye, water did not cross the fracture. Rather, it moved upward thus forming what appeared to be a convection cell. The dye became too diluted beyond this point to be useful as an indicator of water flow direction or of the existence of the upper portion of the suspected convection cell.

The second observation of interest in Test 5 was the effect that the simulated fracture had upon flow within the test container. Water appeared to flow from the cool boundary up to but not across the fracture. Late in the experiment, after sufficient water had migrated to the cool side of the test container, the moisture content of the bead mixture medium next to the fracture became sufficiently high so that the relatively large-sized pores of the simulated fracture became saturated at

isolated locations and water appeared to traverse the fracture to the other side of the container. Photographs illustrating these two observations are presented in Figure 1.

IV. Simulation of Experiment Using TOUGH

A version of TOUGH that was adapted for use for the NRC has been further adapted for use at the CNWRA. TOUGH has been modified to facilitate data entry and interpretation of the simulation results. In particular, it has been the intention of these numerical exercises to evaluate the capabilities of TOUGH to simulate the two significant flow patterns observed in Test 5, the apparent formation of a convection cell and the reluctance to flow across the simulated fracture under partially-saturated conditions. Although the difficulty of simulating these complex processes has been documented (Runchal et al., 1985; Nitao and Buscheck, 1989; and Pruess et al., 1990), it is thought that such an assessment will provide valuable insight into the thermohydrological phenomena expected in the geologic medium near high-level waste.

The simulated medium is a vertically-oriented, two-dimensional (20.7 cm x 14.6 cm) grid with variably-sized elements that decrease in width proximal to the vertically-oriented, simulated fracture. The two vertical edges of the container are simulated as constant-temperature (20 and 60°C), no-flow boundaries and the two horizontal edges are treated as adiabatic, no-flow boundaries. The simulated fracture is vertically located approximately half-way between the two vertical edges.

The hydraulic characteristics of the matrix and the simulated fracture have been assigned values that approximate those of the media in Test. The permeability of the matrix and fracture are 1.2×10^{-14} m^2 and 1.2×10^{-12} m^2, respectively. The van Genuchten parameters of the matrix were the same as those determined experimentally. Several different sets of van Genuchten parameters were assigned to the fracture in an attempt to accurately portray the physical nature of the fracture relative to the matrix. Among these data sets were a prescribed set of values (alpha = 0.920 m^{-1} and n = 7.38) and a set of values from Peters et al., (1984) (alpha = 1.2851 m^{-1} and n = 4.23). The residual saturation was nominally set to 0.03 for these data sets.

V. Simulation Exercise Results

The experiment was simulated using the TOUGH code for different sets of hydraulic properties assigned to the fracture. The simulations were designed for a period of up to about 35 days, similar to the duration of Test 5. The simulated movement of water and water vapor for the different cases responded to the effect of the heated boundaries in a manner similar to what was observed in the laboratory. However, water and water vapor

movement has not been adequately simulated in the region near the fracture. Parameters that proved to be difficult to determine were the van Genuchten parameters assigned to the fracture elements. Close inspection of the fracture elements which were assigned the prescribed van Genuchten parameters revealed that the simulated fracture had liquid saturation levels greater than adjoining matrix elements. This is in contrast to what would be expected with respect to capillary forces and the relatively large-sized pores of the fracture.

The simulated fracture in a second set of simulations was assigned van Genuchten parameter values that were calculated for a fracture in tuffaceous materials (Peters et al., 1984). In these simulations, the fracture elements attained moisture contents that were lower than the adjoining matrix elements, as was observed in the laboratory experiments. Of interest was the observation that liquid water appeared to dam up on the side of the fracture closest to the heated boundary (Figure 2). Unfortunately, these simulations were computationally intensive and only about one-half day of the experiment was simulated.

VI Summary

Preliminary analyses using the numerical simulations have provided results with potentially important implications. The hydrologic effect of fractures in a partially-saturated, fractured porous medium is not entirely understood. Preliminary analyses of fractures investigated at a regional scale under isothermal conditions have indicated that partially-saturated fractures will not act as impediments to flow of liquid water from matrix block to matrix block if there is even a low level of connectivity between the blocks (e.g. 10 percent)(Buscheck and Nitao, 1990). However, preliminary analysis of the numerical simulation of the Test 5 case has provided results that have been interpreted to suggest that fractures proximal to heat-generating waste may respond differently than in an isothermal medium at a regional scale. Because fractures have lower air-entry levels than the pores in the matrix, they remained unsaturated for particular moisture contents while the adjoining matrix was essentially saturated. Consequently, as demonstrated in Test 5 and simulated with the TOUGH code, the movement of water vapor was not impeded by the presence of a fracture, however, the movement of liquid water was.

Based on these analyses and observations, the following scenario has been identified. A heat-pipe process will occur only in the matrix block nearest the heat-generating source during the early stages after waste emplacement. Heat will be more efficiently removed from the heat source by phase change resulting from the water vaporization, thus maintaining the temperature near the heat source near 100°C. As additional water is vaporized near the heat source and as the heat regime migrates into the medium, water vapor will be expected to move past the initial fracture and outward into the next matrix

block. The matrix block nearest the heat source will become desaturated as the return flow of liquid water in the outer matrix block is arrested by the presence of the fracture. Liquid water will only cross the fracture when the moisture content of the matrix adjacent to the fracture is sufficiently high (and the suction pressure is sufficiently low) to cause the fracture to saturate. Prior to this, the matrix block on the heated side of the fracture will desaturate thus denying the heat-pipe process the return flow of liquid water necessary to continue.

Without the removal of heat by phase change, temperatures at the heat source boundary will tend to increase. The same process was predicted by Pruess et al. (1985) in an investigation of the heat-pipe effect where liquid water was assumed to be immobile. The phenomenon of heat pipe collapse with associated elevated temperatures could be expected to migrate outward if multiple vertical fractures are present near the heat source. This phenomenon has been investigated in only limited laboratory and numerical experiments and requires additional investigation to be verified.

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Figure 1. Photographs of the test chamber at days 7, 14 and 23 (left to right) of Test 5. Dye movement was downward at day 7, to the right (toward the heated half of the chamber) at day 14 and upward at day 23. Note that there is no indication that the dye (and associated liquid water) crossed the fracture in these photographs.

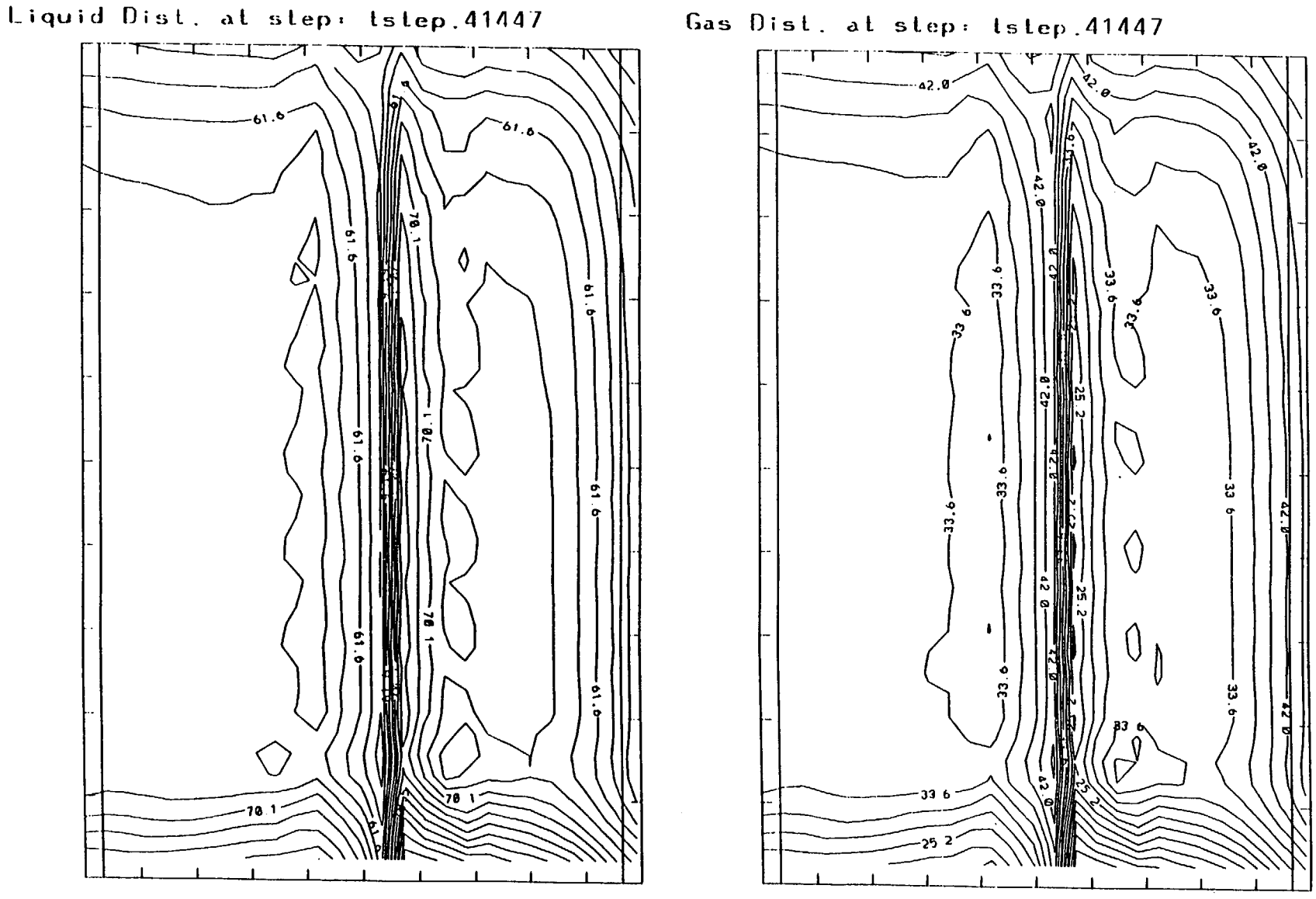

Figure 2. Simulations of gas and liquid concentrations at 41447 seconds (approximately one-half day).

FLOW THROUGH NONHOMOGENEOUS POROUS MEDIA*

Roger R. Eaton, Ronald C.Dykhuizen, and Katherine M. Hansen
Sandia National Laboratories

ABSTRACT

Modeling studies were conducted to determine the effects of material heterogeneities on the flow of water through rock. Multiple numerical calculations were made using random variations in spatial distributions of material properties. The results of these material variations on flow resistance, mechanical dispersion, and channeling were determined. Computed results were compared with a linear analytical model. Good agreement was obtained in the majority of the flow cases investigated.

INTRODUCTION

Yucca Mountain, located in southwestern Nevada, is the site for a proposed high-level nuclear waste repository. The hydrologic units at Yucca Mountain appear to have quite different material characteristics.[1] Additionally, measurements show that the material properties within each hydrologic unit vary significantly. Rock core samples taken from this site indicate that the volcanic tuff is highly fractured and nonhomogeneous. Numerical modeling has been used to study the water infiltration from the ground surface, past the location of the proposed repository, to the underlying water table. Because the material characteristics used in the modeling result in nonlinear partial differential equations, multidimensional computations can be computer-time intensive. Consequently, the majority of the calculations made to date have been made using one-dimensional geometries. It is anticipated that the flow could be significantly influenced by the heterogeneities of the rock, and one-dimensional calculations may not yield accurate flow predictions.

The purpose of this study is to investigate the effect of uncorrelated rock heterogeneities on predominately one-dimensional water flow through partially saturated rock. This is modeled by computing multiple realizations of two-dimensional Darcy flow through rock whose randomly assigned saturated hydraulic conductivities vary in space by as much as four orders of magnitude. This work is the first step towards our ultimate goal of determining effective material property values that can be used in one-dimensional calculations to give accurate flow predictions in multi-dimensional nonhomogeneous regions.

Numerous studies have been reported in the literature that are applicable for the related saturated flow problem (linear systems).[2,3,4,5] Calculations for partially saturated flow are more difficult and consequently have received considerably less attention. For unsaturated cases, material characteristics, such as conductivity and moisture capacitance, can vary by several orders of magnitude over the problem domain. Eaton and Dykhuizen calculated the effect of a single impermeable obstruction on the partially saturated flow around the obstruction.[6] That study concluded that the nonlinearity of the material characteristics significantly reduced the effect of the impermeable region on the overall flow rate.

The current work extends earlier studies to include randomly-distributed low-conductivity two-dimensional regions and allows for the effect of nonlinear material properties. A procedure is proposed for predicting effective material conductivities for a range of material mixes.

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It was found that the numerical results agree well with Kirkpatrick's analytic approximation for the effect of random inhomogenities in materials with constant properties.[2]

PROBLEM FORMULATION

It has been proposed that the underground nuclear waste repository be placed in the Topopah Spring unit. This study is limited to meter-scale investigations in that unit. For the purpose of this exercise it was assumed that the rock within this layer was interlaced with randomly located cells having lower-than-average hydraulic conductivities. One such set of random distributions is shown in Figure 1 for low conductivity regions extending over 25, 50 and 75% of the total area.

Material Properties

Material property values were taken from the recent PACE-90 study repository unit.[7] The value given in the PACE-90 study for saturated hydraulic conductivity, $K_s = 2 \times 10^{-11}$ m/s, was assigned to the high conductivity (nonhatched) regions shown in Figure 1. The value of hydraulic conductivity arbitrarily assigned to the low conductivity (hatched) regions was between one and three orders of magnitude smaller. Values of alpha and beta required by the van Genuchten[8] and Mualem[9] models to define matrix conductivity and saturation as a function of pore pressure, were 0.01 1/m and 1.7, respectively. The matrix porosity was 0.12. Both the low and high conductivity regions were assumed to be fractured and the fractures to be full of sand-like material with a saturated conductivity of 4×10^{-5} m/s. The matrix/fracture material properties were area weighted. Values of alpha and beta for the fractures were 1.285 1/m and 4.23, respectively. The fracture density was 3×10^{-5}.

Numerical formulation

Numerical solutions were obtained by solving Richards equation.[10] which describes the isothermal flow of water through porous media. Steady-state numerical solutions were obtained using a finite-difference, two-dimensional method-of-lines code. Spatial derivatives were approximated using first order finite differences. The resulting matrix of ordinary differential equations in time were solved using routines developed by Shampine and Watts.[11] The code is well suited for calculating flows through media whose material characteristics are extremely nonlinear. Numerical meshes as large as 64×64 were used (see Figure 1 where the small squares show the size of the mesh grid spacing). A single run using a 64×64 mesh required approximately 5 minutes of computer time on the Cray-XMP.

Linear Case

Although the material properties and boundary conditions used in this study result in nonlinear solutions, it was useful to compare these results with averaging methods for the linear case. Many equations have been proposed to find average conductivities that falls between the limiting cases of arithmetic and harmonic averaging.[3] Kirkpatrick provides a power averaging for random geometric mixtures of materials which falls between arithmetic and harmonic averaging for materials with constant conductivities.[2] Kirkpatrick presented the following transcendental equation for approximating the effective conductivity of a random mesh of resistors:

$$\int_0^{+\infty} \frac{(K_e - K)f(K)}{(c/2 - 1)K_e + K} dk = 0$$

where K_e is the effective conductivity, $f(K)$ is the probability density function for the conductivity, and c is the connectivity of the resistor mesh. For a continuous region, the connectivity is twice the number of dimensions. This allows use of this averaging equation for one, two and three dimensional continuum problems.

It was assumed in deriving the above equation that the medium is of infinite extent and has the various conductivity levels distributed randomly. When these conditions are met, the equation has been demonstrated to be reasonably accurate by Kirkpatrick,[2] Burganos and Sotirchos.[5]

RESULTS

The primary indicator of the effect of material heterogeneities is the change of flow rate as reflected by effective conductivity, K_{eff}. This is defined as the equivalent conductivity for one-dimensional flow and is given by

$$K_{eff} = q_y \times (y_{top} - y_{bottom})/(P_{top} - P_{bottom}),$$

where q_y = vertical mass flux, $y_{top} - y_{bottom}$ = vertical length of numerical grid, and $P_{top} - P_{bottom}$ = pressure drop across the grid in the y direction.

The prescribed pressure drop across the region, $P_{top} - P_{bottom}$, was held constant for all runs. It was determined from a baseline run using all high conductivity material (zero mix) with a 0.01 mm/yr flux applied at the top boundary. The bottom boundary pressure was fixed such that the saturation equaled 0.88. This is consistent with the nominal PACE-90 case.[7]

To obtain a reasonable conductivity ratio for use in the random material mix investigations, a set of calculations was run using a single obstruction with a range of conductivity ratios, Figure 2. The conductivity of the obstruction was varied from 2×10^{-14} to 2×10^{-11} m/s. Figure 2 shows the resulting pathlines. The calculations show that to reduce the flow of water, the reduction of the obstruction's conductivity by one order of magnitude is almost as effective as a reduction of three orders of magnitude. For example, the reduction of conductivity by one order of magnitude reduced the through flux by 30%, while reducing the conductivity by three orders reduced the flow by 39%. The remainder of the calculations made in this study were made using a conductivity ratio of 1000.

Effect of Mesh Size

In order to compute realistic two-dimensional results, the minimum resolution of a cell was determined, that is, the minimum number of computation mesh points for each cell of low or high conductivity material. This was approximated by making a series of runs using the four region geometry shown in Figure 3 and varying the number of mesh points per region from two to 64. Effective conductivities resulting from cell refinement is shown in Figure 4. Because of the preliminary nature of this study and the anticipated computer time requirements, it was decided that 16 mesh points per cell would give adequate resolution.

A second investigation was made in which the resolution per cell was held constant at 16 node points, while the total number of cells in the entire region was varied from four to 256. The effective conductivity was nearly constant for meshes greater than 32×32 (64 cells), Figure 5. The balance of the two-dimensional calculations was made using a 64×64 mesh (256 cells). For this mesh resolution it was found that the mean effective conductivity

for 15 runs and 20 runs varied less than than 15%. Therefore, the results of 20 realizations were averaged for each mix considered in the following investigations to obtain the mean effective conductivities.

Effect of Conductivity Mix

The effect of the material mix on effective conductivity was obtained by making a series of runs in which the percent of high conductivity material was varied from 0 to 100% in seven steps. Multiple realizations were computed at each mix by randomly locating the low conductivity regions on the numerical grid. The resulting mean effective conductivities obtained from averaging the effective conductivity calculated for 20 runs at each mix are given in Figure 6. The range of the values at each mix is also given. The two highest values and the two lowest values are not included in the plot resulting in 80% confidence intervals. A single run was used for the 0 and the 100% mixes since they only involved a single material. Also shown on Figure 6 are the results of Kirkpatrick's analytical solution.

The analytical and numerical results are within a factor of three. Error bars are reasonably small except near the 50% mix. Our finite-size domain yields quite diverse results depending upon an occurrence of a continuous path through the domain that avoids the low conductivity material. Thus, bimodal distributions of effective conductivities were found. Even though the error bar is large compared to the mean, the average of the effective conductivities for the 20 runs is in reasonable agreement with Kirkpatrick's analytical approximation.

The random distributions of the flow obstructions give the flow a tortuous path, as shown by pathlines given in Figure 7. The starting locations of the flow paths are specified to give even increments of mass flow between adjacent pathlines. Flow channeling for the distributions calculated is most prominent for mixes in the 50% range. Mechanical dispersion of the flow was most dominate for the 50% cases. The ratios of the maximum to the minimum particle path travel times was approximately ten.

SUMMARY OF RESULTS AND CONCLUSIONS

A conceptual understanding of the effect of material heterogeneities on the flow of water through hard rock has been obtained through the use of multiple realizations of the Richards equation for materials randomly located within a meter-scale region. For a large range of material mixes the effective conductivities obtained using Kirkpatrick's analytical solution and those obtained from numerical results were in good agreement. The poorest agreement occurred for material mixes in the 50% range. The 50% mix also tends to result in noticeable flow channeling and the largest mechanical dispersion based on maximum and minimum particle pathline travel times. For the types of geometries and material mixes considered in this study, two-dimensional flow can be reasonably approximated using one-dimensional calculations and the effective conductivity obtained from Kirkpatrick's theory.

FUTURE WORK

In order to further evaluate the feasibility of using effective conductivities in numerical calculations, it will be necessary to gain a better understanding of the Yucca Mountain geometry and in particular to determine the extent to which low-conductivity cells and other heterogeneities might exist in the various geologic regions. Currently numerous investigations are being done by Rautman,[12] in which the mountain is being statistically analyzed using existing drill hole data. Specifically, he is studying a single correlated variable to demonstrate dispersion of travel times. The incorporation of the results of these statistical investigations into an analysis procedure given herein should provide additional insight into

the development of improved computational procedures for Yucca Mountain.

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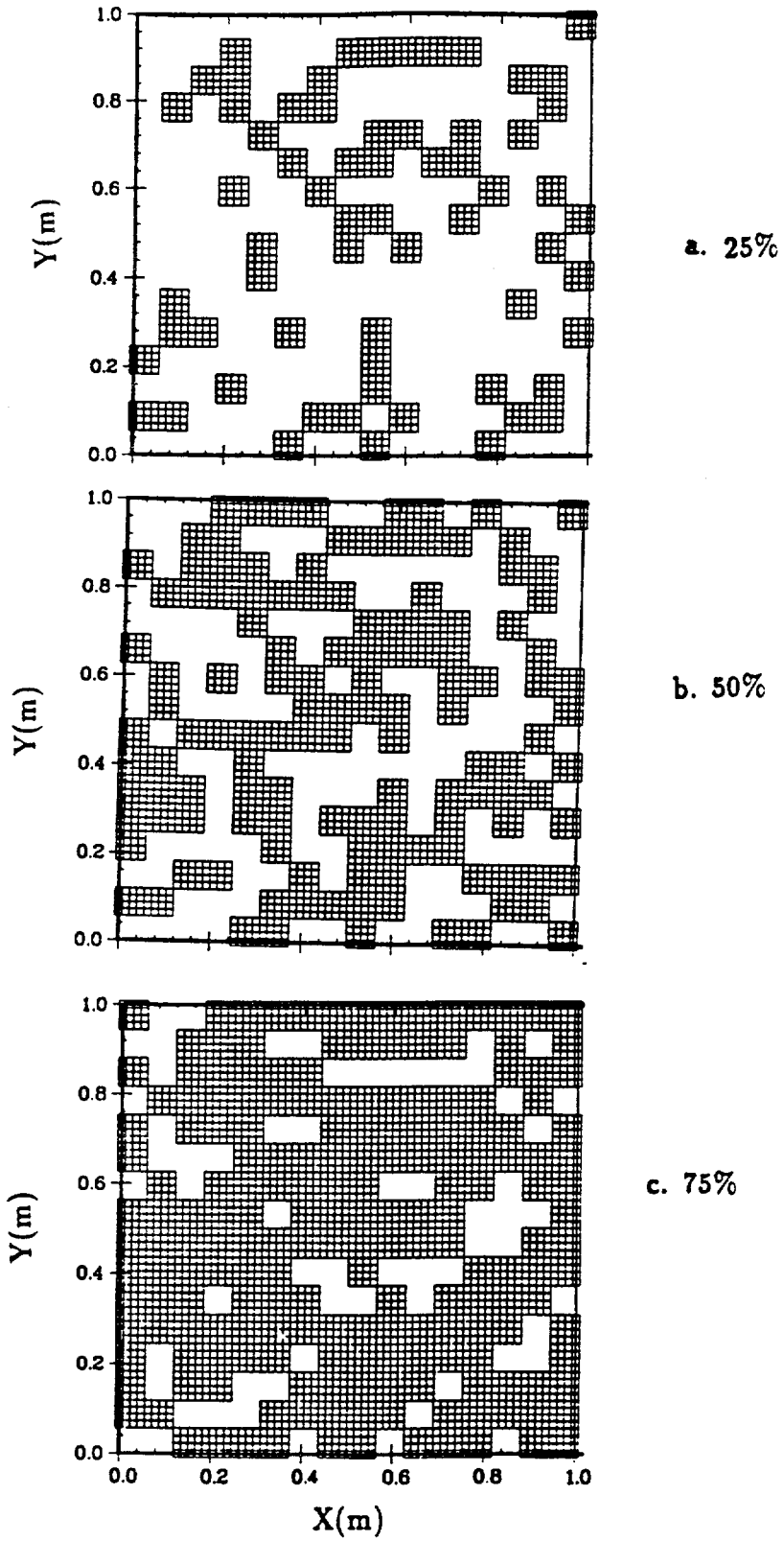

Figure 1: RANDOM DISTRIBUTIONS OF LOW CONDUCTIVITY. MATERIAL: a. 25%, b. 50%, c. 75% mix.

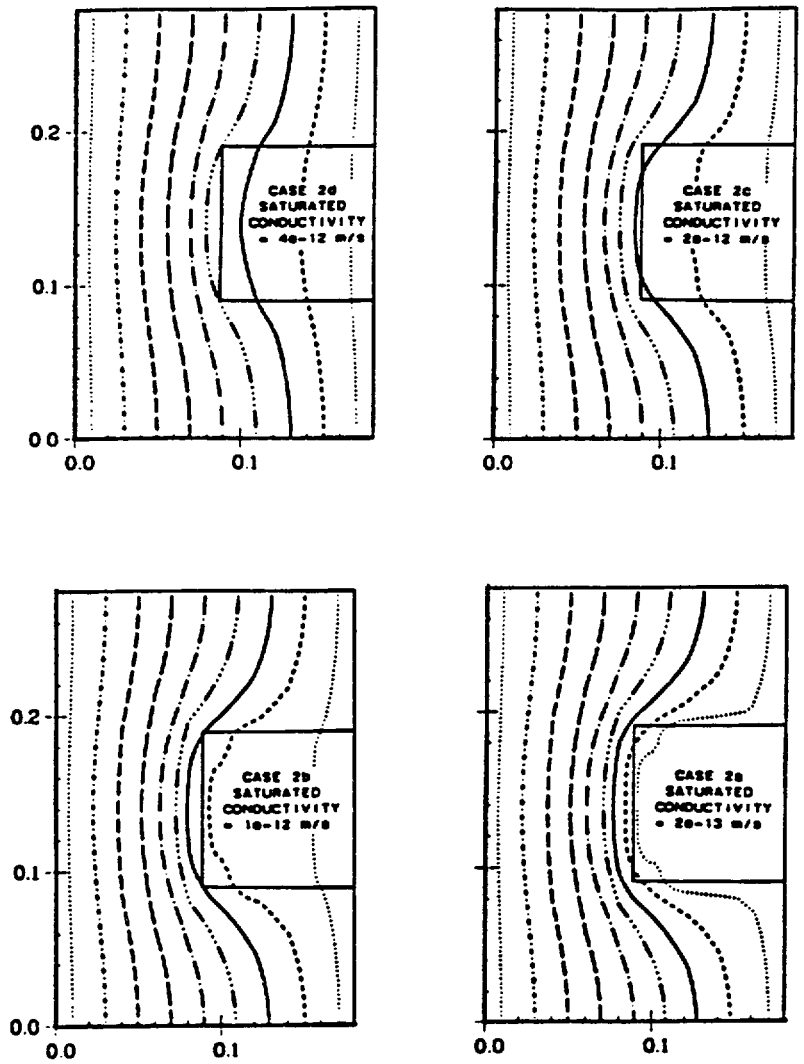

Figure 2: EFFECT OF SINGLE LOW CONDUCTIVITY OBSTRUCTION.

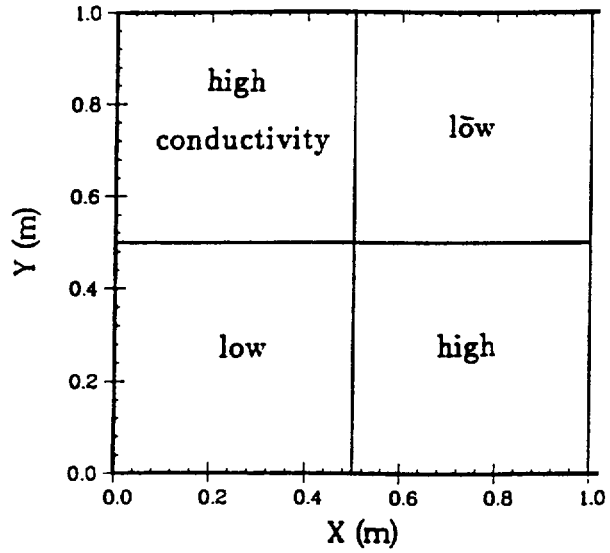

Figure 3: FOUR CELL REGION USED TO INVESTIGATE NUMERICAL GRID RESOLUTION.

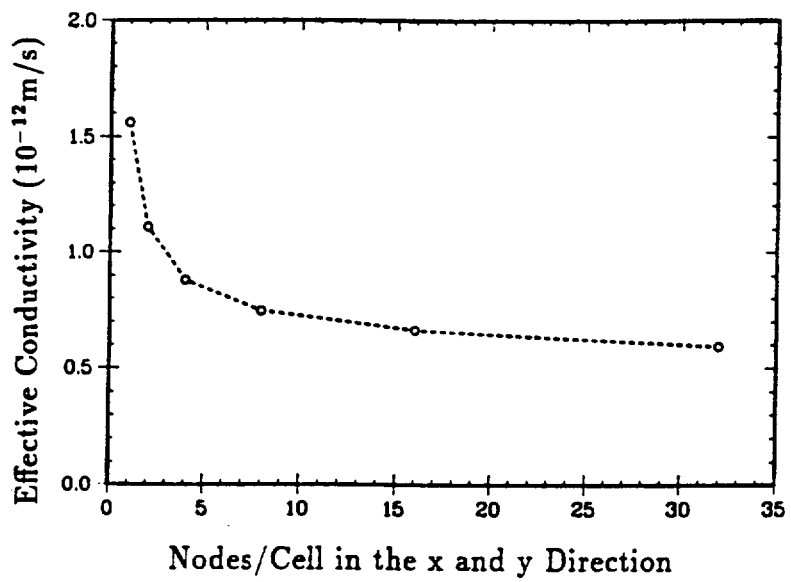

Figure 4: EFFECTIVE CONDUCTIVITY AS FUNCTION OF CELL REFINEMENT.

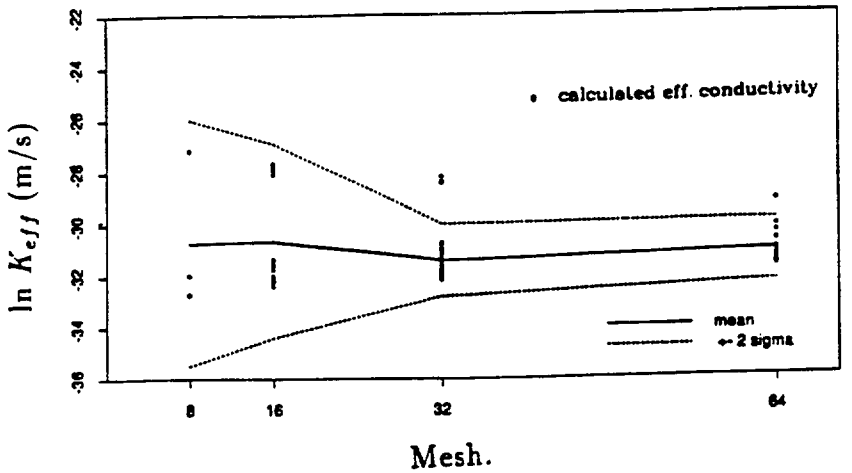

Figure 5: EFFECTIVE CONDUCTIVITY AS FUNCTION OF MESH.

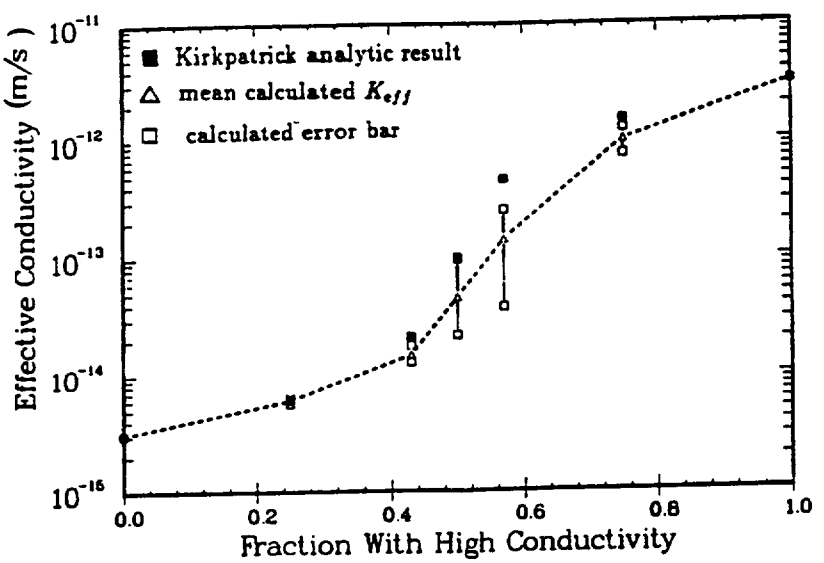

Figure 6: EFFECTIVE CONDUCTIVITY AS FUNCTION OF MATERIAL MIX.

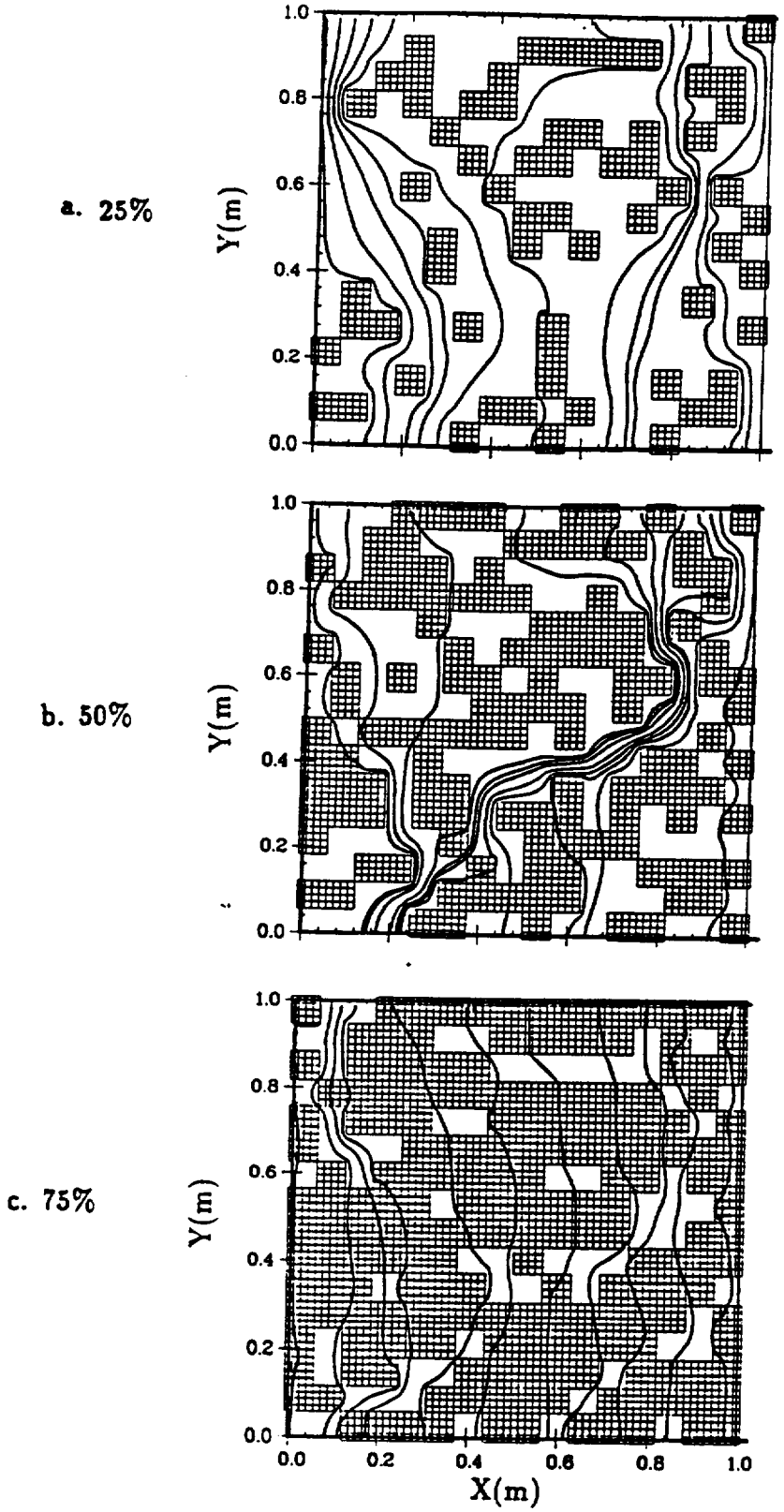

Figure 7: FLOW PATHLINES FOR THREE MATERIAL MIXES: a. 25%, b. 50%, c. 75% mix.

Evaluation of Tracers for Hydrologic Studies at Yucca Mountain

R.S. Bowman, G.W. Gross, and R.L. Liddle

New Mexico Institute of Mining and Technology

1. INTRODUCTION

In order to individually label different water inputs during site characterization and construction of a repository at Yucca Mountain, as many as 30 unique chemical tracers may be required. Only a handful of tracers has been proven suitable for investigations under a broad range of hydrologic and geochemical conditions. An effective tracer is nonreactive, i.e., it is not significantly sorbed nor transformed chemcially during the time frame of interest, and it is present naturally at low levels or not at all. Other considerations in choosing a tracer include ease of quantitation, detection limit, environmental hazards, and cost. Tracers to be used under unsaturated conditions must be nonvolatile.

Due to the need for more proven tracers for testing at Yucca Mountain (and for hydrological investigations in general), a series of laboratory experiments was performed to evaluate some new and/or little-utilized water tracers. The tracers tested included bromide, iodide, borate, and four fluorinated derivatives of benzoic acid. The emphasis was on testing tracers which could be used under unsaturated as well as saturated conditons.

A complete report on the experiments described below (Bowman et al., 1990) is available from the senior author or from the U.S. Geological Survey.

2. MATERIALS AND METHODS

Five lithologically different crushed volcanic tuffs (supplied by the U.S. Geological Survey in Denver) were used in the tests. Three of these were from different locations in "G" tunnel near the proposed Yucca Mountain repository. The other two were synthetic mixtures designed to simulate the different mineralogies of fractures present in the native tuffs.

Sieved samples in the 75-μm to 250-μm size range were packed into 5-cm I.D. by 30-cm long Plexiglas leaching columns equipped with porous plates at both ends. Leaching solution was applied to each of the five columns simultaneously using a multi-channel syringe pump. Column effluents were directed to automated fraction collectors. For leaching experiments under unsaturated conditions, column outlets were attached to vacuum chambers which housed the fraction collectors. For these unsaturated experiments a constant pressure of 0.8 atm to 0.9 atm was maintained in the vacuum chambers. The Plexiglas columns, syringe pump, and vacuum chambers were purchased from Soil Measurement Systems, Tucson, Arizona. The methodology for performing unsaturated flow experiments is described in detail by Wierenga et al. (1975).

Eight separate transport experiments were conducted with each column. Four experiments each were conducted using either synthetic J-13

well water (TDS = 220 mg/L) or synthetic pore water (TDS = 400 mg/L) as the leaching solution. For each leaching solution, transport experiments were performed under both saturated and unsaturated conditions. Finally, for both leaching solutions under both degrees of saturation, two different initial tracer concentrations were used.

For each transport experiment, columns were leached at a given flow rate and applied outlet vacuum until steady-state conditions were obtained. Steady-state was indicated by constant column water contents and constant tensions measured by tensiometers emplaced 5 cm from the top and bottom of the columns. At this point, a one pore volume (PV) slug of tracer solution was added to each column under the same flow conditions. Effluent was collected until all applied tracers had eluted from the columns.

Tracers were applied as mixtures prepared in the appropriate leaching solution. All tracer mixtures contained tritiated water (tritium), which served as an index tracer to which the behavior of the other compounds was compared. The tracers evaluated included bromide, iodide, and borate, which were each at nominal a concentration of 10 mg/L in one set of experiments, and at a nominal concentration of 20 mg/L in the other set. In addition, the synthetic organic tracers pentafluorobenzoic acid (PFBA), 2,6-difluorobenzoic acid (2,6-DFBA), m-trifluoromethylbenzoic acid (m-TFMBA), and o-trifluoromethylbenzoic acid (o-TFMBA), at concentrations of 20, 15, 10, and 10 mg/L, respectively, were included in one of the unsaturated flow experiments. These compounds have been proven effective as soil and groundwater tracers in a variety of hydrologic environments (Bowman, 1984; Bowman and Gibbens, 1991).

Tracer concentrations were determined in every 0.10 PV fraction of effluent. Selected effluent samples were also analyzed for major cations and anions, electrical conductivity, and pH.

The breakthrough curves (BTCs) of the test tracers were plotted and compared to those derived for tritium under the same experimental conditions.

3. RESULTS AND DISCUSSION

Figures 1 and 2 show BTCs for the test tracers and tritium for one of the porous media under unsaturated conditions. These examples are representative of results obtained for each of the porous media under the various experimental conditions. Referring to Fig. 1, bromide and iodide always eluted somewhat before tritium, indicating that anion exclusion occurred during transport through the tuff. Borate always eluted at the same time or, as in the case illustrated, slightly later than tritium. This suggests that borate was subject to sorption in at least some of the tuff samples. Referring to Fig. 2, all of the fluorobenzoates behaved identical to bromide.

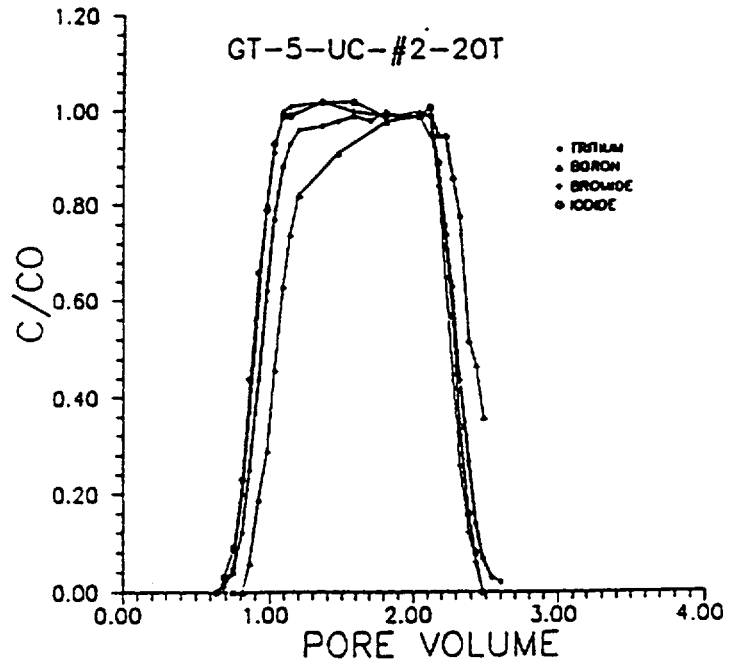

Figure 1. Breakthrough curves for tritium, bromide, iodide, and borate in column GT-5 under unsaturated conditions.

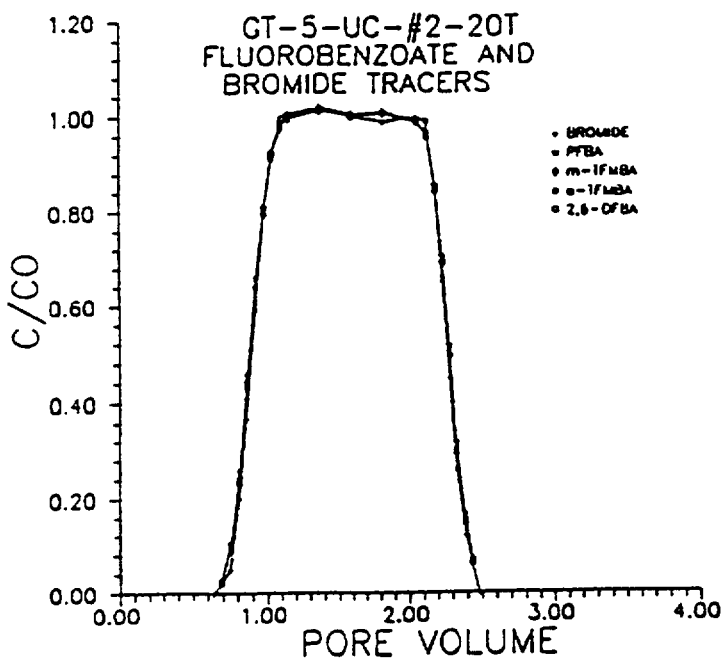

Figure 2. Breakthrough curves for bromide and four fluorobenzoate tracers in column GT-5 under unsaturated conditions.

Each of the tracer BTCs was fitted with the one-dimensional advection-dispersion equation, using the optimization algorithm of Parker and van Genuchten (1984) to yield best-fit values of the solute dispersion coefficient and retardation factor. The analytical solution used assumed equilibrium, linear solute sorption, as well as physical equilibrium (no immobile water). The mean pore water velocity was fixed at the value of the column specific discharge divided by the volumetric water content. There was no effect of background electrolyte composition or initial tracer concentration on the BTCs observed for a given tracer in a given porous medium. There was an effect of saturation, however. The averaged (over both leaching solutions and both tracer input concentrations) fitted tracer retardation factors from all the experiments are summarized in Table 1.

Table 1

Average Retardation Factors for the Tracers in Five Porous Media

Porous Medium	Bromide		Iodide		Borate	
	Sat	Unsat	Sat	Unsat	Sat	Unsat
GT-2	0.844	0.748	0.848	0.752	1.09	1.15
GT-5	0.957	0.883	0.957	0.884	1.07	1.08
GT-7	0.972	0.876	0.974	0.876	1.00	0.941
COL-1	0.874	0.747	0.873	0.746	1.03	1.03
COL-2	0.870	0.832	0.868	0.833	1.05	1.04

Retardation factors for bromide and for iodide were identical under the same experimental conditions and always less than 1.0, indicating anion exclusion of these species. Anion exclusion was more pronounced under unsaturated versus saturated conditions, as expected. Borate retardation factors exceeded 1.0 under all conditions save one (Table 1), indicating that borate is subject to sorption reactions in these media. Borate sorption was not extreme, however. Within experimental error, mass recoveries were 100 % for all tracers under all conditions, indicating that all are conservative at least on the time scale of these experiments (several weeks).

The BTCs for the fluorobenzoate tracers in all cases were indistinguishable from those of bromide under the same conditions.

4. SUMMARY AND CONCLUSIONS

Based on the somewhat limited range of conditions examined in these experiments, it appears that bromide, iodide, borate, PFBA, 2,6-DFBA, m-TFMBA, and o-TFMBA would each be a useful tracer for hydrological investigations at Yucca Mountain or in formations having similar lithologies. The range of retardation factors observed (0.75 to 1.15) is negligibly different from 1.0 given the variability encountered in measuring hydrologic characteristics in the field. Additional experiments to determine the magnitude of anion exclusion at very low saturation levels, and to determine the long-term stability of the fluorobenzoates in tuff, could yield greater confidence in field data derived from the use of these tracers.

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THE COMPOSITION AND CO_2 CARBON ISOTOPE SIGNATURE OF GASES FROM BOREHOLE USW UZ-6, YUCCA MOUNTAIN, NEVADA

Donald C. Thorstenson

U.S. Geological Survey
National Center, MS 432
Reston, VA 22092

The monitoring of gas composition and/or flow at a number of unsaturated-zone boreholes at Yucca Mountain has been carried out since 1983 by the U.S. Geological Survey (USGS). This paper reports the first depth profile of ^{13}C and ^{14}C (from CO_2) from the deepest of these boreholes, USW UZ-6. Much of the significance of the data from UZ-6 lies in its relation to data already obtained from other UZ boreholes.

Boreholes USW UZ-6 (UZ-6) and USW UZ-6s (UZ-6s) were drilled at the crest of Yucca Mountain, and at present remain open through thick sections of unsaturated fractured rock. Borehole UZ-6 was drilled using a reverse air vacuum method to a depth of 575 m (Whitfield, 1985) and is cased to a depth of 99 m. The borehole is open for the remainder of its depth and is completed in the ash-flow tuffs of the Prow Pass Member of the Crater Flat Tuff Formation. Borehole UZ-6s was drilled to a depth of 158 m with casing to a depth of 1 m, and is completed in the non-welded tuffs underlying the Tiva Canyon Member of the Paintbrush Tuff Formation. A third borehole, USW UZ-1 (UZ-1), in Drillhole Wash roughly 3.5 km NNE of UZ-6 and UZ-6s, was also drilled with reverse air vacuum to a depth of 387 m (Whitfield, 1985). UZ-1 has been instrumented at 15 levels, including gas sampling tubes, and is grouted throughout its depth (Montazer and others, 1985). From 78 m to its bottom at 387 m, UZ-1 taps the moderately to densely welded tuffs of the Topopah Spring Member of the Paintbrush Tuff Formation (Whitfield and others, 1990).

In the two open boreholes, UZ-6 and UZ-6s, gas flow to/from the boreholes, and thus through the mountain, is governed by a combination of barometric and thermal-topographic driving forces. At UZ-6s flow reverses frequently during the summer. During the winter months (roughly November to April) thermal effects predominate, and flow out of UZ-6s is essentially continuous. The physical and chemical characteristics of UZ-6s have been reported on by Weeks (1987) and by Thorstenson and others (1990). At UZ-6, however, barometric effects predominate even in winter, because of the fact that 200 m of fractured rock tapped by UZ-6 lie at an altitude below the floor of Solitario Canyon. Most gas samples from UZ-6 were collected at the following depths: 61 m (in the casing), 168, 244, 364, 376, 404, and 549 m (26 m above bottom) in the uncased hole. These depths were selected at high-permeability zones observed during borehole flow surveys (E.P. Weeks, personal communication). The sampling depths from 168 to 404 m are in the fractured welded tuffs of the Topopah Spring Member. The 549 m level is in the underlying bedded tuffs. One or more gas composition-depth profiles were collected in September and December 1986, March, May, June, July, August, and December 1987, March 1988, and March 1990. In March 1990 carbon isotope data were also collected. Additional UZ-6 carbon isotope samples at the surface and/or 549 m were collected in January 1987, January 1989, and March 1989.

On a time scale perhaps reaching months, CH_4 appears to be non-reactive in the Yucca Mountain unsaturated zone, and provides a convenient estimator of the mixture of atmospheric air into the system. A plot of all paired CO_2-CH_4 data from fractured tuff in UZ-6 (61 to 404 m) shows a linear relationship indicative of mixing of two end-member gases, air (with CO_2 - 0.036%; CH_4 - 1.7 ppmv) and a "rock gas" whose approximate composition is: CO_2 - 0.12% ± 0.01%, and $CH_4 \leqq 0.4$ ppmv (Figure 1). The relative number of data points near each member is greater than the number of intermediate points, suggesting that mixing is generally not complete, and that the flow in and out of the borehole occurs in part by piston flow. Samples from the underlying non-welded tuff also have CH_4 concentrations $\leqq 0.4$ ppmv, with CO_2 concentrations up to 0.5%.

When air is flowing into UZ-6 there is a rapid input of rock gas from the shallow Tiva Canyon Member, perhaps in part from the annulus around the casing, in spite of the large diameter (0.45 m ID) of the open casing itself. This was recognized early in the study, and is illustrated by the data in Figure 2, from September 11, 1986. These data show that at depths of 168 m and below, gas composition is unchanged during diurnal inhalation/exhalation cycles, and thus during inflow the air input through the casing is overwhelmed by rock gas by the time the 168 m depth is reached. This provides a qualitative indication of the extremely high permeability of the shallow fractured rock flow system.

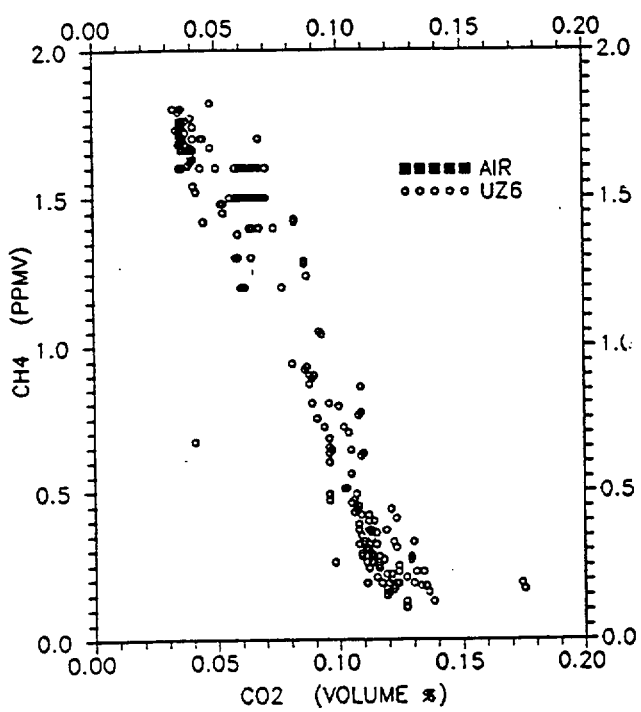

Figure 1. All CO_2-CH_4 data from UZ-6 fractured tuff; 397 samples from depths of 61 to 404 m.

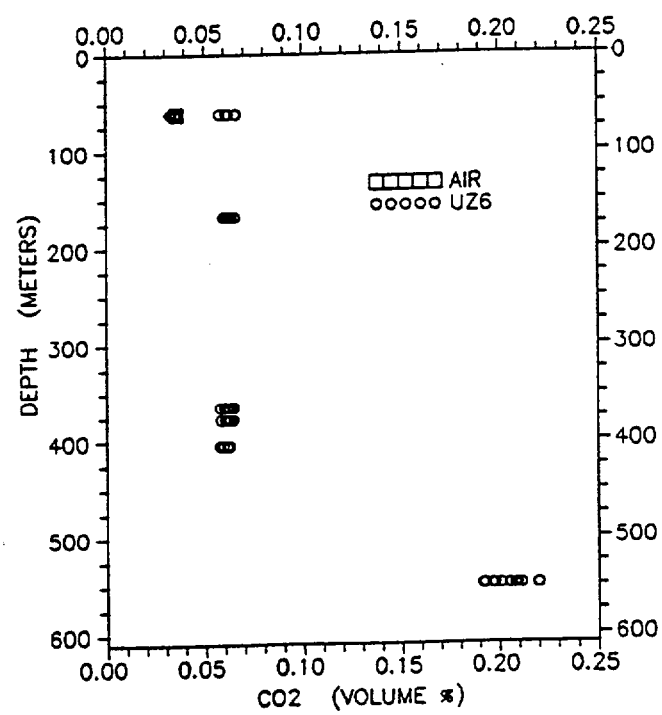

Figure 2. CO_2-depth, 9/11/86; 8 profiles: 5 inflow, 3 outflow

No systematic attempt at carbon isotope collection at UZ-6 was made for several years, on the assumption that interpretation would be rendered meaningless by the mixing of air and rock gas. On January 10, 1990, a check valve in an 8 cm I.D. pipe was installed on the surface cap of UZ-6, allowing flow out, but essentially stopping return flow. Although the check valve cannot stop the abundant cross-formational gas flow in the borehole, it was hoped that preventing direct input of atmospheric air through the casing would at least partially flush the UZ-6 flow system of air in time for isotope sampling during March 1990. Throughout the isotope sampling, March 1 to March 8, 1990, UZ-6 was pumped continuously at the surface (approximately 1,000 m^3/day), to maintain upward gas flow and thus to provide a sampling profile similar to those obtained for several years at UZ-6s. The results (Table 1), when compared with data from boreholes UZ-6s and UZ-1, suggest that the experiment was at least partially successful.

The composition and $^{13}C(CO_2)$ content of rock gas in the fractured tuff flow system are similar throughout the Yucca Mountain unsaturated zone. The concentrations of N_2, O_2, and Ar are at atmospheric levels in all samples from all boreholes. Concentrations of CO_2 and CH_4, and values of $\delta^{13}C(CO_2)$, from the following boreholes fall within the ranges $0.10 < \text{percent } CO_2 < 0.14$; $0 < \text{ppmv } CH_4 < 0.4$; and $-20 < \delta^{13}C < -16$: A) the 1990 UZ-6 data to 376 m; B) the UZ-6 rock gas end member in Figure 2; C) all March/April 1987-1990 UZ-6s data to 107 m; D) all March/April 1987-1990 data from shallow neutron-logging holes at Yucca Mountain crest; and E) most data from the Topopah Spring Member sampling interval (100 m to 387 m) at UZ-1. Data from the non-welded tuff intervals at UZ-6 (549 m) and UZ-6s (122-137 m) generally show higher CO_2 concentrations and slightly more negative $\delta^{13}C$ values than in the fractured tuffs. The data sources are - UZ-6s and neutron-holes: Thorstenson and others (1990); UZ-6 : Table 1, and Hass and others, written commun. (1990); UZ-1 : Yang and others (1985), and C.A. Peters and others, written commun. (1990).

In contrast to the uniformity of gas composition and ^{13}C content, the ^{14}C contents of CO_2 differ markedly between the shallow Tiva Canyon Member and deeper Topopah Spring Member flow systems. Figure 3 presents depth plots of the ^{14}C data from UZ-6, UZ-6s, UZ-1, and the nine neutron holes at the crest of Yucca Mountain. The depths in both boreholes are equated stratigraphically at the top of the Topopah Spring Member. Physical and chemical observations show that flow in the shallow Tiva Canyon Member is very rapid; all samples at depths of 100 m below Yucca Mountain crest have ^{14}C contents >100 pmc. The similarity of composition and $\delta^{13}C$ values in all gas samples from fractured tuff suggest that geochemical reactions in the CO_2-carbonate system are similar throughout the fractured-rock unsaturated zone at Yucca Mountain. If so, the differences in ^{14}C signature between shallow and deep flow systems must be attributable, at least in part, to differences in age. The deep Topopah Spring Member flow system thus appears to be operating on a far slower time scale than the shallow Tiva Canyon Member, and the intervening non-welded tuffs must constitute a substantial barrier to gas flow in the system. The natural (pre-borehole) residence time of gases in the Topopah Spring Member system may be thousands of years. Additional sampling is planned to see if continued flushing of UZ-6 may bring its ^{14}C profile into greater agreement with that of UZ-1.

Table 1. UZ-6 DATA: MARCH 1-8, 1990

DEPTH (m)	CO_2 ±1σ (vol%)	CH_4 ±1σ (ppmv)	$\delta^{13}C$ gas[1] KOH[2] (°/∞)	^{14}C ±1σ (pmc)
61	0.123	0.22	[1]-17.0	86.5
	±0.005	±0.09	[2]-17.5	±0.5
168	0.108	0.52	[1]-16.9	87.9
	±0.029	±0.27	[2]-16.9	±0.6
244	0.118	0.32	[1]-16.9	86.2
	±0.008	±0.13	[2]-18.0	±0.6
364	0.122	0.21	[1]-16.9	87.6
	±0.008	±0.06	[2]-16.0	±0.6
376	0.122	0.25	[1]-17.0	86.1
	±0.012	±0.17	[2]-17.6	±0.6
404	0.083	0.22	[1]-10.4	85.9
	±0.022	±0.15	[2]-14.3	±0.5
549	0.124	0.31	[1]-14.7	45.2
	±0.022	±0.18	[2]-18.0	±0.4

[1]Analysis of 500 cc gas samples.
[2]Analysis of ^{14}C aliquots.

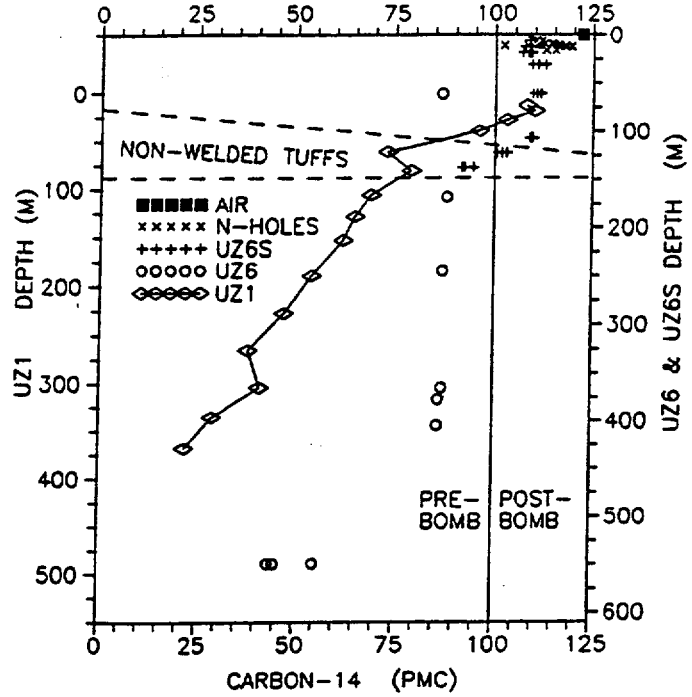

FIGURE 3. Carbon-14 vs depth. Neutron holes, UZ-6, UZ-6s: all data; UZ-1: 1990 data.

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Stable and Tracer Isotopic Studies of Hydrogenic Deposits Exposed at Trench 14, Nevada test Site

John S. Stuckless
U.S. Geological Survey

Reference: An Evaluation of Evidence Pertaining to the Origin of Vein Deposits Exposed in Trench 14, Nevada Test Site, Nevada. Proceedings of the International High-Level Radioactive Waste Management Symposium, April 28 to May 2, 1991 in Las Vegas, Nevada, by John S. Stuckless

Isotopic Tracers for Water and Solute Movement in Desert Soils

Fred M. Phillips
New Mexico Tech

Up to the present time, most soil-physics investigations have focused on agricultural soils. As a result, the physics of soil-water processes in desert soils are comparatively poorly understood. The difficulties of understanding soil-water processes in desert soils are compounded by the typical low water content in these soils. As a result, the physics of water flow in desert soils is much less linear than in agricultural soils and the rates of water movement are often orders of magnitude slower.

Since traditional soil-physics approaches are of limited applicability to desert soils, long-term tracer experiments provide a valuable alternative. Given typical rates of water movement in desert soils, tracer experiments on the time scale of decades are required. Artificial tracer tests of such duration are typically not practical, and so environmental tracers must be used.

Among the most useful environmental tracers for this purpose are those injected into the stratosphere by atmospheric nuclear weapons testing in the 1950's and 1960's. Many of the radionuclides produced by the nuclear testing are strongly adsorbed on soil particles, and so are not useful as water tracers, but tritium (^{3}H) actually enters the water molecule and chlorine-36 (^{36}Cl) is very conservative. Phillips et al. (1984, 1988, 1990) investigated the distribution of these "bomb" radionuclides with depth in New Mexico soils. They found most of the bomb chlorine-36 within the top 1.5 m of soil, but the tritium peak was found at 1.5 to 3.0 meters depth. This discrepancy in the penetration of the two bomb tracers is particularly striking in light of the fact that the bomb chlorine-36 fallout peaked in the mid-to-late 1950's and the bomb tritium in the mid 1960's. We attributed the greater net displacement of the tritium peak to downward thermal diffusion of the tritiated water vapor under the strong downward temperature gradients of mid-summer. The chlorine-36, which is not volatile, can move only by advection or diffusion in the liquid phase. Summer matric potential gradients are upward, toward the drying front, and thus the chlorine-36 tends to be refluxed upward at the same time that the tritium is being driven downward in the vapor phase.

In order to test this hypothesis, Knowlton (1990) measured profiles of deuterium (^{2}H) and oxygen-18 (^{18}O) in some of the same soils investigated for tritium and chlorine-36. Deuterium and oxygen-18 are stable isotopes of hydrogen and oxygen that are naturally found in the water molecule. Both of these minor isotopes are less volatile than their respective major isotopes and can thus serve as tracers for evaporation, condensation, and diffusion processes. Knowlton (1990) found that the depth profiles for both stable isotopes were characterized by minima at depths between 1.0 and 1.5 meters. Numerical modeling showed that these minima could be reproduced only by including the vaporization of water near the soil surface, downward thermal diffusion, and recondensation in the cooler soil below 1 meter. This result strongly supports the thermal vapor diffusion hypothesis for the separation of the tritium and chlorine-36 peaks.

Conclusions from these studies include the following: (1) Isotopic tracers are indeed very useful for understanding the soil-water physics of desert

soils, (2) Thermal vapor diffusion plays a very important (perhaps in many cases a dominant role) in water movement in these soils, (3) Upward refluxing of the liquid phase during the summer tends to separate volatile from non-volatile components and retain the non-volatile ones near the soil surface, and (4) Net infiltration rates over the past 30 years amount to a few millimeters or less in all soils investigated.

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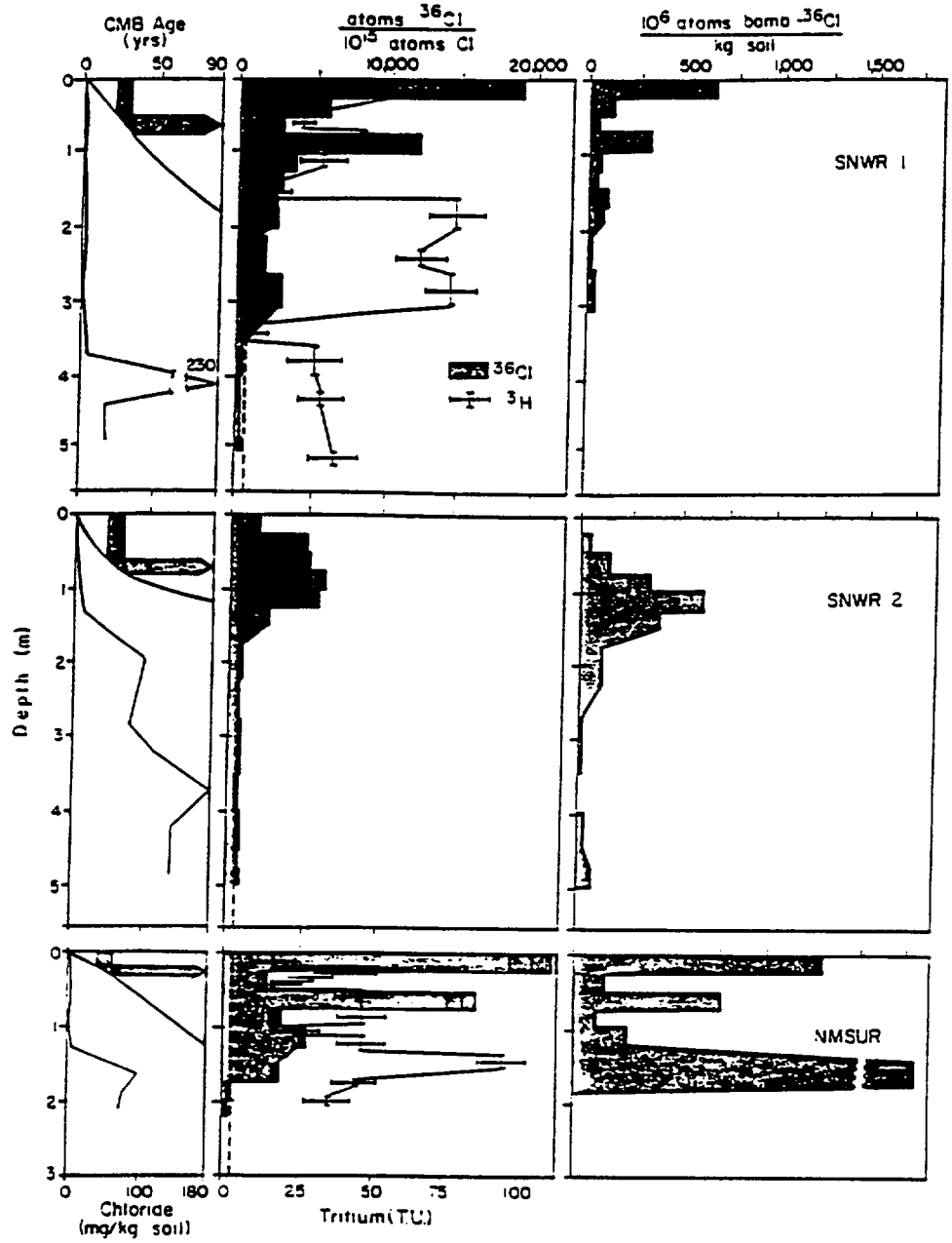


Fig. 1. Chloride, chloride mass balance age, ^3H, $^{36}Cl/Cl$ ratio, and ^{36}Cl content as a function of depth at the SNWR 1, SNWR 2 and NMSUR sites. The heavy arrow connecting the CMB age axis in the left-hand columns to the depth axis indicates the period of bomb ^{36}Cl fallout. The lower curves in the left-hand columns are the chloride concentration.

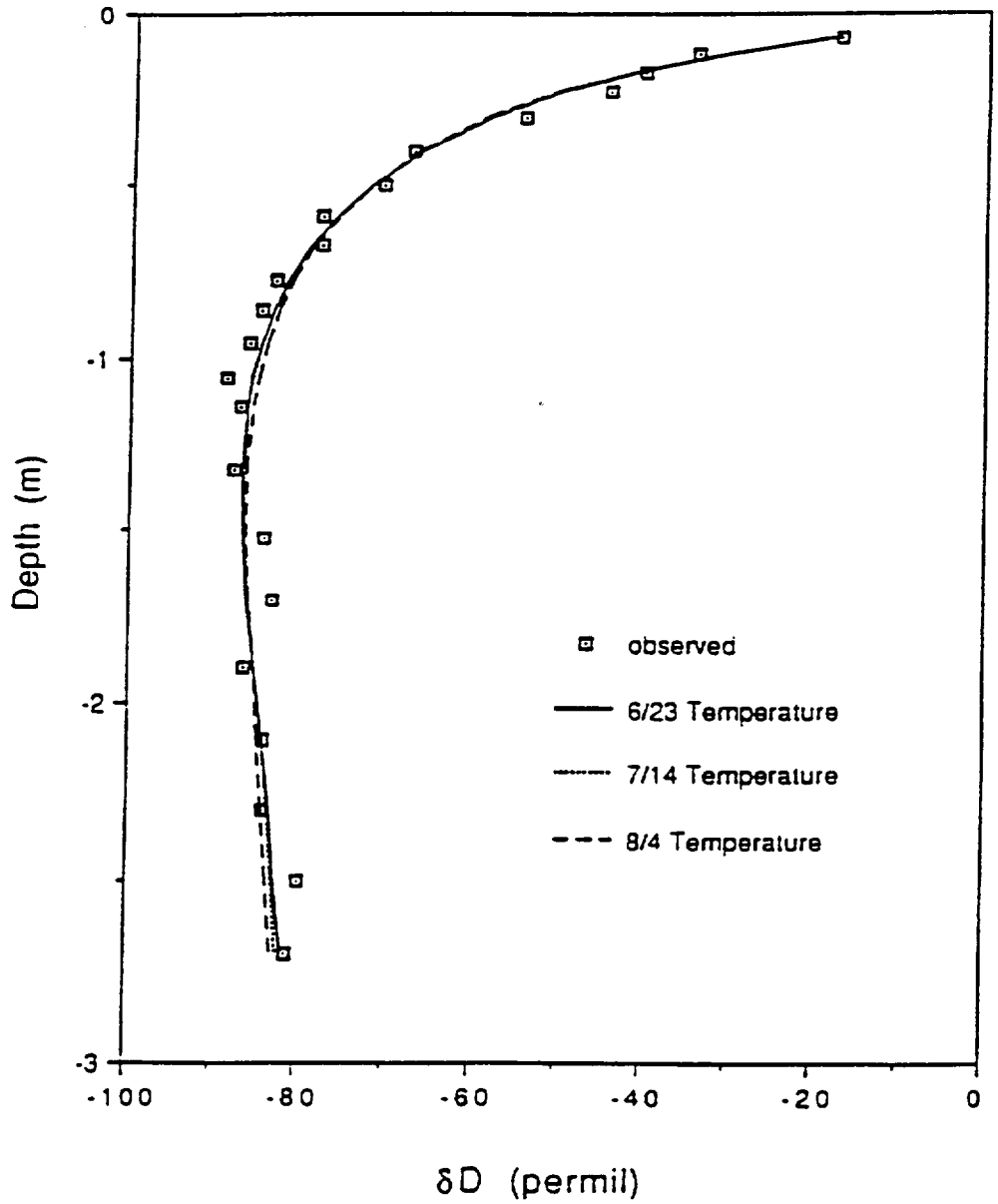


Figure 2. - NIR model calculated versus observed SSIP5 δD profile for three simulated temperature realizations

APPRAISING THE USE OF ENVIRONMENTAL TRACERS TO DETERMINE GROUNDWATER RECHARGE RATES: THE IMPACT OF MEDIA ANISOTROPY

J.T. McCord[1], C.K. Keller[2], and S.H. Conrad[1]

1. Sandia National Laboratories, Div. 6416, Waste Management Systems, Albuquerque, NM 87185-5800
2. Washington State University, Department of Geology, Pullman, WA 99164

INTRODUCTION

In the past couple of decades various environmental tracers have been utilized by hydrologists to estimate long-term recharge rates to groundwater aquifers. In general, environmental tracers are readily identifiable constituents of atmospheric precipitation which move through geological media along with the percolating water. These constituents can either be part of the water molecules themselves (such as isotopes of hydrogen and oxygen) or they may be highly soluble, non-reactive solutes (such as chloride). Such constituents are referred to as environmental tracers because they are naturally occurring and because some near-surface process (either natural or anthropogenic) induces some quantifiable characteristic signature in the water. This characteristic signature effectively labels the water, and the label either remains unchanged or else it changes in a predictable fashion as that parcel of water passes through the subsurface environment. Assuming: (1) that the tracer is uniformly applied in space at the field scale, and (2) that one-dimensional vertical downward flow predominates, a variety of models have been developed to estimate average groundwater recharge rates through the unsaturated zone based on environmental tracer concentration versus depth profiles.

In recent years there has been a growing recognition that fluid flux rates through geologic materials may vary significantly from point to point in space. With regard to groundwater recharge fluxes, there is abundant evidence for topographic localization or "focussing" of recharge at the scale of topographic variability (i.e., Meyboom, 1967; Lissey, 1971; Keller et al., 1988). Even where application of water to the ground surface is relatively spatially uniform, unsaturated fluid fluxes in the underlying soils are often highly spatially variable (e.g., Biggar and Nielsen, 1976). Based on the growing awareness of spatial variability in unsaturated soil water movement, a number of researchers have developed new stochastic mathematical models to predict flow and transport through heterogeneous media.

With regard to this study, the physically-based stochastic models of variably saturated flow developed by several researchers (Mualem, 1984; Yeh et al., 1985a,b,c; Mantoglou and Gelhar, 1987; Bear et al., 1987) have very significant implications. One important finding is that the hydraulic conductivity, or permeability, anisotropy ratio of a layered porous material can vary dramatically as its water content changes. Some soils which are nearly isotropic at complete saturation may be highly anisotropic under unsaturated conditions. Given that layering is a characteristic of many sedimentary deposits, this

result should be applicable under a wide variety of field situations. A net effect of this variable or "state-dependent" anisotropy phenomenon is that unsaturated flow paths through dipping layered deposits can develop significant horizontal components, even where the mean hydraulic gradient is vertical. McCord and Stephens (1987) and McCord et al. (1991) performed a number of soil-water tracer experiments on a sandy hillslope to validate these physically-based stochastic flow models in a natural field setting. Their experiments clearly demonstrated that there was a significant horizontal downslope component to the vadose water flow paths despite the absence of any pervasive "impeding" sublayers. Furthermore, depending on the geologic and topographic setting, large lateral flows can develop in some relatively flat-lying deposits (McCord, 1988). If this is true, then the one-dimensional models invoked to interpret unsaturated environmental tracer concentration profiles may require a reappraisal.

The physically-based stochastic theories and the field experimental validations cited above clearly suggest that in topographically variable terrain (even fairly mild topography) underlain by stratified geologic deposits, multidimensional unsaturated flow is the rule rather than the exception. Since recharge estimation techniques using environmental tracer profiles are based on the 1-D assumption, recharge estimates may be in error. In addition, environmental soil-water tracer analyses have been proposed to determine paleoclimatic conditions (Phillips and Stone, 1985), and are currently being applied to do so at the Sevilleta Long Term Ecological Research (LTER) Site in New Mexico (Phillips, 1989, personal communication). Once again, the 1-D assumption will provide a cornerstone for the paleoclimatic interpretive analyses. Therefore, it is vital that we assess the effect of multidimensional flow on the resulting subsurface distribution of the tracer.

IMPACT OF ANISOTROPY ON SUBSURFACE DISTRIBUTION OF TRACERS

A very simple demonstration of the effect of anisotropy on flow directions and environmental tracer distributions is provided below. For a two dimensional (x,z) cartesian coordinate system (with computational coordinates aligned with principal directions of permeability) the directional water fluxes can be computed by Darcy's law:

$$q_x = K_{xx}J_x \qquad\qquad q_z = K_{zz}J_z \tag{1}$$

where q_i is the flux in direction i, K_{ii} is the hydraulic conductivity in direction i, and J_i is the hydraulic gradient in the i direction. Applying this coordinate system to the hillslope setting depicted in Figure 1, where H is the horizontal direction and V is the vertical direction, and the medium dips at angle B. If $J_V = -1$ and $J_H = 0$ (which is a reasonable assumption: the average long-term hydraulic gradient is dominated by gravity), then q_x/q_z can be estimated using (1) above to obtain the curves depicted in Figure 2. Clearly, anisotropy dramatically impacts flow directions.

We can see how this may affect the subsurface distribution of a uniformly applied tracer by an application of the advection-dispersion equation. If advective flux dominates over dispersive flux and assuming steady conditions, we obtain for a two-dimensional (x,z) flow system

$$(v_xC)_x + (v_zC)_z = 0 \tag{2}$$

where v_i is the pore water velocity in the i direction, C is the solute concentration, and $()_i$ is the spatial derivative operator for the i direction. This steady-flow advective transport equation is solved here using finite difference techniques for a variety of hillslope configurations and constant material anisotropy ratios. Velocities are specified to be constant and uniform, and backward-differencing was used to calculate the concentration gradients. Figure 3 shows a schematic diagram of the system modeled. Note that water is applied uniformly at the ground surface at a constant concentration, $C=1$, and that a 25% evapotranspiration enrichment occurs every meter of depth in the top 3 meters. Below 3 meters no evapotranspiration influences are felt. At all locations constant values are assigned for v_x and v_z (based on calculations similar to those presented in Eqn. 1 and Fig. 2).

The resulting subsurface solute distributions for three different cases are presented in Figure 4. For the trivial case of a constant 1:1 anisotropy ratio, Figure 4a shows that the solute concentration versus depth profile would be the same for all locations along the hillslope. In essence, all flow is vertical and thus interpretations based on the 1-D piston flow assumption would be valid. This is the result one would expect for any isotropic material under a unitary, vertical hydraulic gradient, regardless of slope angle B. Figures 4b and 4c show solute profiles along the hillslope for two different topographic and material property combinations. The resulting distributions are quite different from the 1-D flow solute profile depicted in 4a. However, they bear a strong resemblance to the chloride profiles observed by Stone (1984) at a site in western New Mexico, as well as those observed by Sharma (1986) in his sampling along a hillslope in western Australia: the chloride concentration "peaks out" at a shallow depth and drops off somewhat below that depth. Stone suggested the profiles are indicative of a previous wetter paleoclimatic regime. Sharma suggests a couple factors which may have contributed to the solute profile characteristics, including soil layering and varying vegetation, but he felt he lacked the information necessary to draw any firm conclusions. Although these simulations are highly simplified and idealized, they suggest an alternative interpretation and they underline the substantial impact of anisotropy on the subsurface distribution of uniformly applied solutes.

FUTURE WORK

The above calculations represent the first preliminary steps in an ongoing integrated study which addresses the impact of media heterogeneity and resulting flow spatial variability on environmental tracer transport. As part of this study we will perform more rigorous flow and transport simulations with explicit consideration of stochastic heterogeneity. In addition an intensive field investigation of environmental tracer distributions (including Cl^-, ^3H, ^{36}Cl, and possibly ^2H and ^{18}O) is proceeding in Frenchman Flat in southern Nevada.

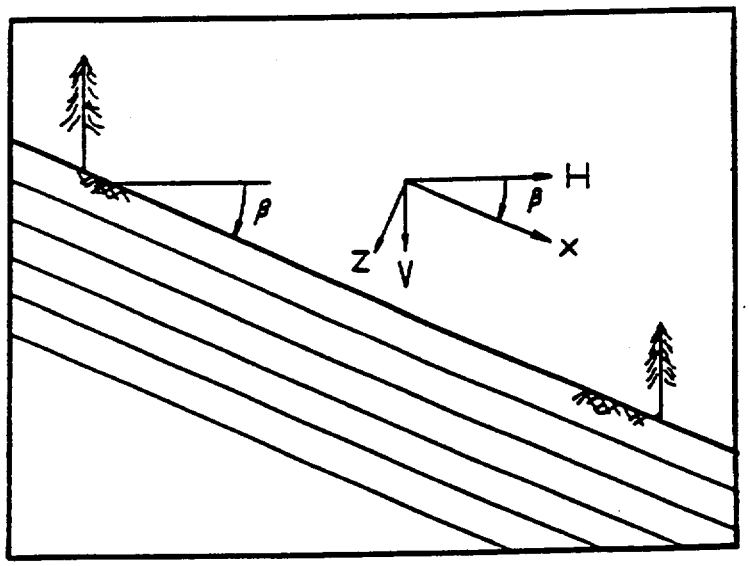


Fig. 1. Schematic diagram of a hillslope of angle *B* underlain by a layered medium with stratifications parallel to the ground surface.

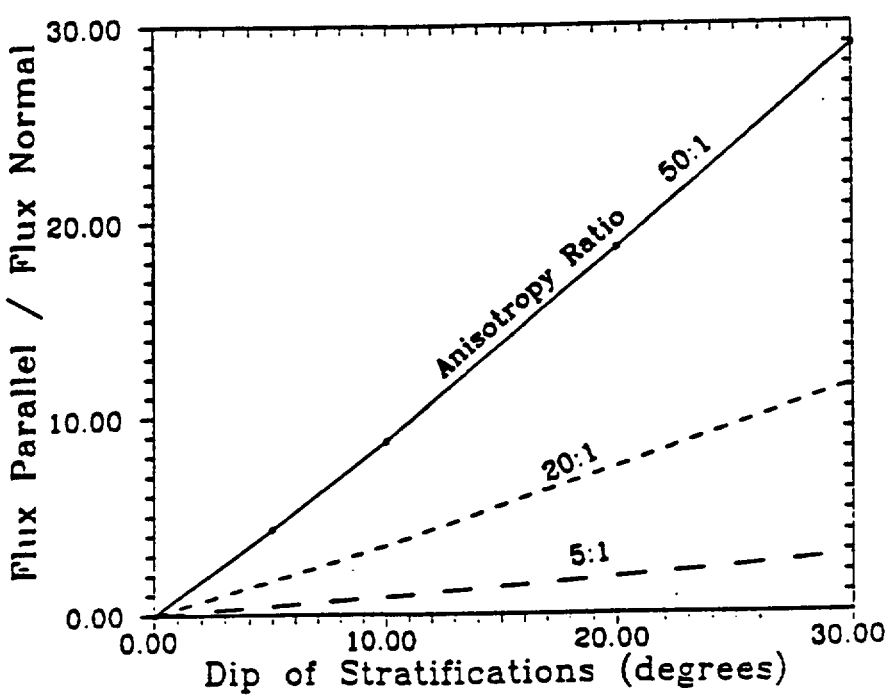
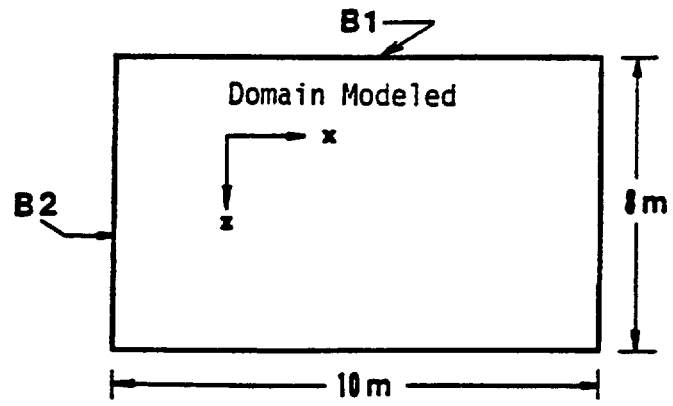


Fig. 2. Fluid flux parallel to medium stratifications divided by flux normal to stratifications as a function of dip for three different anisotropic materials under steady-flow conditions.



Flow Conditions

- steady flux specified for all nodes below the ground surface:
  $qx = \hat{q}x \qquad qz = \hat{q}z$
- all flow is down and to the right

Evapotranspiration Conditions

- water uniformly extracted from shallow profile:
  $\frac{\text{25\% of water removed}}{\text{meter}}$ for top 3 meters

Solute Boundary Conditions (BC's)

B1 $C = 1$

B2 $\partial C/\partial x = 0$

- no solute BC's are needed for bottom and right boundaries due to upstream weighting finite difference formulation.

Fig. 3. Schematic diagram of system modeled to demonstrate the importance of anisotropy on the subsurface distribution of an environmental tracer.

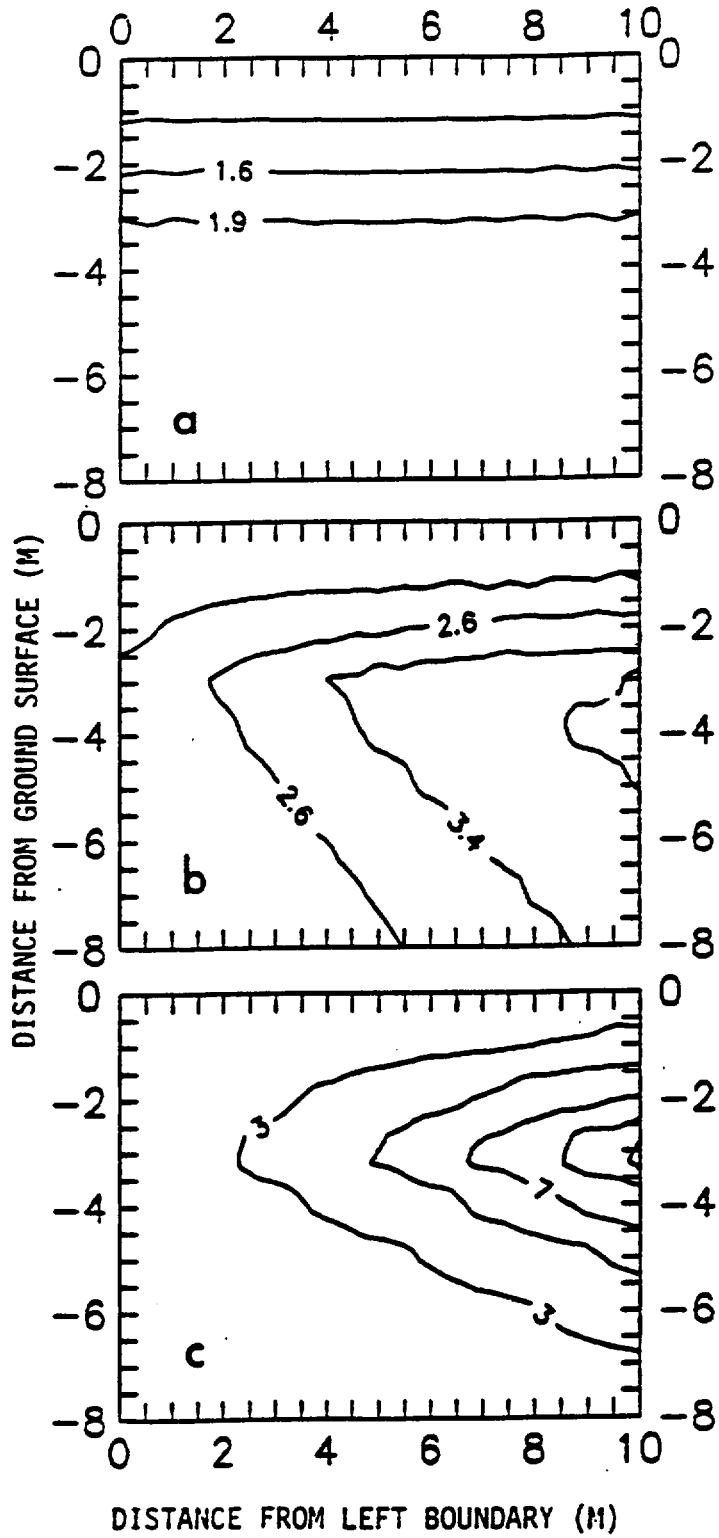


Fig. 4. Contours of profile solute concentrations from steady flow and transport simulations for three material and topographic combinations: (a) isotropic medium regardless of slope angle, (b) anisotropy = 5:1 and hillslope = 12 degrees, and (c) anisotropy ratio = 20:1 and slope = 10 degrees.

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UNSATURATED FLOW AND TRANSPORT RESEARCH QUESTIONS AND PRIORITIES; CONSIDERATIONS FOR WORKSHOP V

by

Donald L. Chery, Jr.
Division of High-Level Waste Management
U.S. Nuclear Regulatory Commission

December 1990

INTRODUCTION

A little over two years ago, a similar meeting (Workshop IV - Flow and Transport through Unsaturated Fractured Rock; Related to High-Level Radioactive Waste Disposal) was held here in Tucson, Arizona, to discuss the same issues that everyone here has been ruminating on again these past 4 days. It may be of some value to revisit what was said 2 years ago, to review research needs that have been articulated by the licensing staff of the Division of High-Level Waste Management, Nuclear Regulatory Commission, and to extract some of the thoughts on research needs resulting from the deliberations of a special committee of the National Research Council. These revisitations have been provided in the following three section of this report. We can then ask ourselves what has been accomplished in the past 2 years and where we should focus our attention and energies in the coming few years.

SUMMARY OF RESEARCH NEEDS FROM THE 12/12-15/1988 TUCSON WORKSHOP

At the end of the 12/12-15/1988 workshop on flow and transport in unsaturated media, an overall summary list (Silberberg, 1988) of research issues and thoughts was presented for discussion. That summary was organized in four sections - Issues, Processes/Mechanisms, Parameters/Measurements, and Models. I have also appended to the overall summary list a set of issues that was written down during the meeting. It is the summary from the Geochemistry Session, which was nicely prepared and illustrates the type of information that was incorporated in the overall summary. The overall summary, as prepared by Joe Wang at the December 1988 meeting, follows:

<u>Summary List prepared by Joe Wang</u>

Issues

* Ambient Liquid Flow at Depth

* Infiltration Distribution
* Long Term Evolution of [the] Vadose Zone
* Radionuclide Transport
* Spatial Variability
* Vapor Transport
* Responses to Extreme Precipitation
* Responses to Thermal Loading

A secondary list of issues

* Relative permeabilities of paths
* Treatment of fracture-porous flow system
* Solution efficiency (3D problems)
* Chemical, mechanical, and thermal couplings
* Tracer transport
* Code modification
* Field observation vs. experimentation

Processes/Mechanisms

* Understand precipitation - infiltration relationship
* Resolve fracture flow vs. matrix flow [issue]
* Need to better evaluate lumped parameters in lumped models for dual porosity
* Assess change of flow paths with saturation
* Need better understanding [of] interaction among geophysics, geomechanics, geology, hydrology and geochemistry
* Coupled gas, water, rock reactions
* Vapor phase transport
* Spatial distribution of phases and reactions
  Temporal distribution of phases and reactions

* Need more studies on field sites and natural analogs
  Need more infiltration studies
  Need more studies with natural/man-made tracers
  Need more studies of mineral coatings on fractures

* Understand retardation mechanisms

* Thermally induced [effects in] nearly saturated zone
  Thermally induced fast gas velocity?

Parameters/Measurements

* Need to measure relative permeabilities for matrix and fracture

* Quantify long tails in permeability distributions

* Assess influence of wet vs. dry drilling

* Compare mercury intrusion, nitrogen condensation, water adsorption methods

* Develop guidelines/standards for unsaturated sampling/testing

* Apply CAT scan tomography to unsaturated fractured rock
  Use seismic tomography for unsaturated fractured rock

* Need more work to measure hydraulic heads and tensions in fractured, unsaturated media

* Assess the scaling of water content and hydraulic conductivity functions of hydraulic potential

* Need work on water-retention prediction on aggregated soils (and fractured, consolidated medium) with fractal analyses

* Need thermodynamic data on secondary minerals

* Need baseline information on compositions of all phases
  - liquid phase - pores, fractures
  - gas phase
  - solids - fracture coatings, matrix mineralogy

* Identify exotic tracers - halogenated hydrocarbons

* Extrapolate lab data to field scale (i.e. crushed samples)

* Determine number of data points needed to define distribution

---

Models

* Use models more in experimental design in addition to predictions

* Assess the influence of sand layer near boundary in percolation experiments

* Compare numerical solutions with analytical solutions

* Evaluate double-porosity models to handle matrix - matrix cross flow and matrix to fracture flow

* Need coupled hydro chemical transport codes (dissolution, precipitation effects of mineral redistribution on flow paths, temperature, and pressure around repository)

* Develop more sophisticated sorption models

* Code verification

* Develop simple models to approximate complex models

* Develop models to understand processes/mechanisms

* Develop stochastic (fractal) models to handle spatial heterogeneity

* Check modeling results with experiments

* Evaluate 1D results with 2D and 3D results

* Uncertainty quantification - parameter, scale, temporal, process

* Model validation

Summary of Geochemistry Session Research Needs (incorporated in the overall summary)

Two major areas where geochemistry can support hydrologic processes -

1. Flow: Where and how water flows
2. Transport

Research Needs:

A. Coupled hydrochemical transport codes to study interaction of geochemical process - dissolution, precipitation and flow. What effect does mineral redistribution have on flow paths, temperature, and pressure around repository.

   Needs - thermodynamic data on secondary minerals
   solid-solution surface reactions
   data on reaction rates, kinetics of relevant phases

B. Baseline information for modeling
   - composition of all phases
     - liquid(groundwater) phase in pores and fractures
     - gas phase
     - solids, both for fracture coatings and the matrix mineralogy
   - gas, water, rock reactions
   - vapor-phase transport
   - spatial distribution of phases and reactions
   - temporal distribution of phases and reactions

C. Understanding flow
   - studies on field sites (natural analogs)
     - infiltration studies/natural or man-made tracers
     - mineral coatings on fractures
     - isotope studies

D. Retardation mechanisms
   - understanding mechanisms
   - development of more sophisticated sorption models - i.e., constant capacitance models
   - comparison of sophisticated models with the Kd model
   - identification of tracers - exotic tracers, halogenated hydrocarbons
   - extrapolation of lab tests to field

SUMMARY OF NUCLEAR REGULATORY COMMISSION (NRC)/DIVISION OF HIGH-LEVEL WASTE MANAGEMENT (DHLWM) RESEARCH NEEDS

In 1989, the Hydrologic Transport Section, DHLWM, NRC, prepared a set of research needs for the NRC Office of Nuclear Regulatory Research (Browning, 1989). For your reference, the statements

of those research needs, pertaining to unsaturated flow and flow/transport issues, are given in the following listing:

1. The Hydrologic Transport Section staff needs to have a description and understanding of recommended surface and subsurface methods, to determine water flux in unsaturated fractured rock medial in climates similar to that at Yucca Mountain.

2. The Hydrologic Transport Section staff has a need for definite criteria to evaluate the appropriateness and accuracy of pneumatic tests (use of air or gases) for determining hydraulic parameters of water flow in the unsaturated zone.

3. The Hydrologic Transport Section staff has a need to understand how to establish a representative elementary volume for flow and transport in unsaturated fractured rocks.

4. The Hydrologic Transport Section staff needs facts about flow and transport process and knowledge about parameter measurement techniques, to evaluate the current concepts of moisture characteristic relations for fracture/matrix flow in unsaturated fractured rocks.

5. The Hydrologic Transport Section staff needs an appraisal of the appropriateness and the precision/accuracy of using anthropogenic contaminants such as tritium, technetium-99, iodine-129, and chlorine-36 (bomb pulse radioisotopes), to directly assess pre-waste-emplacement groundwater travel time.

6. The Hydrologic Transport Section staff needs an appraisal of the applicability of existing coupled flow and transport codes, to model the performance of a proposed HLW repository at Yucca Mountain.

RESEARCH NEEDS FROM THE NATIONAL RESEARCH COUNCIL STUDY

In 1987, the Water Science and Technology Board of the National Research Council assembled a committee of 14 distinguished water science practitioners and academicians to address two questions: "To what extent can the current generation of groundwater models accurately predict complex hydrogeologic and chemical phenomena?" and "Given the accuracy of these models, is it reasonable to assign liability for specific groundwater contamination incidents to individual parties or make regulatory decisions based on long-term prediction?" After an 18 month study, the committee produced a report in early 1990 titled, "Ground Water Models; Scientific and Regulatory Applications." The last chapter of its report is devoted to "Research Needs."

For your reference, I have copied some of the "hopefully" seminal thoughts from that chapter.

The committee introduces its thoughts on research needs by commenting -

> "Concern exists that until one can predict with confidence the migration of a conservative solute within a heterogeneous medium, one will not be able to convince a great many people of the veracity of reactive solute migration predictions. (p. 251)
>
> Or in general that "...something less than a predictive capability exists at this time." (p. 255)
>
> And that "Modeling needs to be redefined as a cost-effective way of interpreting all available data, to the extent that the interpretation provided by that modeling effort enables one to be comfortable in making a decision. (p. 251)

Given these concerns, the committee contends that the present state of subsurface hydrologic modeling is evolving and is "...on the threshold of a significant change in how the subsurface environment is interpreted." (p. 250) It is the committee's opinion that "...current transport theory developments based on statistical interpretations of subsurface deposits may, in time, replace much of the deterministic theory. At issue are the characterization and simulation of dispersive phenomena."

Under a section titled "Basic Understanding and Process Models," it made the following comments:

> "While relatively better understood than geochemical and microbiological processes, present conceptual and mathematical models of convection and dispersion do not provide accurate results or inspire confidence when applied to highly heterogeneous or otherwise complex environments." (p. 255)
>
> A need "...to extend modeling capabilities to new classes of problems [such as] ... the commonly encountered problem of multiphase fluid flow and transport accompanied by dissolved component transport in water." (p. 256)
>
> [Given that] "...considerable success has been achieved in modeling the geochemistry of natural waters and in modeling the movement of ground water[,] it is logical to take the next step and link an equilibrium geochemical model with a ground water transport model." (p. 258)
>
> "We have probably reached the stage of development in modeling at which it is imperative to gather more and

better empirical data to demonstrate the validity of geochemical and transport models." (p. 260)

"...geochemical models are quite complex and computationally demanding to solve for only equilibrium calculations. Incorporation in their present form into solute transport modeling is impractical because of computing demand. Therefore the available geochemical models with comprehensive reactions and databases do not seem to be appropriate for solute transport modeling. Instead, simpler versions of these comprehensive codes have been developed and incorporated into transport [models]. ... Ideally, these more streamlined and efficient daughter codes could be tailored to include only the species and components of known importance to the site being studied." (p. 260)

"Biological reactions present a major modeling challenge. ... [in that] the biological reaction affects the pressure distribution and water flow paths, which in turn can affect the biological reaction." (p. 261)

Before biological and chemical models can be used routinely in solute transport, the fundamental mechanisms must be studied and better understood, and the models must be tested in controlled field studies." (p. 262)

"Methods available in ground water hydrology for obtaining estimates of uncertainty involve two general approaches: deterministic porous-media models, where the probability component enters primarily through parameter variations, and stochastic porous-media models, where the probability component enters through the treatment of the medium itself as well as through parameter variations." (p. 262) "Research is ongoing and should continue to develop both probabilistic approaches to modeling ground water systems." (p. 263)

"...neither the stochastic nor the deterministic method has satisfactorily resolved the role of scale-dependent dispersion." (p. 263)

Under the Section - "Translation of State of the Art to State of the Practice," the committee made the following comments:

"Major field-scale experiments conducted in the recent past ... have not provided data sufficient to discriminate between alternative [flow/transport] theories. Thus, the question of validity, especially for extrapolations to predict future events, remains unanswered." (p. 265)

"Calibration is undertaken in two ways: automated as an inverse or parameter identification method or ad hoc as a trial-and-error method."

"Both approaches benefit from advances made in the last decade in the interpretation of field data. [I.e. kriging methods.] Recently, research has been directed toward nonparametric methods that will enable the blending of soft (qualitative) and hard (quantitative) data." (p. 266)

The requirement for increasingly greater computational resources for linked hydrologic/geochemical models may be reduced by "...new mathematical methods for improving the computational efficiency of existing codes..." or by limiting "...the magnitude of the problems to be studied and, with such a limitation, to reduce the overhead of computing resources that must be carried." (p. 267)

"Another important theoretical push in modeling could come from the field of artificial intelligence, more specifically, expert systems. Expert systems are an emerging technology that could have a significant impact on ground water modeling methodologies as they exist at the present time.

Under the section, "Interdisciplinary Efforts," the committee made these comments:

"Currently, risk assessment methods applied to ground water systems are simply based and are used for screening or scoping newly discovered problems; however, more sophisticated modeling capabilities are needed for remediation studies. Essentially, the decisionmakers are more interested in a quantification of risk than in a quantification of contamination level." (p. 272)

"One aspect of characterization is sampling to independently define process model parameters. The identification of necessary data, suitable instrumentation, appropriate sample network design, and data interpretation methods is an interdisciplinary effort. Research should proceed toward highly integrated interdisciplinary methods in order to sample the subsurface environment." (p.273)

CONCLUDING THOUGHTS

I have summarized here, from three sources, the expression of research needed to better understand the processes occurring in underground fluid flow and contaminate transport and the modeling of these processes and the natural systems in which they occur. Repetition of needs can be found in all three sources, and we can continue making the same lists. The issue for this workshop is to move beyond the making of another comprehensive list, do some real focusing, and come forth with well expressed needed research endeavors that, if done, would contribute significantly to understanding the physical processes and how to model the systems of interest.

The participants of this workshop should attempt to:

- be aware of what have already been stated as needs
- assess if efforts have been made to respond to the previously expressed needs
- determine what progress has been made in resolving the previously stated research needs in the past 2 years
- keep in mind a general time constraint of about 8 years for research to contribute to the siting and performance evaluations for the Yucca Mountain site
- keep in mind that what ever is proposed must be relevant to the license application demonstration needs of the Department of Energy (DOE) and the license application determination needs of NRC.

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TECHNICAL QUESTIONS RELATED TO MODELING GROUNDWATER FLOW AND RADIONUCLIDE TRANSPORT IN UNSATURATED FRACTURED ROCK

Group 2 - Experimental (mainly physical) Research Area

Leader: R. Baca
Reporter: R. Green
Members: R. Baca, A. Flint, R. Green, J. McCray, P. Pohl, T. Rasmussen, V. Tidwell

1. Liquid/Vapor Flow in Unsaturated Fractures

Question:
What additional information is required to adequately characterize fractures and assess their importance to flow and transport in unsaturated, fractured rock?

Discussion:
An area of technical uncertainty in evaluating the propensity for flow and transport through unsaturated fracture rock is the effect of fractures on flow and transport under various conditions. Specific areas of technical uncertainty regarding fractures include the following: characterization, parameterization, observation and measurement of fractures; representative modeling of fractures; matrix/fracture interaction; characterization of fracture networks; and the effect of fracture coatings. A further understanding of these topics may be gained through theoretical analyses and numerical, laboratory and field experimentation. This additional information would help evaluate the role fractures or fracture networks have on flow and transport over a range of flow conditions and media properties (e.g. do fractures act as simple media, heterogeneous media, primary conduit or barrier to flow).

The effect of physics and geochemistry must be understood to evaluate liquid/vapor flow in unsaturated fractures. Sufficient information is not currently available to understand if and when fractures act as barriers or as conduits. It appears that they could act as either a barrier or a conduit under different sets of conditions. In particular, fracture coatings could cause a fracture to impede imbibition into the rock matrix and result in rapid infiltration to greater depths. Laboratory and field experiments are needed to determine which fractures act as conduits or as barriers to liquid flow.

2. Scaling of Processes, Properties and Parameters

Question:
Is it possible to assess relationships between observations, measurements and predictions/simulations of processes at a smaller scale and then use scaled parameters for site characterization and assessment at the field scale.

Discussion:

Full-scale observations and measurements of key parameters, properties and processes at the proposed repository site are difficult and typically impractical. One potential method to overcome this dilemma is through the use of scaled parameters and dimensional analysis. In this approach, laboratory-scale experiments and numerical and analytical evaluations of the specific processes of interest are performed. Next, assessments are made of how well this information can be used to understand the same processes at full scale. Part of this assessment is performed by scaling from laboratory-scale experiments to predict large, laboratory-scale experimental results and eventually extend to field-scale experiments. Those dimensionless terms which prove to be sensitive to variations in parameters will require further study before they can be used to make predictions at the repository scale. Dimensionless terms that are not sensitive can be identified as not critical and omitted from future investigations.

3. Coupled Processes

Question:

Which of the coupled processes have a significant impact on HLW emplaced in a repository located in unsaturated, fractured rock and what is the significance and influence of these coupled processes on travel times and release rates?

Discussion:

Several general areas of coupled processes have been identified as having a potentially significant impact on travel times and release rates from a geologic repository. These include: thermal/vapor effects - enhanced diffusion; air/water interactions; geochemical/thermal interactions; thermal/mechanical interactions; and, in general, the effect of high-temperature versus low-temperature HLW. These technical areas need to be investigated to determine the extent to which each has to be taken into account and to determine the extent to which decoupling is possible or allowable.

Possible approaches to this problem are as follows. Conduct fully-coupled, partially-coupled and uncoupled experiments at both laboratory scale and field scale, for various geometries and time scales.

Perform sensitivity (performance assessment) analyses of parameters associated with different coupled processes. Of benefit is the identification of those coupled processes and parameters which are not important. This will permit the application of limited resources to address those parameters which are important. Laboratory- and possibly field-scale experiments are of great importance because theoretical analyses may incorrectly assess the importance of a particular process at the repository scale. Theoretical analyses are, however, an important component of this evaluation.

4. Prioritize Importance of Pathways of Groundwater Travel Time or Release Rates

Question:

What are the significant pathways (e.g. air, water, matrix, fractures, etc.) by which the performance measures may be violated.

Discussion:

Dimensionless, scaling or sensitivity (performance assessment) analyses ultimately need to be performed to resolve this issue. It is doubtful that a sufficient data base is currently available to complete this task. However, the data base should be expanded and preliminary scoping evaluations need to be performed at this time to help prioritize future data collection efforts. Additionally, systematic physical and numerical experimentation of the processes governing flow and transport should be performed. Included in the experimentation is the investigation of gas and liquid flow through media associated with localized saturation.

5. Liquid and Vapor Flow Through Fault Zones

Question:

How are flow and transport in fault zones characterized?

Discussion:

The presence of fault zones near a geologic repository may provide significant pathways for flow and transport. It appears imperative that flow and transport through fault zones be characterized to adequately evaluate a geologic HLW repository. Included in the characterization is the ability to parameterize, collect data and model flow and transport of water, vapor and gas through fault zones.

This characterization may proceed along several directions. The integrated or cumulative flux through a fault zone needs to be determined. In order to accomplish this, large-scale volume averaging measurement techniques are required. Point measurements, while useful, are not adequate to evaluate fault-zone properties. Cross-hole or surface-borehole geophysical methods may be useful to measure volume-averaged properties. Environmental tracers may also be useful, particularly when sampled regionally and at depth. Large-scale water or air injection tests may be useful. Geologic/paleontologic evaluations may provide information concerning the nature of a fault zone.

6. Model Validation

Question:

How can models (e.g. conceptual and/or mathematical) be validated in order to develop confidence in the travel time and release rate predictions?

Discussion:

Many scientific hypotheses have been (and will be) developed to explain and describe physical and chemical processes that are important to travel time and release rate predictions. A systematic, experimentally-based approach is needed to establish the degree of validity of these hypotheses. Research should be conducted to formulate a quantitative approach and acceptance criteria for assessing model validity. Validation exercises, in which experiment outcomes are predicted in advance of physical experiment results, need to be conducted.

Experiments that directly yield representations of travel times and release rates should be selected and conducted. Results of these tests could be evaluated to determine the degree of validity of the existing hypotheses upon which travel time and release rates are made. Experiments for validation should be improved over time in terms of scale (bigger not smaller) and complexity (more not less) to test the robustness of the model. Models should be tested against site-specific criteria. Confidence in the models can be increased or augmented by means of a series of such validation experiments or through the use of natural analogs.

7. Techniques for Designing and Evaluating Sample Representativeness as Well as Measurement Precision and Accuracy

Question:

One of the foremost questions in the assessment of a geologic site is how to define a "representative" sample. Inexorably associated with this question is the definition of the "representative elemental volume" of a heterogeneous site. Associated with this topic is the determination of whether laboratory-measured properties are statistically significant as a measure of the performance of a particular geologic site.

Discussion:

In the performance of large-scale field experiments, it is important to 1) insure the reproducibility of site-specific experiments and 2) perform a sufficient number of experiments to assess spatial variability. This assessment should be performed with respect to the importance of the parameters to the performance measure. Those parameters that prove to be most sensitive should be identified and the experimental reproducibility and accuracy of these parameters should be stressed.

Geostatistical analysis can be used to investigate the correlation length of measured properties. Conditional simulations can be performed to investigate data uncertainty and the spatial structure. The distribution of model results can provide insight into the representativeness and sensitivity of the data.

8. Instrumentation for Moisture Content and Suction Pressure Measurement at the Laboratory and Field Scale

Question:

How can the instrumentation and measurement technologies for determining moisture content and suction pressure measurements at both the laboratory and field scale be improved?

Discussion:

The measurement of moisture content and suction pressure is difficult at either the laboratory or field scale. Better understanding of these parameters is imperative to be able to accurately understand flow and transport processes. An improvement in the accuracy, ease of use and reliability of the measurement techniques is needed. This ability is important to the investigation of both the matrix and fractures of dual-porosity media and under non-isothermal conditions. The techniques for laboratory-scale applications may differ from those appropriate for field-scale applications.

Prototype instruments are reported in the literature. These methodologies and instruments need to be developed to a sufficient level of confidence and reliability (e.g. those used with limited success to date but which appear promising). Instruments already designed, need to be made available to the technical community.

Technologies available in other disciplines may provide possibilities. Most prominent are the technologies available in the oil/gas industry (more applicable to field-scale applications) and the medical industry (more applicable to laboratory-scale applications).

9. Long-Term Climatic Effects

Question:

What are the potential impacts of climatic changes on long-term HLW isolation emplaced in a geologic repository in terms of travel times and release rates?

Discussion:

To assess the performance of a geologic repository it is necessary to identify anticipated and unanticipated climatic changes for the required time frame of the repository. It is necessary to assess the effect of these climatic changes on travel time and release rates. Climatologically associated parameters and processes include the past/present/future rainfall, evaporation, infiltration, barometric pressure, temperature and wind velocity at the proposed site.

Possible approaches to this evaluation include: the use of natural analog studies; numerical experiments; isotope studies; and paleontological studies. Remote-sensing and field-inspection techniques can be useful to identify any

historical evidence of recent (Quaternary) features (e.g. soils, varnishes, geomorphic features, geochemical evidence, flora, etc.) that would suggest that past climatic conditions were sufficiently different to indicate that future conditions could also be dramatically different.

10. Depth and Rates of Infiltration in Fractures and Faults at both the Surface and the Repository Elevation

Question:

Is it possible to quantify and characterize infiltration and percolation rates at the atmospheric boundary and at the repository horizon within the rock mass. What is the effect of fractures and faults on infiltration rates?

Discussion:

This research question is important for determining the impact of precipitation events upon travel times of fluids through the subsurface. An important aspect of characterizing the basic hydrologic nature of a site is to determine the depth of infiltrating water in response to a precipitation event. It may be possible to investigate infiltration rates and depth at either the laboratory or the field scale. Simulation/modeling experiments may also be used in this investigation. Additional associated questions are raised in this investigation such as the size of representative elemental volumes and the hydraulic properties of fractures. The variation of the hydrologic response of the fractures and faults could be large, that is, different fracture or fault sets could have dramatically different responses to a precipitation event. Thereby, single measurements or limited investigations may prove to be misleading. Representative measurements at sufficiently large scales are required. Natural analogs may again be useful in the investigation of basic flow and transport processes.

TECHNICAL QUESTIONS RELATED TO MODELING GROUND WATER FLOW AND RADIONUCLIDE TRANSPORT IN UNSATURATED, FRACTURED ROCK

Group 3 - Modeling Research Area

Leader: C. Voss
Reporter: D. Gallegos
Members: R. Ababou, D. Chery, W. Ford, S. Gomberg, D. Hoxie, L. Lehman, K. Pruess, S. Wurstner

Modeling Research Group 3 has identified a number of general areas for which technical questions remain unanswered. The group further ranked the areas in order of perceived importance. In each area a number of specific questions were raised and in some cases, a strategy was proposed to address those questions. What follows is a discussion of these issues and concerns.

1. Flow Behavior in Fractures and Fracture/Matrix Interactions

Question:

What is the nature of liquid flow in fractures on different scales, and how can it be modeled?

Discussion:

Concerns about the suitability of the Yucca Mountain site arise mainly from the possibility of liquid phase flow along preferential pathways, such as fractures and faults. Generally, it is thought that without fracture flow, the site is safe in terms of liquid phase transport. On one hand, laboratory and field experimentation is needed to identify mechanisms of liquid-phase flow in fractures, including fracture-matrix interactions. On the other hand, conceptual and numerical models need to be developed for describing such flows qualitatively and quantitatively. The two must then be combined to address important site performance issues and to develop a sound understanding of ground water flow. For instance, this includes the important issue as to the feasibility and limitations of approximating a fractured, porous medium as a single effective continuum. Addressing this specific question will require not only an understanding of the flow mechanisms in the fracture and the matrix, in different types of rock and at different scales, but also an understanding of the flow/pressure boundary condition at the fracture-matrix interface. Conditions also need to be identified under which fracture flow is unimportant. For example, does there exist a well-defined parameter region under which the role of fractures is negligible, and can that region be identified?

2. Model Validation

Questions:

Can a generic, systematic model validation strategy or methodology be developed which can address all aspects of model development?

Discussion:

A number of issues concerning model development and testing could perhaps be addressed through the use of a generic, systematic model validation strategy. However, it is not clear whether or not a single strategy would be acceptable. Instead a number of different approaches may be necessary to look at different issues. As an example, the approach to model validation for deterministic and stochastic models may not be the same. Also, could the validation strategy used to judge the adequacy of a given model be used to identify controlling processes and performance measures? The idea of model refutation was suggested as one possible alternative to model validation. The potential utility and limitations of any of these approaches need to be identified.

A number of specific issues concerning models and experiments used during validation were also raised. For instance, is a continuum approach to ground water flow modeling based on Darcy's Law adequate for modeling ground water flow in an unsaturated, fractured rock? Or conversely, under what conditions would such an approach be acceptable? While possibly appropriate at the laboratory scale, the model may not be appropriate at the site scale. Also, can an ideal field experimental site be identified to be used to validate flow and transport models on large scales? In general, experimentation is needed to increase confidence in unsaturated zone modeling. Pertinent experiments need to be identified, depending on the processes considered.

3. Need for New and Improved Modeling

Question:

What aspects of modeling capabilities are in most need of improvement and where are new modeling capabilities needed?

Discussion:

The improvement of modeling capabilities is a key to the overall improvement of our understanding of flow and transport in unsaturated, fractured rock. Improved modeling can help narrow the gaps between measurement (including experimentation), conceptual models, mathematical models and numerical models. Particular modeling needs include a means to include more realistic geologic heterogeneities and coupled (multiphase) processes in numerical simulations. Effect of heterogeneities, discontinuities, and coupled thermo-hydro-mechanical and chemical processes were viewed as the most important areas to be examined and better understood through

improved modeling. Other related questions were the effect of space dimensionality on simulation results, the combination/coupling of several numerical and/or theoretical models, and discrepancy between model sophistication and data input. For example, the recommendation was made that perhaps simpler modeling approaches rather than more complex could be investigated for ground water flow in unsaturated, fractured rock. Some of the specific goals of modeling were large-scale analysis of unsaturated zone fluxes, alternative techniques for analyzing unsaturated zone flux, calculation of ground water travel times, and the calculation of probability distributions of ground water travel time.

4. Treatment of Uncertainty

Question:

How can we determine what are acceptable levels of uncertainty for performance assessment modeling, and, specifically, how can we treat and represent conceptual model uncertainty in performance assessment analyses?

Discussion:

Performance assessment analysis necessarily involves the treatment of uncertainty in models, data and parameters, and future states of the system. Uncertainty in data and parameters and future states of the system must therefore be quantified and propagated through the performance assessment models. The question that has arisen is "how do we determine what are the acceptable levels of uncertainty at each step of the analysis?" For instance, stochastic modeling, because of uncertainty, will result in a range of predictions in system behavior, whereas the real physical system is operating under a single set of conditions. If the range of predictions encompasses reality, it does not necessarily mean that the model is valid. Through reduction of uncertainty, the range in predictions can be narrowed. Determination of the level of reduction of uncertainty is thus critical to the issue of model validation.

In addition to uncertainty in data and parameters and future states of the system, is uncertainty in models. Formal, systematic treatment of model uncertainty will need to be addressed as part of performance assessment analyses. Currently, no well-defined methods for resolving conceptual model uncertainty exist. Techniques for reducing model uncertainty include model validation with the assistance of experimentation and site characterization. However, because of insufficient data or modeling limitations, these may not guarantee resolution of the issue of multiple, plausible conceptual models for a given system. Consequently, methods for representing alternative conceptual models in performance assessment analyses are needed.

5. Scale Effects

Question:

For sensitive model parameters, can scaling relationships be identified which can: a) span the range of possible measurement scales, and b) allow extrapolation to larger scales necessary for repository performance assessments, either in a single model or in a sequence of models?

Discussion:

In nature, processes and heterogeneities occur at several different scales. Observation (i.e., measurement), experimentation, and modeling also occur at different scales. Modeling and measurement approaches need to be developed or identified which can correctly capture different natural scales and be able to consistently translate interpretation from one scale to another.

A unique opportunity exists to pursue scaling effects at the Apache Leap Site in Arizona. Work to date has included both laboratory and field scale studies of matrix and fracture flow. Further, two other opportunities exist to go to larger scales in a phased sequence. First, the Never Sweat Tunnel is nearby and may possibly directly underlie certain ongoing research areas. This tunnel is at a depth of several hundred meters below the surface. Secondly, the Magma Mine lies at a depth of approximately 1500-2000 m below and nearby the Apache Leap site. The mine is currently in the process of dewatering, so other hydraulic analyses may be feasible. Both the tunnel and the mine may provide the opportunity to determine scaling relationships in terms of flux (or other parameters) from the laboratory scale through the larger field scale. The larger scales can be used to support estimates of flux derived at the smaller scales.

6. Preferential Pathways for Flow and Transport

Question:

To what extent do preferential pathways, such as fractures, faults, and associated high-permeability zones, control flow in the unsaturated zone and how can we account for these pathways in our models?

Discussion:

High conductivity, preferential pathways are likely to occur within unsaturated zones that could be activated, for example, by episodic, high-intensity, land-surface infiltration events. These pathways and flows within them could lead to localized perched-water zones, in addition to being major conduits for flow. These pathways need to be identified in the field and, if their occurrence is proven, methods need to be developed to account for these pathways within flow and transport models. Examples of such pathways have been observed near the Apache Leap tuff site, for example, within

the Magma Mine haulage tunnel.

Field evidence for preferential pathways would include examination of saturation distributions around faults and fracture zones, as well as, seeking occurrences of perched water within the unsaturated zone. Natural tracers (for example, ^{3}H, ^{36}Cl, and ^{14}C) also could be used to identify the likely presence of preferential pathways.

Preferential pathways between the repository and the water table could lead to short ground-water travel times and to possible significant radionuclide transport and releases to the accessible environment.

7. Scenario Development and Description

Question:

Can a methodology or approach be developed to provide for the quantitative definition and identification of potentially significant disruptive scenarios, including volcanism, climate change, and faulting? Can the events comprising a scenario be simplified from event trees, and the parameters to evaluate performance be identified and quantified, to allow for meaningful modeling of a particular disruption scenario?

Discussion:

Developing scenarios from our conceptual understanding of a site is a significant part of quantifying and modeling the performance of the site under different, credible events and processes. Development of relevant scenarios is a complex process requiring site data, expert judgement, and qualitative information. Several important issues have been raised with regard to scenarios, as characterized by the above questions.

Particular concerns related to scenario development and modeling included describing the existing features of the site under a nominal set of conditions. For example, under current conditions, what would be the significance of the elevated water table to the north of the site on the performance of the site proper? Additional concerns included the identification of a complete set of disruptive scenarios, defining a set of parameters to experimentally test for such information, development of scenario probabilities estimating the occurrence of each scenario, and estimating parameter uncertainties to allow for meaningful modeling.

As indicated above, inclusion of scenarios in performance assessment analysis not only requires modeling the disposal system under the set of conditions imposed by the scenario, but modeling the scenario itself so that the set of conditions is meaningful. For example, climate change is generally considered to impose a change in the upper boundary condition (i.e., flux at the surface) of the system and possibly a change in the location of the lower boundary condition (i.e., change in water table elevation). Only a reliable model for climate change will provide meaningful values for these boundary conditions. Other scenarios, such as volcanism-related, may require that very different conceptual models of the system be used in the performance assessment analysis.

8. Definition and Treatment of Model Boundary Conditions

Question:

For the unsaturated and saturated zone, how can present and future boundary conditions (above, below, and lateral) be established?

Discussion:

To adequately model an unsaturated repository site, boundary conditions will have to be established for both the unsaturated and saturated ground water flow systems. In the unsaturated zone, the upper boundary condition location will probably be established by the land surface. The lower boundary condition will probably be defined as the water table. However, the nature of the boundary conditions is highly uncertain. For example, the spatial and temporal distribution of both flux at the land surface and recharge to the water table can have a significant impact on modeling results. Additionally, it may not always be apparent where in the model to locate lateral boundaries or what their nature should be (no-flow, constant pressure, etc.).

In the saturated zone, the upper boundary would likely be the water table. However, it may not be readily apparent at what location lateral and bottom boundaries should be established and what type of behavior they exhibit. In terms of solute transport, the unsaturated zone provides an upper boundary condition for the saturated zone. The spatial and temporal distribution of solute (i.e., radionuclides) at this boundary could be critical to site performance.

Also, over time, all boundaries in both the saturated and unsaturated zone may change location (for example, location of water table), type (for example, constant pressure), and magnitude (for example, change in pressure distribution). These changes could have a significant impact on the ground water flow system at the repository site.

9. Treatment of System Heterogeneity

Question:

How can we effectively measure and model heterogeneity while considering different scales occurring within the same system?

Discussion:

The fact that the natural geologic system is heterogeneous is a major complicating factor in site characterization and modeling. Spatial heterogeneity is present within, as well as, between geohydrologic units. In fact, the designation of geohydrologic units or layers is a direct consequence of property differences in the vertical direction. These vertically occurring differences are usually easy to observe in detail (in core samples), but are generally, difficult to incorporate into numerical site-scale models. That is, for

numerical modeling purposes, relatively large hydrogeologic units are defined, each encompassing a number of similar small units. Perhaps this is acceptable, assuming that at some scale, small heterogeneities will not make a difference in larger scale behavior, and consequently effective property values can be used to describe behavior at the larger scale. Lateral heterogeneities are perhaps even more difficult to characterize and treat because of the nature of the sampling techniques (boreholes are usually drilled vertically and far apart). Nevertheless, a method for defining the point at which the assumption of an effective property value can be used needs to be developed. By doing so, the effect of heterogeneity on bulk (effective) properties may be assessed. This can be particularly import for flow and transport in unsaturated, fractured rock. Improved numerical modeling techniques may help resolve the issue to a certain extent.

10. Experimentation Related to Modeling

Question:

What experimentation (at all scales) should be applied to assist in the validation of models, site characterization, and parameter estimation?

Discussion:

Laboratory and field experimentation is needed to resolve a number of important conceptual issues, and to assist in site characterization and evaluation of site suitability. Areas identified that could be addressed through use of experimentation include the multiphase behavior of fractures, fracture-matrix interactions, and the applicability of pneumatic tests for evaluating hydrologic parameters. Experimental tests could also be used to test the applicability of the representative elementary volume (REV) concept for modeling flow in an unsaturated, fractured rock. Experimentation may also help determine the appropriate size of an REV for a given model. Development of techniques to measure large-scale flux in the unsaturated zone and to detect important isolated features such as fractures, is also considered necessary. In general, development and design of experimental efforts, and selection of sites for field experimentation, should be directed toward understanding flow and transport mechanisms, should be related to site performance issues, and should make use of available modeling techniques.

11. Engineering Measures to Improve Performance of the Natural Barrier

Question:

Can the site be engineered to alter the hydrologic conditions around the repository to improve the overall performance of the site?

Discussion:

It may be possible to alter the *in situ* conditions around a repository to improve the overall performance of the site. For example, it may be feasible to lower the water content in the rock to increase the ground water travel time by circulating air through the rock prior to closure. Other possibilities are engineered materials for backfilling the emplacement rooms to divert water away from the underlying waste containers (i.e., for vertically emplaced waste). Surface (topographic) features can be created (or eliminated) to produce favorable infiltration conditions.

This effort consists of tasks to identify different feasible engineered systems that potentially would improve site performance. These ideas are explored further using analytical models to determine their impact on the nominal system behavior. The analyses should consider a range of ambient conditions, geologic structures and boundary conditions.

TECHNICAL QUESTIONS RELATED TO MODELING GROUNDWATER FLOW AND RADIONUCLIDE TRANSPORT IN UNSATURATED, FRACTURED ROCK

Group 4 - Modeling Research Area

Leader: R. Eaton
Reporter: J. Wang
Members: P. Kaplan, S. Magnuson, M. McGraw, B. Sagar, Y. Tsang, D. Updegraff, R. Wescott, G. Wittmeyer, R. Zimmerman

Group 4 has identified, discussed, and ranked the priority for further study of technical issues in the modeling research area. After listing 42 issues from the members, the group collectively discussed, combined, and casted the issues into 17 questions which were then ranked by voting. The top 10 issues identified by the group are reported in this summary. Justification and possible approaches to study each issue were briefly addressed by the members before these technical questions were presented to the whole workshop. For each issue, the mean value and the standard deviation (as a measure of consensus) of the ranking votes are enclosed in parentheses following the title.

1. **Fracture-Matrix Interaction** (1.9 ± 1.4)

Question:

What are the dominant physical processes that should be included in the modeling of fracture-matrix interactions with discrete and continuum models ?

Discussion:

The group reached a good consensus on this issue which was addressed from different perspectives 6 out of 42 times in the initial assemblage of issues. Short travel time and fast radionuclide transport, most likely through the fractures, are the main concern. The transition between fracture flow and matrix flow depends on the coupling between the discrete fractures and the porous matrix blocks. In addition to liquid capillarity and gravity, do we need to take into account the effects of vapor flow, phase transition, wettability, fracture surface coating, and other processes? There is great interest in developing and testing dual-porosity and multiple-continuum type models for transient flow through fractured, porous media under variably-saturated conditions. In addition to flow and transport between fractures and matrix blocks, the block-to-block processes need to be modeled. There is a great need to determine the scale at which the equivalent continuum or multiple continuum models can produce similiar results of discrete models with fractures explicitly taken into account. For large scale studies, it is not practical and probably not necessary to explicitly model all the fractures.

2. Boundary and Initial Conditions (4.9 ± 2.0)

Question:

How can the types, location, and values of the boundary and initial conditions be determined ?

Discussion:

Changes of boundary and initial conditions can change the modeling results of travel time, amount of water contacting the wastes, etc. Recharge is not spatially uniform and is not constant in time on the undulating ground surface. Lateral infiltration may exist through side slopes. There is also concern about the effects of possible seepage boundary conditions and drainage in fractured or faulted zones. Numerical experiments (see issue 5) can be run to determine the sensitivity of the models to various conditions. Within the formation, for the initial ambient conditions or in the postemplacement period, there is a need to improve field estimations of the direction and magnitude of liquid and gaseous fluxes and other state variables. It is desirable to have a direct measurement of fluxes to check the current approach of estimating fluxes from the product of conductivity values and potential gradients.

3. Unsaturated and Fracture Parameters (5.7 ± 4.9)

Question:

How to determine unsaturated parameters (moisture characteristic curve, relative permeability, etc.) and functional forms of these relationships for porous rock matrix and rough fractures ?

Discussion:

The moisture characteristic curves and the relative permeability functions of both the matrix and the fractures are needed for modeling unsaturated flows in fractured, porous media. There are concerns about the choice of proper functional forms of these relationships and the problems associated with nonuniqueness and nonidentifiability in parameter estimation. There is also concern about the correlations among different parameters. Some existing functional forms allow different groups of model parameters to describe the same moisture characteristic curve. While existing models may be adequate to fit the data, there is a need to develop models with parameters tied to physically measurable quantities and with unique curve for each set of parameters. For the fractures, can we relate the unsaturated curves to distributions of geometric parameters such as aperture, roughness, surface contact, width, etc. ? In a more general context, we need to know what measurable parameters will be used by the models for the flow and transport processes. We should put more emphasis on the measurements of parameters which will actually be used in the models.

4. **Formation Heterogeneity** (6.0 ± 3.8)

Question:

What are the impacts of formation heterogeneity on model analysis and borehole testing of flow channeling and tracer breakthrough ?

Discussion:

There is a need to improve our understanding of advective transport in heterogeneous media under variably-saturated conditions so that proper bounds can be established for the tracer residence time, degree of flow channeling, and tortuosity of flow paths. The presence of very heterogeneous flow and transport makes interpretation difficult for point measurements from individual boreholes in the field. Formation heterogeneity will affect the testing requirements and evaluation of site suitability with boreholes. We need to evaluate the consequences of using parameters from point measurements on field scale modeling results.

5. **Numerical Experiments** (7.0 ± 3.5)

Question:

What numerical experiments need to be run to determine the mechanisms, conditions and parameters likely to control flow processes and influence performance calculations ?

Discussion:

Before formal performance calculations are made, numerical models can be used to identify the different mechanisms, boundary and initial conditions, and parameter variations most likely to influence the calculations of travel times and other performance criteria. For example, we can use numerical experiments to determine the conditions and mechanisms of maintaining fracture flow with the porous matrix blocks remaining in unsaturated conditions. If the travel time or other performance criteria is sensitive to some mechanisms, conditions, or parameters, we should put higher priorities on the measurements of these factors. The modelers running the numerical studies need to interact closely with lab and field investigators to gain insight of the physical reality and incorporate the knowledge into the models. The numerical simulations can then be used to help design tests to measure meaningful parameters and variables so that models can be validated.

6. **Model Complexity vs. Data Availability** (8.1 ± 4.1)

Question:

How can a proper balance between model complexity and data availability be maintained ?

Discussion:

The complexity of a numerical model should be compatible with the type and amount of data available for a given task. A complex model without support from adequate data tends to generate voluminous results representing information which does not really exist. An oversimplified model tends to neglect data and reality and generate oversimplified predictions. There is a need to develop rationale to decide the adequacy of model complexity based on data availabilty. However, model development should not be restricted by presently existing data since the amount of data will change over time. The amount of data needed can best be estimated by the modelers working with the experimentalists. Close interaction between modelers and experimentalists is crucial for maintaining a balance between modeling and testing.

7. **Computational Efficiency** (8.3 ± 3.8)

Question:

How can we obtain computational efficiency adequate for large scale analyses requiring multiple realizations ?

Discussion:

Both the geometric complexity (fractured porous media) and the property nonlinearity (unsaturated characteristic curves) introduce computational difficulties. Small grid blocks and nonlinear changes can limit the size of time steps. We need to model large systems over long terms and we need to carry out the calculations many times to quantify the effects of model and parameter uncertainties. While we implement new computing technologies (parallel, vectorizing algorithms), we need to develop more efficient approaches specifically designed for solving unsaturated flow and coupled process problems in fractured, porous rock. The group briefly discussed stiff matrix solvers, time step maximization schemes, higher order discretization elements, boundary integral methods, path integration formulations, and stochastic models. Some or all of these methods may need to be developed before run times for multi-dimensional computations can be made cost effective.

8. **Coupled Processes** (9.5 ± 4.6)

Question:

What is the importance of coupling mechanical and geochemical processes to thermohydrology ?

Discussion:

Thermally induced stresses may significantly change the permeability and other hydraulic properties of fractures. Dissolution and precipitation of rock minerals can change the geometry of flow channels. Multiple phase and heat pipe effects can enhance

heat transfer efficiency. Coupling mechanical and geochemical processes to thermohydrology adds complexities to the models. We need to evaluate the importance of including these couplings in performance assessment models. Carefully designed experiments are needed to quantify the coupling effects and to develop the relationships needed in coupled models.

9. **Continuum Mechanics and Darcy's Law** (10.0 ± 5.5)

Question:

Is the concept of classical continuum mechanics combined with the Darcy's law adequate for flow modeling ?

Discussion:

Most of the unsaturated flow models are based on Darcy's law modified by the relative permeability function and on Richard's equation for conservation of mass in partially saturated conditions. These classical equations based on continuum mechanics were developed and well-established for uniform cores in saturated porous media. We need to test these fundamental equations and concepts for partially saturated, fractured rocks with strong contrast in hydraulic properties between fractures and tight porous rock matrix. We need to separate the effects due to heterogeneity from the fundamental processes using simple experiments specifically designed for testing the continuum concepts. The comparison between experiments with fractured samples and modeling results based on Darcy's law can help us to determine if highly transient fracture flow, film flow along fracture surfaces, very tortuous channeling flow, and other processes can be modeled by continuum mechanics.

10. **Coupled Testing** (10.5 ± 5.1)

Question:

How can geophysical and hydraulic testing methods be combined to locate and measure large contrasts in hydraulic conductivity ?

Discussion:

Tomographic imaging and geophysical testing can supplement hydraulic testing to determine the heterogeneity of fractured formations. For saturated formations, geophysical methods such as ground penetrating radar, seismic profiling, and electromagentic surveys have been used to study fractured zones. We need to couple these geophysical studies with hydraulic or pneumatic tests from the boreholes for partially saturated formations. Coupled testings can greatly enhance our ability to characterize fractured porous systems with strong contrasts in hydraulic conductivity between fractures and matrix.

TECHNICAL ISSUES RELATED TO GROUNDWATER FLOW AND RADIONUCLIDE TRANSPORT IN UNSATURATED FRACTURED ROCK

Group 6 - Geochemistry

Leader: J. S. Stuckless
Reporter: W. M. Murphy
Members: A. Arredondo, A. Freeze, A. Meijer, F. Phillips, K. Richards, P. Striffler.

Six high priority issues selected from over twenty technical subjects compiled by the group are summarized in this report. No judgement of relative priority is intended by the order of presentation. Technical issues focus primarily on the Yucca Mountain, Nevada proposed repository environment.

1. Regional Distribution of Chemical and Isotopic Tracers in Deep Vadose Environments

Investigations are required to evaluate the distribution of chemical and isotopic tracers in regional deep vadose zones. Comparisons and interpretations of natural chemical and isotopic tracer data are presently limited by the sparsity of data from deep vadose environments. A basis of regional field data is required for development of conceptual models for interpretation of data to be obtained at Yucca Mountain. The feasibility of addressing several important problems in unsaturated flow and transport could be assessed. For example, do $^{234}U/^{238}U$ ratios reflect the water-rock ratio and/or contact time in the vadose zone; does the distribution of ^{36}Cl offer constraints on fluxes, flow directions, or preferential flow paths in deep unsaturated environments; can climatic effects, e.g. variations in temperature or recharge, or geothermal gradient effects be interpreted from $^{18}O/^{16}O$ or D/H ratios in these environments? A regional context is required for the proper interpretation of natural isotopic and geochemical tracer data from the vadose zone at Yucca Mountain.

2. Detailed Isotopic Data Base for Comparison with Model Results

Isotopic data from Yucca Mountain are necessary to place constraints on groundwater sources, residence/travel times, recharge rates, and mixing. A three-dimensional data base of groundwater isotopic data from saturated and unsaturated environments should be generated in sufficient density to permit analysis by transport modeling. The suite of data should include H, C, O, Ca, Sr, Pb, and U analyses. Models for groundwater sources, flow, and mixing should be consistent with and/or constrained by the isotopic data. Geochemical data may be used to evaluate whether a water sample can be

regarded conceptually as the product of movement of a water packet along a well defined flow tube or must be interpreted as the result of continual mixing of waters from many sources and paths. Bulk chemical and mineralogic data should be useful in the interpretation of the isotopic data and groundwater flow and transport processes, and should be integrated in the modeling.

3. Development of Isotopic Techniques for Constraining Groundwater Flow in Unsaturated Media

Isotopic techniques should be explored to distinguish instantaneous/episodic groundwater recharge and continuous/gradual recharge. Basic questions to be addressed are: Does water introduced in episodic events carry an isotopic or tracer signature; do isotopic data constrain the relative significance of fracture versus matrix flow during recharge; can rapid infiltration in fractures or fracture networks be identified by observations of bomb pulse ^{36}Cl or by other methods? Bulk water chemistry may also reflect fracture versus matrix environments, and could be used in conjunction with the isotopic data. Radiometric dating of hydrogenic deposits may also identify episodic or continual processes.

4. Investigation of the Significance of Fracture Coatings for Radionuclide Transport in Unsaturated Media

The occurrence, distribution, mineralogy, hydraulic properties, and geochemistry of fracture coatings must be investigated to evaluate their significance for flow and transport processes. Fracture coatings may affect moisture transport between matrix and fracture environments in unsaturated media. Radionuclide sorption at fracture surfaces may occur by mechanisms that differ from matrix sorption, and the systematics of retardation may differ significantly between fracture and matrix flow. In addition, the groundwater composition in the unsaturated environment may be influenced or reflected by fracture mineralogy. The properties of fracture coatings must be known to assess whether or under which conditions the fracture coatings are a barrier or a conduit for unsaturated flow. The mineralogy of fracture fillings and coatings may provide traces of flow paths. Investigations of fracture petrography should be linked to analyses of flow and transport phenomena.

5. Radionuclide Speciation and Solubilities in Aqueous Solutions

Radionuclide speciation in aqueous solution and solubilities of radionuclide-bearing solids must be studied because of the controls these phenomena have on radioelement source concentrations and aqueous transport. Important questions include: how does speciation depend on bulk fluid composition and temperature; how does sorption/solid-liquid

exchange/precipitation depend on speciation; can a limited number of significant aqueous species be identified; can aqueous speciation be regarded strictly as an equilibrium phenomenon, or are metastabilities significant (e.g., among electron transfer reactions); what complexing agents in the natural or perturbed environment affect solubilities; what solids will control the concentrations of waste elements, and what are their properties? Solubility studies as a function of solution composition are valuable for identifying aqueous species as well as constraining source concentrations of radionuclides. Reversed solubility studies could lead to the identification of metastable phases that sustain elevated radionuclide concentrations generated by releases from an unstable source (e.g. spent fuel or waste glass). Detailed site data on water chemistry are necessary to justify detailed aqueous speciations in transport codes. The extent to which it is necessary to incorporate detailed aqueous speciations in transport codes must be evaluated.

6. Appropriate Mathematical Formulation for Radionuclide Retardation

An appropriate treatment of retardation must be devised. Although the K_d formulation is practical and widely invoked, it is unclear that it is capable of adequately describing retardation in unsaturated geologic media. Retardation can be expected to depend on fracture flow versus matrix flow, variable water composition, nonisothermal flow paths, time dependent dispersion, variable hydrologic saturation, gas composition, mineralogic and petrographic characteristics, etc. Furthermore, a variety of chemical processes governed by different physical relations are expected to contribute to retardation (e.g., adsorption, ion exchange, coprecipitation, exclusion). Important questions include: to what extent can the anticipated complexity be reliably represented by simplified relations; can minimum or conservative K_d values be confidently established for individual radionuclides in the range of possible environments; can nonlinear sorption effects be practically incorporated in transport models?

APPENDIX A

List of Participants

WORKSHOP V

Rachid Ababou
Center for Nuclear Waste Regulatory Analyses
6220 Culebra Road, P.O. Drawer 28510
San Antonio, TX 78284
(512) 552-2583

Alonzo Arredondo
Dept of Geosciences, Box 164
Texas A&I University
Kingsville, TX 78363
(512) 595-3310

Robert Baca
EG&G Idaho
P.O. Box 1625, MS 2107
Idaho Falls, ID 83415
(208) 526-1295

Robert Bowman
Department of Geoscience
New Mexico Inst. of Mining and Technology
Socorro, NM 87801
(505) 835-5992

John Bradburg
U.S. Nuclear Regulatory Commission
NMSS/HLGP, MS 4H3
Washington, D.C. 20555
(301) 492-0535

Adrian Brown
AB Consults, Inc.
155 S. Madison St., #302
Denver, CO 80209
(303) 399-9630

Tom Buscheck
Lawrence Livermore N.L., MS L 208
P.O. Box 808
Livermore, CA 94550
(415) 423-9390

Donald L. Chery, Jr.
NMSS/TR, MS 4H3
U.S. Nuclear Regulatory Commission
Washington, D.C. 20555
(301) 492-3461

John Cushman
Department of Agronomy
Purdue University
West Lafayette, IN 47907
(317) 494-8040

Jack Daemen
Department of Mining Engineering
University of Nevada - Reno
Reno, NV 89557-0139
(702) 784-6961

Roger Eaton, Division 1511
Sandia National Laboratories
P.O. Box 5800
Albuquerque, NM 87185
(505) 844-4063

Alan Flint
U.S. Geological Survey
P.O. Box 327
Mercury, NV 89023
(702) 295-5805

Lorraine Flint
Fenix and Scisson, Inc.
P.O. Box 327
Mercury, NV 89023
(702) 295-5805

William H. Ford
NMSS/TR, MS 4H3
U.S. Nuclear Regulatory Commission
Washington, D.C. 20555
(301) 492-0506

Allan Freeze
3755 Nico Wynd Drive
White Rock, British Columbia
Canada V4A5Z4
(604) 943-4828

David Gallegos, Division 6416
Sandia National Laboratories
P.O. Box 5800
Albuquerque, NM 87185
(505) 844-6218

Glendon Gee
Pacific Northwest Laboratory
P.O. Box 999
Richland, WA 99352
(509) 376-8424

Ronald Green
Center for Nuclear Waste Regulatory Analyses
6220 Culebra Road, P.O. Drawer 28510
San Antonio, TX 78284
(512) 522-5305

Richard Hill
Department of Mechanical Engineering
New Mexico State University
Las Cruces, NM 88004
(505) 646-4342

Dwight Hoxie, U.S. Geological Survey
Box 25046, MS 421
Denver Federal Center
Denver, CO 80225
(303) 236-5019

Paul Kaplan, Division 6312
Sandia National Laboratories
P.O. Box 5800
Albuquerque, NM 87185
(505) 846-1815

Charles Kincaid
Pacific Northwest Laboratories
Battelle Blvd.
Richland, WA 99352
(509) 376-8324

Ed Kwicklis, U.S. Geological Survey
Box 25046, MS 421
Denver Federal Center
Denver, CO 80225
(303) 236-6280

Linda Lehman
L. Lehman and Associates, Inc.
1103 W. Burnsville Pkwy #209
Minneapolis, MN 55337
(612) 894-0357

Mark S. Logsdon
Adrian Brown Consultants
155 S. Madison St., Suite 302
Denver, CO 80209
(303) 399-9630

Roy C. Long, Department of Energy
Yucca Mountain Project Office
P.O. Box 98608
Las Vegas, NV 89193-8606
(702) 794-7503

Swen O. Magnuson
EG&G Idaho, Inc.
P.O. Box 1625/MS 2107
Idaho Falls, ID 83402
(208) 526-1816

Tim Margulies
RES/WMB, MS NL/S-206
U.S. Nuclear Regulatory Commission
Washington, D.C. 20555
(301) 492-3847

James McCord, Division 6416
Sandia National Laboratories
P.O. Box 5800
Albuquerque, NM 87185
(505) 844-5157

Maureen McGraw
Pacific Northwest Laboratory
P.O. Box 999, MS K6-96
Richland, WA 99352
(509) 376-3454

Alan Mitchell
MS J514
Los Alamos National Laboratory
Los Alamos, NM 87545
(505) 667-4085

Bill Murphy
Center for Nuclear Waste Regulatory Analyses
6220 Culebra Road, P.O. Drawer 28510
San Antonio, TX 78284
(512) 522-5263

Claudia Newbury
U.S. Department of Energy
Las Vegas, NV
(702) 794-7942

Thomas J. Nicholson
RES/WMB NL/S-260
U.S. Nuclear Regulatory Commission
Washington, D.C. 20555
(301) 492-3856

John Nitao
Lawrence Livermore National Laboratory
P.O. Box 808, MS 206
Livermore, CA 94566
(415) 423-0297

Natale Olague, Division 6415
Sandia National Laboratories
P.O. Box 5800
Albuquerque, NM 87185
(505) 846-5935

Gary Olhoeft, U.S. Geological Survey
Box 25046, MS 964, Bldg. 2
Denver Federal Center
Denver, CO 80225
(303) 236-1302

Martin Ott
MS J514
Los Alamos National Laboratory
Los Alamos, NM 87545
(505) 667-3631

Ned Patera
MS 514
Los Alamos National Laboratory
Los Alamos, NM 87545
(505) 665-3465

F.J. Pearson, Jr.
1304 Walnut Hill Lane, Suite 210
Irving, TX 75038
(214) 550-1688

Fred Phillips
Department of Geosciences
New Mexico Inst. of Mining and Technology
Socorro, NM 87801
(505) 835-5540

Phillip Pohl, Division 6416
Sandia National Laboratories
P.O. Box 5800
Albuquerque, NM 87185
(505) 844-2992

Karsten Pruess, MS 50E
Earth Science Division, LBL
University of California
Berkeley, CA 94720
(415) 486-6732

Kenneth Richards
Fenix and Scisson, Inc.
P.O. Box 327
Mercury, NV 89023
(702) 295-5998

Ben Ross
Disposal Safety, Inc.
1660 L. St., NW, #314
Washington, D.C. 20036
(202) 293-3993

John L. Russell
Center for Nuclear Waste Regulatory Analyses
6220 Culebra Road, P.O. Drawer 28510
San Antonio, TX 78284
(512) 522-5183

Budhi Sagar
Center for Nuclear Waste Regulatory Analyses
6220 Culebra Road, P.O. Drawer 28510
San Antonio, TX 78284
(512) 522-5252

Marvin (Nick) Saines
Harza Engineering Co.
101 Convention Center Dr., Suite 407
Las Vegas, NV 89109
(702) 794-7191

John Smoot
Battelle PNL, MS K6-77
P.O. Box 999
Richland, WA 99352
(509) 376-8331

Dave Stock
Mechanical and Materials Engineering
Washington State University
Pullman, WA 99163-2920
(509) 335-3223

Peter Striffler, U.S. Geological Survey
Box 25046, MS 421
Denver Federal Center
Denver, CO 80225
(303) 236-6258

John S. Stuckless, U.S. Geological Survey
Box 25046, MS 963
Denver Federal Center
Denver, CO 80225
(303) 236-7886

Falah Thamir, U.S. Geological Survey
Box 25046, MS 421
Denver Federal Center
Denver, CO 80225
(303) 236-5189

Molly Thompson, Division 6233
Sandia National Laboratories
P.O. Box 5800
Albuquerque, NM 87185
(505) 844-7146

Donald C. Thorstenson, U.S. Geological Survey
National Center, MS 432
12201 Sunrise Valley Drive
Reston, VA 22092
(703) 648-5847

Vince Tidwell, Division 6315
Sandia National Laboratories
P.O. Box 5800
Albuquerque, NM 87185
(505) 845-8956

Ines Triay, MS J514
Los Alamos National Laboratory
Los Alamos, NM 87545
(505) 665-1755

Yvonne Tsang, MS 50E
Earth Science Division, LBL
University of California
Berkeley, CA 94720
(415) 486-7047

Chin Fu Tsang, MS 50E
Earth Science Division, LBL
University of California
Berkeley, CA 94720
(415) 486-5782

David Updegraff, Division 6416
Sandia National Laboratories
P.O. Box 5800
Albuquerque, NM 87185

Tilak Verma
NMSS, 4H-3
U.S. Nuclear Regulatory Commission
Washington, D.C. 20555
(301) 492-3465

Charles Voss
Golder and Associates
4104 148th Avenue, NE
Redmond, WA 98052
(206) 391-1655

J.S.Y. Wang, MS 50E
Earth Science Division, LBL
University of California
Berkeley, CA 94720
(415) 486-6753

Ed Weeks, U.S. Geological Survey
Box 25046, MS 421
Denver Federal Center
Denver, CO 80225
(303) 236-4981

Rex Wescott
NMSS/TR, MS 4 H3
Nuclear Regulatory Commission
Washington, D.C. 20555
(301) 492-0755

Roy Williams, Consultant
P.O. Box 15
Viola, ID 83872
(208) 885-6259

Gordon Wittmeyer
Center for Nuclear Waste Regulatory Analyses
6220 Culebra Road, P.O. Drawer 28510
San Antonio, TX 78284
(512) 522-5082

Signe Worstner
Pacific Northwest
P.O. Box 999, MS K6-77
Richland, WA 99352
(509) 376-9758

Al Yang, U.S. Geological Survey
Box 25046, MS 421
Denver Federal Center
Denver, CO 80225
(303) 236-5178

Robert Zimmerman
Lawrence Berkeley Lab
University of California
Berkeley, CA 94720
(415) 486-7106

University of Arizona

Dept. of Hydrology and Water Resources

Randy Bassett
(602) 621-6215

Daniel Evans
(602) 621-7118

Dave Anderson

Amado Guzman
(602) 621-8792

Charles Lohrstorfer

Shlomo Neuman
(602) 621-7114

Shlomo Or

Todd Rasmussen
(602) 621-6216

Mike Sully
(602) 621-7609

Jim Yeh
(602) 621-5943

Dept. of Nuclear and Energy Engineering

Jim McCray
(602) 621-4985

Dept. of Soil and Water Science

Art Warrick
(602) 621-4985

Pete Wierenga
(602) 621-7228

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Department of Hydrology & Water Resources
University of Arizona
Tucson, AZ 85721

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Division of Regulatory Applications
Office of Nuclear Regulatory Research
U.S. Nuclear Regulatory Commission
Washington, DC 20555

Center for Nuclear Waste
Regulatory Analyses
6220 Culebra Road
San Antonio, TX 78228-0510

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The "Workshop on Flow and Transport Through Unsaturated Fractured Rock Related to High-Level Radioactive Waste Disposal" was cosponsored by the NRC, the Center for Nuclear Waste Regulatory Analyses, and the University of Arizona (UAZ) and was held in Tucson, Arizona, on January 7-10, 1991. The focus of this workshop, similar to the earlier four (the first being in 1982), related to hydrogeologic technical issues associated with possible disposal of commercial high-level nuclear waste (HLW) in a geologic repository within an unsaturated fractured rock system which coincides with the UAZ field studies on HLW disposal. The presentations and discussions centered on flow and transport processes and conditions, relevant parameters, as well as state-of-the-art measurement techniques, and modeling capabilities. The workshop consisted of: four half-day technical meetings, a one day field visit to the Apache Leap test site to review ongoing field studies that are examining site characterization techniques and developing data sets for model validation studies, and a final half-day session devoted to examining research needs related to modeling groundwater flow and radionuclide transport in unsaturated, fractured rock. These proceedings provide extended abstracts of the technical presentations and short summaries of the research group reports.

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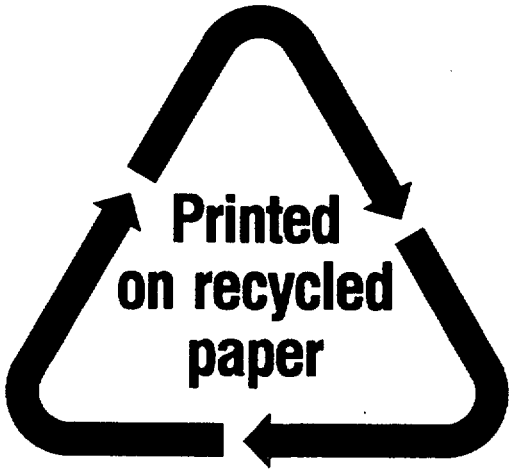

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