In: Hydrgeology of Low Permeability Environments, Vol 2, S.P. Neuman and I. Neretnieks editors, International Association of Hydrogeologists, pp. 239-268

PREDICTING FLOW THROUGH LOW-PERMEABILITY, PARTIALLY SATURATED, FRACTURED ROCK—A REVIEW OF MODELING AND EXPERIMENTAL EFFORTS AT YUCCA MOUNTAIN

R. R. Eaton and N. E. Bixler
Fluid and Thermal Sciences Department

R. J. Glass
Nuclear Waste Repository Technology Department
Sandia National Laboratories, Albuquerque, NM 87185

ABSTRACT

Current interest in storing high-level nuclear waste in underground repositories has resulted in an increased effort to understand the physics of water flow through low-permeability rock. The U.S. Department of Energy is investigating a prospective repository site located in volcanic ash (tuff) hundreds of meters above the water table at Yucca Mountain, Nevada. Consequently, mathematical models and experimental procedures are being developed to provide a better understanding of the hydrology of this low-permeability, partially saturated, fractured rock. Modeling water flow in the vadose zone in soils and in relatively permeable rocks such as sandstone has received considerable attention for many years. The treatment of flow (including nonisothermal conditions) through materials such as the Yucca Mountain tuffs, however, has not received the same level of attention, primarily because it is outside the domain of agricultural and petroleum technology. This paper reviews the status of modeling and experimentation currently being used to understand and predict water flow at the proposed repository site. Several areas of research needs emphasized by the review are outlined. The extremely nonlinear hydraulic properties of these tuffs in combination with their heterogeneous nature makes it a challenging and unique problem from a computational and experimental viewpoint.

INTRODUCTION

Mathematical description of flow through porous media had its origin over a century ago. Early steady-state experiments and analyses were documented by Darcy (1856) during his work to design a water supply system for the city of Dijon, France. Later, Richards (1931) addressed the transient, isothermal, porous-flow problem. Since that time a number of disciplines have cultivated the understanding of flow through porous media. These disciplines include agriculture, mining, groundwater management, toxic waste disposal, landfill safety, reservoir management, geothermal energy, oil recovery, soils stability in construction, pesticide control, and filter design. The general scope of flow through porous media has been discussed in a previous review paper by Nielsen *et al.* (1986), who point out that in the past few decades a great deal of effort has been expended to understand the complexities of various interactive physical, chemical, and microbiological mechanisms affecting unsaturated flow. The lack of experimental and theoretical understanding of the unsaturated zone, however, has limited accurate predictions and in their view, increased the need for basic research in this complex field.

Long-term underground storage of high-level nuclear waste in geologic formations has recently generated international interest in better understanding how water flows through fractured rock. Several countries, including the United States, Sweden, France, Canada, Britain, and Japan, are all investigating the possibilities of underground waste storage.

The U. S. Department of Energy (DOE) has proposed to locate a repository in the unsaturated zone of Yucca Mountain in Nevada. Several positive attributes are associated with locating a repository in the unsaturated zone (Winograd, 1981). For example, the nature of unsaturated rock is thought to significantly reduce the mechanisms for dissolving and transporting radionuclides from the repository to the accessible environment. In an unsaturated state, the fractures are thought to remain dry and create natural barriers to the flow of water and dissolved radionuclides. Computational and experimental aspects of the problem, however, are significantly more complicated in the unsaturated zone than in the saturated zone. The U. S. Nuclear Regulatory Commission (NRC) has stipulated licensing requirements for waste repositories built in the United States. To assess the performance of the repository with respect to these requirements, travel times for water to move from the repository to the accessible environment must be determined. Accumulative probability density function for radionuclide release to the accessible environment also is required as a part of total system performance assessment. Because under many scenarios, the transport of the radionuclide dissolved in the liquid phase is the major vector for radionuclide migration, understanding of water flow through unsaturated rock is of considerable importance.

Yucca Mountain is located in West-Central Nevada on land managed by three government agencies: the DOE (Nevada Test Site), the Bureau of Land Management, and the United States Air Force (Nellis Base) (See Figure 1). It forms a north-south trending ridge with a steep western scarp rising about 250 m above the adjacent basin floor. Yucca Mountain is an eastward dipping fault block predominantly composed of ash flow and ash fall tuffs, which create alternating welded, nonwelded, and bedded layers. The proposed repository will be located 150 to 400 m above the water table and greater then 200 m below the ground surface, where the *in situ* saturation has been measured at 47 to 89% (Weeks and Wilson, 1984). Although the local annual rainfall is nearly 20 cm, the average infiltration rate has been predicted to be less than 0.1 mm/yr (Montazer *et al.*, 1988). The densely welded tuff units have low saturated matrix conductivities, on the order of 10^{-11} m/s, and high saturated fracture conductivities (Peters and Klavetter, 1988). Matrix porosity ranges from 0.03 to 0.30. Fracture porosity ranges from 10^{-5} to 10^{-3}. The nonwelded, vitric tuffs have few fractures and relatively high saturated matrix conductivities in the range of 10^{-8} to

10^{-6} m/s. The nonwelded zeolitized tuffs have low saturated matrix conductivities, 10^{-11} m/s or less, and matrix porosity ranging from about 0.20 to 0.40. Additional heterogeneity and anisotropy exist within each of the units as a result of such processes as microlayering, fracturing, inclusion of fragments and air pockets, cross-bed vitrification, and others.

Test wells drilled at the crest of Yucca Mountain show that the mountain is capped by about 125 m of highly fractured welded tuff that make up the Tiva Canyon welded unit (Montazer and Wilson, 1984). This is underlain by about 30 m of sparsely fractured nonwelded and bedded tuff overlying about 300 m of highly fractured, moderately to densely welded tuffs of the Topopah Spring unit. Underlying this unit and extending down below the water table is the Calico Hills nonwelded and bedded unit. A cross section of the mountain with the proposed repository location is shown in Figure 2.

Because of the importance of this proposed underground waste repository and the need for credible model development and validation, this paper will be devoted to a review of our present understanding and capability to predict water flow through low-permeability, partially saturated, fractured or unfractured tuff. A number of physical processes must be considered to model water movement through the layers of unsaturated tuff at Yucca Mountain. Nonisothermal conditions may result from naturally occurring geothermal gradients, daily and yearly temperature cycles at the surface and from nuclear waste emplaced in the repository. Vapor transport carrying solutes toward the waste containers may occur in the near field (Evans and Nicholson, 1987). Vapor transport resulting from geothermal gradients may also be important (Ross, 1984). Topographic effects on gas flow in unsaturated fractured rock may cause air flow through Yucca Mountain (Weeks, 1987; Kipp, 1987). Barometric pumping at the site may be an effective process for drying out the mountain according to Tsang and Pruess (1987). Large-scale density plumes above a warm repository may generate air circulation. Geochemical processes will most likely influence the motion of the water and hydraulic properties of the tuff at least in the vicinity of the repository. The conditions for instability of unsaturated flows may exist within the layered formation as well as within individual unsaturated fractures (Glass *et al.*, 1989 a, b). Process time scales, which describe the repository problem, range from minutes for rainstorms to thousands of years for groundwater travel times.

The Yucca Mountain Project (YMP) has unique computational challenges. The hydraulic properties of the unsaturated rock are extremely nonlinear. In a typical calculation, the permeability used in the transient partial differential equation that mathematically describes the flow varies by orders of magnitude. Futhermore, in the vicinity of the buried waste containers the temperatures may be high enough to result in multiphase flow conditions. Because time scales of interest are as long as 10,000 yr, extrapolations from known data will have to be made through numerical calculations that typically require large computer central processor unit (CPU) times.

Experimentally, the project has unique challenges as well. The low permeabilities of the welded units usually require very long elapsed times for experiments and extreme boundary condition pressures or initial conditions, far from the *in situ* conditions in Yucca Mountain. An underground laboratory for field-scale testing (experimental shaft facility) is planned, however, emphasis will also be placed on laboratory-scale experimentation followed by extrapolation to the repository scale.

The unique characteristics of the nonlinear unsaturated flow problem have fostered the development of numerical procedures to investigate waste storage at an underground repository. A summary of the early stages of modeling capabilities applicable to the design and performance evaluation of underground repositories was given by Golder Associates (1979). They focused primarily on saturated flow. Evans (1983) gave a status of modeling capabilities which included unsaturated flow. He addresses modeling of fluid and heat flow in partially saturated, fractured, porous media for evaluating the option of an unsaturated disposal site. A general overview of flow and transport through unsaturated fractured rock was given by Evans and Nicholson (1987). They outlined many of the concepts of flow in fractured porous rock and summarized their ongoing research program. Additional aspects of the progress in numerical modeling through 1986 were given by Pruess and Wang (1987).

Research supporting YMP emphasizes the understanding of macroscopic, Darcy-scale, nonisothermal water movement in heterogeneous, anisotropic, fractured rock from first principles for the purpose of (1) identifying, evaluating, and bounding mechanisms or combinations of parameters and circumstances that may cause the natural repository barrier to fail to meet the regulatory compliance criteria, and (2) exploring the validity of model simplifications needed for performance assessment calculations. This research approach combines numerical solutions of mathematical models that incorporate the proper physics with systematic experimentation in the laboratory and in the field.

The remainder of this paper covers the following: (1) a summary of the macroscopic models that have been developed to simulate water flow through low permeability, partially saturated highly fractured rock; (2) a review of the numerical approaches that have been used; (3) a description of the verification effort that will assist in giving credence to the existing computational codes; (4) a discussion of the model validation process, with emphasis on completed and needed physical experimentation; (5) a summary of additional areas of needed research; and (6) a review of various repository scenarios that have been computed to date.

MATHEMATICAL MODELING

A number of texts present a basic understanding of flow in porous media (e.g., Freeze and Cherry; 1979, Huyakorn and Pinder, 1983; de Marsily, 1986; Bear and Verruijt, 1988). The basis for the theory of partially saturated flows is classical continuum mechanics, from which are derived expressions for conservation of mass and energy. In addition, a constitutive relation is needed to relate mass flux to pressure gradient. In most cases where flow is sufficiently slow, the linear relationship observed by Darcy (1856) is prescribed, even when the flow is partially saturated. However, the constant of proportionality, permeability, strongly depends on the local saturation when the porous medium is not fully saturated. The nonlinear character of this dependence is what makes partially saturated flows computationally difficult.

The theory of partially saturated flows is even more challenging for fractured rocks where two distinct scales, porosities, and permeabilities are involved. Several approaches have been devised to analyze flow in such media. The simplest and most direct approach is to treat the fractures discretely. Each fracture is ascribed its own characteristics and constitutive relationships. While such an approach is appealing in principle, in practice it becomes overly cumbersome when the number of fractures exceeds a relatively small number, on the order of 10 or 100. This problem has been investigated by Neuman, 1987. He uses a stochastic continuum representation of fractured rock permeability as an alternative to the REV and fracture network concepts. Another approach to the problem is to define an "effective" continuum that accounts for both the properties of the rock matrix and of the fractures. Dual porosity models (e.g., Barenblatt *et al.*, 1960; Warren and Root, 1963; Odeh, 1965; Duguid and Lee, 1977) attempt to do this by overlaying two continua, one to represent the matrix and the other to represent the fractures, that are coupled in some way so that exchange of mass is allowed. When exchange of mass is fast compared with other transients in the flow, the two continua can be collapsed into one with effective properties that represent both (Peters and Klavetter, 1988). This latter approach has been used almost exclusively to model the field-scale hydrology of Yucca Mountain because the flows there are thought to be extremely slow (on the order of 0.1 mm/yr) and transients tend to be quite slow. The assumption that mass exchange between continua is relatively fast compared with other relevant time scales implies that local pressure equilibrium exists between matrix and fractures. This greatly simplifies the modeling of such materials. Figure 3 shows a typical curve of the composite material permeability obtained using area-weighted fracture and matrix permeability.

Most of Yucca Mountain is relatively isothermal below about 10 m depth. However, because of the geothermal gradient, the temperature increases approximately $1°C$ per 40 m of depth (Freeze and Cherry, 1979). Because the thermal variations over the portion of the mountain of interest for performance assessment is only 10° or $20°C$, most modeling to date has not accounted for a balance of energy. However, a region encompassing the proposed repository and extending tens of meters from it would be heated significantly by the spent fuel for 100 or more years after emplacement. The temperature in a portion of this region would probably exceed the boiling point and, thus, water change of phase would occur. Within this region, the porous heat-pipe phenomena would be established, in which water and vapor would flow counter to each other: water along gravity and the capillary pressure gradient toward the repository, and vapor along the vapor pressure gradient away from the repository. This mechanism could also cause minerals to dissolve away from the repository and be transported toward it, thus modifying the permeabilities within the region. In addition, thermal stresses might further modify permeabilities, especially in the fractures.

At the very least, two additional equations are needed to model this zone. The first is algebraic if a vapor/liquid equilibrium is assumed (Pruess, 1987). If a vapor/liquid equilibrium is not precisely demanded, however, then the first equation is a partial differential equation (PDE) representing flow of the vapor component of the gaseous phase (Bixler, 1985; Hadley, 1985). From a computational point of view, both approaches have advantages and disadvantages that will be discussed in the following section. The second equation is a PDE representing flow of the air component of the gaseous phase. A number of mechanisms are likely to be important in the gaseous phase. Darcy flow is important for this phase as well as for the liquid phase. Knudsen diffusion may also be important because average pore diameters are only on the order of 100 $Å$, and the mean free path of a molecule is about 1000 $Å$ at standard conditions (Reda, 1987b). Binary diffusion often controls the motion of the gaseous components where temperatures are less than $100°C$. Thermodiffusion may be important in some cases but is usually neglected.

Scientific understanding of nonisothermal two-phase flows in porous media dates back to the experimental work of Ceaglske and Hougen (1937) on the drying of sand. Philip and de Vries (1957) first formulated a mathematical model for two-phase flow through porous media while Whitaker (1967 and 1973) and Slattery (1970) put the theory on a more formal foundation by deriving governing equations based on an averaging theory. More recent and more complete attempts to model such flows include the works of Hadley (1982) and of Zanotti and Carbonell (1984). Hadley (1984) and Whitaker (1985) have shown that their models describe well the drying experiment performed by Ceaglske and Hougen.

In addition to the mechanisms of two-phase flow, it might be important to model the transport of soluble minerals and mechanical strains resulting from thermal stresses in the heat-pipe regime. Because all of the equations would be coupled, a rather large system would have to be solved simultaneously if these and the above effects were to be accounted for. Although this capability does not currently exist, such a capability would be helpful in determining the significant process for various flow regimes.

SOLUTION TECHNIQUES

A general solution technique for either single- or two-phase flows in porous media should be able to account for complicated domain shapes, for variable properties, and for variable boundary and initial conditions. The technique should also be robust, *i.e.*, useful for a broad spectrum of problems. These requirements necessitate the use of good numerical techniques such as effective iterative solvers and adaptive time-stepping schemes. Especially in two-phase flow problems, natural time scales can change dramatically during the course of a calculation; thus, it is imperative to be able to adaptively choose time-step size to match the natural time scale. As a result of these requirements, computer codes tend to be large and sophisticated. In the remainder of this section, specific techniques and corresponding codes will be highlighted, with emphasis on those that have been applied to YMP performance assessment.

A range of methods is available to solve such problems, depending on dimensionality and other choices. For example, in one-dimensional, single-phase, steady problems and for certain choices of boundary conditions, it is possible to perform a direct integration to obtain a highly accurate, semianalytic solution. This has been done in the code LLUVIA (Hopkins and Eaton, 1989). Solutions of this type are valuable as initial conditions for higher-dimensional problems and for studies where large numbers of cases must be analyzed, such as in Monte Carlo simulations.

Another specialized approach for rapidly obtaining solutions to steady single-phase problems involves the boundary element method. Because this method is limited to problems for which a Green's function is known, it is necessary to make a special choice for the dependence of permeability on capillary pressure, namely an exponential dependence. In one dimension, analytic solutions can be constructed; in higher dimensions, the boundary element method can be applied to obtain fast solutions. The main limitation of this method is that not all permeability data can be fitted well with an exponential curve.

Other less restrictive one-dimensional, single-phase codes are available. For instance, TOSPAC (Dudley *et al.*, 1988) handles both steady and transient problems using standard finite differences and has been used to investigate various repository scenarios.

Many of the analyses that have been done to date for YMP performance assessment are two-dimensional, single-phase, and transient. Among the various codes represented, three methods for spatial discretization have been employed: standard finite differences, integrated finite differences, and Galerkin/finite elements. TRACR3D (Travis, 1984) uses finite differences to solve either two- or three-dimensional problems. TRUST (Narasimhan and Witherspoon, 1977; Narasimhan *et al.*, 1978) uses integrated finite differences and can also handle either two- or three-dimensional problems. Four codes, FEMWATER (Reeves and Duguid, 1975), SAGUARO (Eaton *et al.*, 1983), NAMMU (Atkinson *et al.*, 1983), and NORIA (Bixler, 1985), are based on Galerkin/finite elements and are written to treat two-dimensional problem configurations. (The single-phase version of NORIA is an offshoot of the two-phase version described below.) All of these codes solve Richards equation.

Two-phase flows are considerably more complicated and difficult to solve than single-phase flows. As a result, relatively few two-phase flows have been analyzed as compared with single-phase flows. Three multiphase codes have been developed for YMP performance assessment. NORIA is based on finite elements and is written for two dimensions, as mentioned above. The WAFE code, which was developed by Travis of Los Alamos National Laboratories, is based on standard finite differences and is written for three dimensions. TOUGH (Pruess and Wang, 1983, and Pruess, 1987) is based on integrated finite differences, can handle problem configurations in either two or three dimensions, and is similar in structure to TRUST. All of these codes solve a large system of simultaneous equations in order to track water, vapor, air, and energy transport.

As mentioned in the previous section, either equilibrium or nonequilibrium vaporization models can be used in multiphase-flow codes. The chief advantage of an equilibrium model is that one partial differential equation is eliminated in favor of an algebraic equation, which enhances computational efficiency. The chief disadvantage is that treating dry-out zones, which may form or disappear during the course of a calculation, is unnatural and somewhat cumbersome. When two phases coexist, the governing equation for water flow includes both phases. Phase equilibrium is an auxiliary condition, essentially determining the partial pressure in the vapor phase. However, in regions where only vapor exists (where the vapor is superheated), the equilibrium condition has to be dropped, and the governing equation for flow only includes the vapor phase. This requires some logic to switch equations, depending on the local conditions in the porous medium. In the nonequilibrium model, an extra partial differential equation is needed, but the same system of equations is solved throughout the domain [see Hadley (1985) or Bixler (1985) for a more complete description of this model].

The extremely nonlinear property behavior needed to represent Yucca Mountain tuffs dictates that computer codes used for performance assessment be very robust. Newton's method appears to be ideal for handling the nonlinearities involved in such problems, especially when composite curves are used to represent both matrix and fractures, as explained above. Occasionally, it is desirable to include discrete fractures in order to model faults at the field scale or fractures at the laboratory scale. This modeling requires the ability to have highly irregular meshes with fine resolution in certain regions. The finite element and integrated finite difference methods are best suited for such modeling.

Because current multi-dimensional, time-dependent numerical codes are extremely CPU-intensive, multiple realizations for statistical analyses are prohibitively expensive. What is needed are simplified models that do not overly compromise accuracy. The amount of computer time required for a problem is a function of the nonlinearities in the material characteristic curves. Current work by Gelhar *et al.* (1985) and Mantoglou and Gelhar (1987) to use equivalent material characteristics obtained through stochastic methods is encouraging but will require further application before its usefulness can be fully assessed. The work of Hills *et al.* (1989) shows promise for computing results with considerably less computer time than is required by the currently used codes; however, the method, which solves for moisture content, cannot be used if complete saturation occurs anywhere in the solution domain. He shows that the use of the water content formulation instead of the pressure head formulation is superior for some simulations because of its lack of sensitivity to initial conditions. Therefore the water content-based algorithm is from 1 to 3 orders of magnitude faster than the pressure formulation when applied to infiltration into very dry soils.

SOLUTION VERIFICATION

The use of computer codes for analyzing and characterizing the proposed underground nuclear waste site requires extensive solution verification, which simply demonstrates that the numerical solution solves the mathematical equations correctly. In analogy with analytical solutions, this is equivalent to substitution of the solution back into the solved equation; however, it is much less straightforward to do this when the solutions solve the partial differential equations only approximately. Two general types of verification (benchmarking) exercises can be used: (1) comparison to analytical or semianalytical solutions and (2) code-to-code comparison with independently written codes, which may use different solution algorithms and methods. The former is usually constrained by problem dimensionality, the degree of nonlinearity, and by the types of initial and boundary conditions that can be accommodated; the latter is relatively unconstrained by these aspects.

With respect to both isothermal and nonisothermal flows, exact solutions for some situations are available and are of vital importance for verifying numerical solutions, for pointing out where numerical solutions lack accuracy, and for providing bounds on solution behavior. Analytical/numerical comparisons not only increase understanding of physical processes but can also provide valuable guidance for applying numerical models appropriately, i.e., for choosing proper temporal and spatial resolution to obtain solutions to the accuracy desired.

Verification of numerical solutions by showing correspondence with exact solutions increases our confidence in the code's ability to yield accurate solutions for more complicated problems. It is sometimes assumed that the simplifications needed to obtain analytical solutions do not allow adequate testing of a numerical code. This, however, is not entirely true. Analytical solutions often incorporate at least part of the complications that the numerical solutions must handle when solving more general problems. The process of comparing analytical and numerical solutions has yet to be fully accomplished for the codes currently being used for performance assessment calculations.

For isothermal flow, numerical codes have traditionally been compared with Philip's (1969) perturbation series solution for one-dimensional, transient infiltration into a semi-infinite porous medium at a uniform initial moisture content (see e.g., Haverkamp *et al.*, 1977; Haverkamp and Vauclin, 1981). The top boundary condition is taken as a step change in the supply moisture content at t=0 and is held constant during the infiltration event. Detailed comparisons performed by Haverkamp and Vauclin demonstrate that a large error can occur (on the order of 56% or higher) if temporal and spatial resolutions are not chosen properly. No comparisons have been made for the same problem with a constant flux boundary condition or for time varying boundary conditions. Nonconstant boundary condition solutions for the transient, one-dimensional vertical infiltration problem have been constructed using similarity techniques. One such solution, found by Fleming *et al.* (1986), is currently being used by the authors to systematically explore accuracy constraints on numerical codes as a function of the degree of nonlinearity in hydraulic properties and initial moisture content. In two- and three-dimensional numerical solutions, the influence of grid orientation can be very influential, as demonstrated in oil reservoir simulation (Ewing, 1983). Steady-state solutions by Philip (1969), for special conductivity functions, can be used for verification.

Some progress has been made toward benchmarking nonisothermal two-phase flow codes. To the authors' knowledge, no purely analytical solutions exist, but for steady, one-dimensional problems, a semianalytic solution, for which numerical integration is required, has been developed by Udell and coworkers (Udell, 1985; Udell and Fitch, 1986). This semianalytic solution contains most of the complex physical mechanisms that the codes are equipped to handle and so is a good basis for benchmarking. Pruess has found good agreement between this solution and results using TOUGH.

Four hydrology codes were compared extensively under the auspices of COVE-2A (Code Verification Exercise), (Barnard and Prindle, 1990). The goals of this activity were to: (1) demonstrate and compare the numerical accuracy and sensitivity of certain codes; (2) identify and resolve problems in running typical flow-field codes; and (3) evaluate computer requirements for running the codes. In this exercise, six steady-state and six transient one-dimensional, isothermal cases were analyzed. The four codes used were TRUST (Narasimhan and Witherspoon, 1977; Narasimhan *et al.*, 1978); NORIA (Bixler, 1985); TOSPAC (Dudley *et al.*, 1988); and TRACR3D (Travis, 1984). The comparisons showed that all of the codes were able to solve the 12 cases with reasonable accuracy, although the computer time requirements for the various codes varied by a factor of two as did the magnitude of nonphysical pressure overshoots and undershoots which tended to occur at material interfaces where the material properties varied widely.

Following an initiative by the Swedish Nuclear Power Inspectorate an international study for comparing groundwater hydrology models, HYDROCOIN (Andersson et al., 1988), was started in 1984. The goals of the study were as follows: (1) determine the accuracy of different solution algorithms for calculating groundwater flows, (2) evaluate the capabilities of different models to describe field measurements, and (3) study the importance of various physical phenomena on groundwater flow calculations. At present there are 14 organizations from 11 countries with over 20 project teams participating. Approximately 32 numerical codes are being used by the project teams to work one or all of the problems defined in the study, which range from one-dimensional, saturated, steady-state to partially saturated, transient, two-dimensional problems. The latter class of problems requires tens of Cray X-MP hours for solution.

Most of the participants in the COVE and HYDROCOIN exercises used codes that they had personally developed. Updegraff and Bonano (1988) took a different approach and used three codes (NORIA, PETROS, and TOUGH) with which they had no developmental experience and attempted to work five heat-driven problems. Their results show that even for experienced modelers, successful simulation depends to some extent on the user being familiar with the code being used.

MODEL VALIDATION

Over the past few years, the validity of models (i.e., how well they represent the true physical system) applied to predict long-term transport of water and contaminants in both saturated and unsaturated zones has become a topic of great concern. An international effort to validate hydrologic flow and transport models that relate to radionuclide transport in variably fractured and variably saturated porous media (INTRAVAL, described by Nicholson *et al.*, 1988) was begun in 1987. In addition, conferences and workshops devoted to this issue have been conducted recently (Donigian, 1987; Wierenga and Bachelet, 1988). Philosophical discussions of model validation issues have been given by a variety of researchers, such as Tsang (1987) and Jones and Rao (1988). As part of the Office of Civilian Radioactive Waste Management (OCRWM), a method for model validation has been recently formulated.

Conceptual model formulation begins by making simplifying assumptions; i.e., unimportant physical processes are neglected. The key to the model validation process is listing and understanding, generally through physical and numerical experiments, the assumptions made in a particular conceptual model. An approach to model validation is to challenge these assumptions and bound their validity and thus bound the validity of the model. This approach leads to increased fundamental understanding of the processes incorporated in the model and can guide a site characterization effort by providing key informational needs so that the occurrence of a particular process can be evaluated.

Simplifying assumptions included in a model may be checked by weighing the processes or terms in the full governing equations relative to each other. The coupling between processes must also be understood before terms are neglected. For a model to have a chance of accurately predicting system response, the physics of the major processes that occur for the range of parameter space and boundary conditions within which the model will be applied must be represented correctly.

Model validation requires comparing model prediction to physical system response. As part of a validation effort, laboratory studies fill a critical need to test our understanding of a particular process in isolation from complications due to interaction with other processes. This simplification is a necessary first step toward understanding and should be exploited fully. Field-scale studies must be conducted not only for validating models at the field scale but for identifying and understanding additional processes that may occur and for performing systematic experimentation for adequate evaluation. As a result of its importance in agricultural systems, substantial experimentation has occurred in unconsolidated sediments (soil) in the laboratory and in the field. Because similar physics and validation methods apply for unconsolidated as well as consolidated porous media, validation of models for unsaturated flow and transport in unconsolidated systems is considered a useful first step toward model validation in unsaturated fractured rock. Two field-scale experimental programs are currently underway in unsaturated zones within unconsolidated media in arid New Mexico to provide data sets for model validation exercises (Stephens *et al.*, 1988; Wierenga, 1988).

Essentially no experimentation was performed with respect to water flow in unsaturated, fractured, low-permeability rock before the beginning of YMP in 1978.

Since this time, a small number of laboratory and field-scale experiments have been conducted, and many more are planned. The emphasis of many of the experiments so far has been to demonstrate flow and transport processes expected to occur within these formations. Experimental difficulties arise because of the extremely low pore pressures that exist in the unsaturated rock (about -100 bars for a saturation of 0.5 in the welded units) and the long experimental time scales required. Pressure-saturation models have been fit to data obtained from 1 cm diameter plugs from borehole cores in a number of the strata present at Yucca Mountain (Peters et al., 1984). Hydraulic property data are also being measured on similarly sized samples at a site in the Apache Leap Tuff of Arizona (Yeh *et al.*, 1988). Additional experiments at the Apache Leap Tuff site are currently being conducted as part of INTRAVAL by the University of Arizona.

Several experiments have been conducted to determine the nature of water flow through typical rock cores. The results of these and other field- and laboratory-scale studies are given below. Computational results are compared with experimental results where they are available.

LABORATORY-SCALE STUDIES

Reda (1987a) conducted one of the initial transient, isothermal, unsaturated flow experiments in a 24.8 cm long, 5.1 cm diameter core of densely welded tuff from the Busted Butte outcrop of the Nevada Test Site. Adjacent cores were used to measure the unfractured matrix liquid permeability (Reda 1985; Reda and Hadley, 1986) and gas permeability as a function of pore pressure (Reda, 1987b). Under a confining pressure of 5.5 MPa, water was supplied at a pressure of 0.46 MPa to both ends of an initially dry core evacuated of all gases. The water profile was monitored for a period of 624 hr with a gamma-beam densitometer. The core, which was initially thought to be fracture free, was found to have three significant transverse fractures, which greatly impeded the transient liquid transport. A schematic of the core showing the locations of the transverse fractures is given in Figure 4. Eaton and Bixler (1987) applied the finite element code NORIA (Bixler, 1985) to model Reda's experiment. Their computational mesh consisted of 43 eight-node, subparametric, quadrilateral elements. The measured dependence of saturation on capillary pressure was fit to a van Genuchten (1980) functional form. Using the theory of Mualem (1976), the fitted saturation-capillary pressure curve yields the presumed dependence of liquid permeability on liquid pressure. Results show that the computed time-dependent saturation fronts compare reasonably well with the experimental data, as can be seen in Figures 5, 6, and 7. The largest differences occur near the fractures and have been attributed to the inability of the gamma beam equipment to sufficiently resolve the moisture content in and near a fracture (gamma beam width was 1/16 in.). The other region of discrepancy occurs near the middle of the core at late times where the calculations give filling rates less than those found experimentally.

An isothermal drying experiment was also conducted on the same core by Russo and Reda (1987). Dry nitrogen flowed over each end of the core for a 1400 hr. period during which the water profile was monitored. Fractures were found to be regions of rapid dryout even though they were internal to the core. Computational simulations of this experiment were done by Bixler *et al.* (1987) again using NORIA. Moisture losses were calculated within 5% of experimentally measured values when experimentally measured nonuniform matrix permeability and tuff-like fracture permeabilities were incorporated in the model. Predicted effective saturation profiles were also somewhat different than measured profiles (Figure 8). The measured profiles contain a relatively large amount of "scatter" that appears to be almost periodic. The "scatter" is most likely the result of small-scale property variations in the tuff core. Also, predicted effective saturations fell off sharply near the boundaries, whereas measured ones did not. A possible explanation for this discrepancy is that the presumed permeability curves fall off too rapidly with capillary pressure, i.e., with saturation, making it overly difficult for moisture to flow to the ends of the core in these simulations.

Peters *et al.* (1987) measured and modeled water imbibition in a core of unfractured, nonwelded, highly porous (48%), relatively permeable ($5x10^{-7}$ m/s) Paintbrush tuff. As a result of the high permeability of the sample, the experiment could be conducted in a short period of time (1 week). The structure of the rock showed three distinct pore sizes: submicrometer to micrometer-sized pores within the pumice grains, 10 to 30 micrometer bubbles within the pumice grains, and 100 to 500 micrometer pores between grains. Modeling of the total imbibition using measured pressure-saturation functions and calculated relative permeability functions tended to overestimate the imbibition rate. Connectivity of the pore-size classes obtained from SEM examination was used to explain this result and to adjust the characteristic curves to obtain better agreement between simulated and measured imbibition rates. Implications of such pore structure is also evident for solute transport.

Lin and Daily (1984) and Daily *et al.* (1987) measured the saturated permeabilities of 2.54 cm and 8 cm diameter x 10 cm long cores of both fractured and unfractured Topopah Spring welded tuff subjected to several wetting and dehydration cycles at a confining pressure of 5.0 MPa. Saturated permeability was measured at various temperatures during each saturation period. Permeability of the fractured samples was initially dominated by the fractures; however, with each dehydration/rehydration cycle the permeability decreased by an order of magnitude until it was the same as the unfractured core. The decrease in permeability was attributed to the healing of fractures by the redistribution of silica within the fracture apparently occurring only above $96°C$. Permeability of the unfractured sample did not decrease under similar circumstances. It should be noted, however, that the fractures were initially "healed" with silica and pried apart before the experiment. Electrical resistivity tomography was also used in the studies to qualitatively follow moisture movement during the wetting and drying cycles in the core. During dehydration, the unfractured core dried fairly uniformly while the fractured core dried very nonuniformly. Within the fractured core, two stages were noted in the dehydration process: a rapid dryout of fractures followed by slow dryout of the matrix. During rehydration, a uniform wetting front formed in the unfractured core. However, in the fractured core the wetting front was very nonuniform and moved 100 times faster than in the one in the nonfractured core. The matrix wetted from points along the fracture as well as from the core end. Variability of wetting within the fracture was attributed to surface roughness variability and to "viscous fingering." Viscous fingering, however, cannot occur because the viscosity ratio is stabilizing. Orientation of the fracture in the gravity field was not noted, and so the possibility of a gravity-driven instability cannot be assessed; however, given the large pressure gradients used, it is highly improbable that gravitational fingering would have occurred at the scale of their experiment.

Davies (1987) conducted a transient nonisothermal moisture and solute flow experiment in a small-diameter core of welded tuff. The core was initially at a uniform moisture content and soluble dye concentration. A temperature gradient was placed across the sample and the moisture content distribution measured with gamma beam densitometry. Water content increased at the cool end and decreased to essentially zero at the warm end. Distribution of water along the core became constant in a few days with a steady-state condition of water-vapor flux away from the hot end equaling the water flux in the opposite direction. Soluble tracer in the water concentrated at the dry end of the core as is expected in heat-driven, two-phase transport. Apparently no modeling of this experiment has been done yet. The closed-system porous heat-pipe problem has been simulated, however, by Eaton *et al.* (1987) using NORIA. A schematic of the closed-system heat-pipe problem that they modeled is shown in Figure 9. The saturation distribution along the core was calculated as a function of time for a number of cases that varied the imposed temperature difference between the two ends, the initial saturation of the core, and the core permeability. Again, the relative permeability was calculated from saturation-capillary pressure functions using the method of Mualem (1976). The saturation at the hot end was found to be a strong function of the imposed temperature gradient. In Figure 10, the development of the saturation profile in time is shown for an applied temperature difference of $150°K$. Estimated experimental time scales and predicted saturation profiles were found to be sensitive to the assumed rock permeability. It was also found that as the initial saturation increases, the temperature difference at which dryout at the hot end occurs also increases.

FIELD-SCALE STUDIES

A limited number of field studies have been conducted in tuff at the natural analog sites in G-Tunnel at the Nevada Test Site and at the Apache Leap Tuff Site near Superior, Arizona. At G-Tunnel, Zimmerman *et al.* (1986) conducted a small field-scale experiment that provides field data on thermal, mechanical, thermomechanical, and hydrologic properties of a jointed rock mass of volume 8 m^3 of welded tuff. Three thermal cycles were conducted to study the hydrologic behavior of the block at different moisture contents. Two of the temperature cycles exceeded the boiling point. Permeability of a single fracture was measured before and after excavation of the block and during the thermal cycle. Moisture content was measured using a neutron probe. The experiment has not yet been modeled numerically.

At the Apache Leap Tuff Site, field studies funded by the NRC have been ongoing for several years. The progress of these studies is summarized by Evans (1983), Schrauf and Evans (1984), Huang and Evans (1985), Green and Evans (1987), Rasmussen and Evans (1987), and Yeh *et al.* (1988). A series of nine boreholes inclined at angles of 45°were drilled in echelon to a maximum depth of 30 m. The unsaturated hydraulic properties of this site are being determined from borehole core as well as from various specially developed field measurement techniques. Water- and air-flow experiments are planned as well as small-scale heater experiments. Results of a preliminary heater test indicate a very long recovery time of the moisture field in the surrounding tuff after the shutdown of the heater (Davies, 1987).

EXPERIMENTAL NEEDS FOR MODEL VALIDATION

Many questions and concerns remain regarding the adequacy of the physics incorporated in the models used to predict water flow through low-permeability, fractured rock. In order to address a number of fundamental questions of importance to the YMP, we must continue to integrate physical (laboratory and field) experimentation and numerical (computer-based) experimentation. This effort should not only include experimentation on tuff but also on analogous materials where experimental control and data gathering ability can be maximized. Systematic exploration in an experimental system, which allows high-accuracy data within an entire unsaturated flow field, opens the possibility of discovering and characterizing flow mechanisms, such as gravity-induced instabilities, which may possibly be more important for performance assessment than the ones of initial interest. An example of such a laboratory-based system is described by Glass *et al.* (1989c). With a simple light transmission technique, entire moisture content fields in two-dimensional thin slabs of porous media can be recorded with high spatial and temporal resolution. The method was developed with sand as the medium so that hydraulic properties may be easily and systematically varied. Extension of the method to slabs of fabricated rock is in progress as well as to thin slabs of tuff and individual fractures. The application of x-ray tomography in three-dimensional laboratory experiments has been pioneered by Crestana *et al.* (1985) and also should be implemented as part of the experimental effort.

In addition to the development of laboratory-based experimental systems, emphasis in experimental design should be placed on developing and applying the concepts of nondimensionalization, scaling, and similarity to increase understanding and generalize results. Full understanding and application of these concepts will allow efficient laboratory experimentation as well as numerical experimentation and model validation. In conjunction with proper scaling theory, the possibility for the use of a centrifuge for modifying time scales for certain situations with low-permeability media should also be explored.

From both the wetting and drying experiments on the welded tuff core and the associated numerical simulations discussed above, it may be generally stated that as a consequence of matrix material nonuniformities and the presence of microfractures, detailed characterization of welded tuff on a submeter scale is needed to reasonably predict small-scale system response. This conclusion points to the difficulty of modeling on a repository scale with only small-scale property measurements. We must either measure hydraulic properties on a larger scale or develop models to generate equivalent properties on the scale of model application from smaller-scale measurements.

The work of Lin and Daily (1984) and Daily *et al.* 1987) points to the importance of including geochemistry in models of the near field (where the temperatures will exceed $96°C$). It is highly possible that for very large time scales at lower-temperature, near-isothermal conditions, geochemical processes may also be important and thus should be included. Additional research must be conducted in this area. The geochemistry of fracture healing should be investigated as a function of temperature, pore pressure, confining pressure, and wetting and drying cycles. In addition, the question of flow channeling or fingering within unsaturated fractures should be addressed systematically under realistic boundary conditions. We are currently exploring the various causes of such channeled flow patterns within unsaturated fractures in the laboratory so that their importance for performance assessment may be evaluated.

ADDITIONAL AREAS OF NEEDED RESEARCH

There are several areas in which additional systematic, basic research must be done to obtain a clear understanding of the phenomena that control the flow of water through Yucca Mountain. Many of these areas involve both verification and validation. Here, we emphasize several of these areas as well as the need for assessing alternative conceptual models for water flow at Yucca Mountain. Many of these concerns were addressed by J. S. Y. Wang and by Thomas J. Nicholson (Evans, 1988)

The range of validity for Darcy's law as applied to water flow through low permeability unsaturated rock must be determined. Although the composite model developed by Peters and Klavetter (1988) has been extremely useful in the analysis of many repository associated scenarios, the limits of the applicability of this model also needs further investigation, especially for cases where the results of one-dimensional calculations are being used to investigate scenarios in which two-dimensional flow resulting from material heterogeneities exists. In addition, because nearly all of the material properties being used for computational purposes have been measured using centimeter-scale samples of tuff materials, it is also extremely important to determine the applicability of this data on a larger scale. Investigations to determine the importance of scale will be necessary.

Dissolution of minerals in the tuff near the waste containers appears to be probable when multiphase flow results from the heat from the waste containers. If these minerals are then transported to the inner edge of the two-phase region and recrystalized, the tuff properties could change. This in turn could affect water motion in the vicinity of the waste containers. Additional numerical computations need to be done.

The current conceptual model of unsaturated flow within the fractured, welded tuff at Yucca Mountain hypothesizes that flow is dominated by the low matrix potentials within the partially saturated rock matrix, which pulls water from fractures and ensures no fracture flow. If fracture flow occurs, it does so near the surface but dies out rapidly with depth as water is drawn into the matrix. Thus, fractures are thought to be dry away from the surface and wet only at the surface when occasional intense rainstorms fill the holding capacity of the surface soil and water enters exposed fractures from flow at the surface or the saturated soil cover. Deep within the formation, localized "perched" saturated zones may occur as a result of a combination of hydraulic properties, geometry, and flow rates (Prindle and Hopkins, 1989). Fracture flow instigated from these zones again would dissipate with distance as the fracture passes out of the saturated zone. This conceptualization seems realistic if we consider the hydraulic properties of individual matrix blocks to be uniform and unaltered by the flow of water through them and the confluence mechanisms to be negligible compared with the uniform effects of the low matrix potential.

The possibility exists that the hydraulic properties of the matrix next to the fracture may be altered by the passage of water (*i.e.*, formation of clay, deposition of minerals). This alteration may lead to the "armoring" of the fractures against the effects of low matrix potential. Over a long time with periodic input at the surface, the thickness of fracture armoring should increase with depth and thus the depth of sustained fracture flow should increase with time. In addition, flow processes exist that could cause the confluence of supplied water either at the top of the formation (soil surface) or within the formation, such as the merger of fractures, geometry within a fracture, or the instability of unsaturated fracture flow. The combination of confluence and armoring could cause the formation of localized saturated conduits or "weeps" that may extend to depth and persist in both time and space.

REPOSITORY SCENARIOS

The goal of the numerical and laboratory experiment, as discussed in this paper, is both a better understanding of the conceptual and mathematical models and validation of the underlying processes. As this understanding matures, better estimates of the circumstances under which the site may fail to meet the regulatory compliance criteria can be made and used to guide the collection of site characterization data that will be used to determine whether or not those circumstances exist at Yucca Mountain. To date, most calculations of possible failure scenarios involve broad simplifications to the global three dimensional, transient, nonisothermal problem. Either the scale of the problem has been downsized from the repository scale, the dimensionality of the problem has been reduced (often to one), or the physical mechanisms or driving forces have been simplified or approximated. One example is the heat-pipe problem, which has been analyzed by Doughty and Pruess (1985), Eaton *et al.* (1987), Jennings (1984), and Tsang and Pruess (1987). In each of these analyses, either the scale has been small (laboratory or meter scale) or the problem configuration has been greatly simplified.

Wang and Narasimhan (1985) investigated the effect of cyclic climatic changes on the subsurface variations in moisture content. They found that most variations were damped out at depths well above the proposed repository elevation. Kwicklis investigated the effect of dissolution of elements within the rock pore and its affect on the material properties (Evans, 1988). Peterson *et al.* (1989) investigated the effect of residual drilling water on proposed *in situ* experiments. Because of the predicted low infiltration rate at the proposed repository site (less than 0.1 mm/yr), there is concern regarding the relative influence of upward movement of water vapor. Ross (1984) predicted that for infiltration rates of less than 0.03 mm/yr the upward movement of vapor is equivalent to the downflow of liquid water.

A study recently made by Prindle and Hopkins (1989) involves the influence of the geologic dip in the vicinity of faults on the redistribution of the groundwater infiltration. They found that for infiltration rates less than 0.3 mm/yr the dip has little effect on the water-flow pattern. However, for larger infiltration rates the geologic dip in conjunction with the heterogeneities of the various hydrologic units significantly affects the flow patterns, as shown in Figure 11. A large fraction of infiltrating water flows along strata interfaces and is diverted toward the vertical faults. This transient, two-dimensional analysis, which involves 5000 eight-node finite elements, required several hours of CPU time on a Cray X-MP computer.

A numerical investigation of the effect of material heterogeneities on two-dimensional deterministic calculations of water flow and particle travel times was done by Eaton and Dykhuizen (1988). In this study, upper and lower bounds on the infiltration rates for Dirichlet boundary conditions were defined as a function of the degree of material heterogeneity. The object of the study was to determine whether equivalent material properties could be defined for a wide range of material heterogeneities and to determine the influence of flow obstructions on water transport times. The paper shows that the parallel/series concept for equivalent material properties applies to saturated flows and does not apply to unsaturated flows. A new set of limits was proposed. Figure 12 shows the particle pathlines for two different sizes of obstructions. Although the mass flux rate for these two geometries is the same for the applied pressure boundary conditions, the particle transport times vary by a factor of three as shown in Table 1. The decrease in particle travel time for the large obstruction case results from the material being saturated near the obstruction. The water then flows through the fractures at an increased pore velocity.

Hopkins *et al.* (1987) addressed the issue of mine drift ventilation on the moisture content in the matrix surrounding the buried waste containers (Figure 13). They found that the tuff near the drift walls may dry significantly. The results also showed that this drying aids in the containment of solutes in the repository. Figure 14 shows results for water velocity vectors and saturations near the drift.

CONCLUSIONS

Progress has been made toward developing computational techniques and experimental procedures that aid our understanding of how water flows through fractured hard rock. The capabilities, which now exist, have been helpful in providing insight into the potential performance of Yucca Mountain as a host for the proposed underground nuclear waste repository. However, need exists for continued basic research in this area. Several of the powerful numerical codes that have been developed need additional verification. The much more difficult task of model validation needs increased attention, particularly in the evaluation of flow mechanisms that could cause system failure. The effect of fractures and material heterogeneities on global calculations must also be understood so that proper data may be collected as a part of site characterization.

ACKNOWLEDGMENTS

The Yucca Mountain Project, managed by the Nevada Operations Office of the U.S. Department of Energy, is examining the feasibility of a repository for high-level nuclear waste at Yucca Mountain. This work was funded by the DOE under contract number DE-AC04-76DP00789. This document was prepared under Quality Assurance Level III of the Yucca Mountain Project's quality assurance program.

REFERENCES

Andersson, K. B., B. L. Grunfelt, and C. P. Jackson, HYDROCOIN level 2 final report: validation of groundwater flow models with respect to assessment of radioactive waste disposal, draft report, Swedish Nuclear Power Inspectorate, Stockholm, Sweden, 1988.

Atkinson, R., A. W. Herbert, C. P. Jackson, and P. C. Robinson, NAMMU User Guide, Harwell Laboratory, Oxfordshire, England, 1983.

Barenblatt, G. I., I. P. Zheltov, and I. N. Kochina, Basic concepts in the theory of seepage of homogeneous liquids in fissured rocks [strata], *Journal of Appl. Math. Mech.* (Engl. trans.), 24, 852–864, 1960.

Barnard, R. W., R. W. Prindle, Groundwater flow code verification "benchmarking" activity (COVE-2A): analysis of participants' work, SAND89-2558, Sandia National Laboratories, Albuquerque, NM, 1990.

Bear, J., and A. Verruijt, *Groundwater Flow and Pollution*, D. Reidel Publishing Company, Boston, 1988.

Bixler, N. E., NORIA—a finite element computer program for analyzing water, vapor, air, and energy transport in porous media, SAND84-2057, Sandia National Laboratories, Albuquerque, NM, 1985.

Bixler, N. E., R. R. Eaton, and A. J. Russo, Drying analysis of a multiphase, porous-flow experiment in fractured volcanic tuff, *Fundamentals of Heat Transfer in Drying* (Joint ASME/JSME Meeting, Honolulu, Hawaii), 1987.

Ceaglske, N. H., and O. A. Hougen, Drying granular solids, *Ind. Eng. Chem.*, 29, 805–813, 1937.

Crestana, S., S. Mascarenhas, and R. Possi-Mucelli, Static and dynamic three-dimensional studies of water in soil using computed tomographic scanning, *Soil Science*, 140, 326–332, 1985.

Daily, W., W. Lin, and T. Buschec, Hydrological properties of Topopah Spring Tuff—laboratory measurements, *J. Geophys. Res.*, 92, 7854–7864, 1987.

Darcy, H., *Les fontaines publiques de la ville Dijon*, Victor Dalmont, Paris, France, 1856.

Davies, B., Measurement of thermal conductivity and diffusivity in an unsaturated, welded tuff, M. S. Thesis, University of Arizona, 1987.

de Marsily, G., *Quantitative Hydrogeology*, Academic Press, Inc. Orlando, FL, 1986.

Donigian, A. S., Report of model validation discussion group, Proceedings of Workshop on Research Needs for Unsaturated Zone Transport Modeling of Agricultural Chemicals, Annapolis. MD, Nov. 2–4, 1987.

Doughty, C., and K. Pruess, Heat pipe effects in nuclear waste isolation: a review, LBL-20738, Lawrence Berkeley Laboratory, Berkeley, CA, 1985.

Dudley, A. L., R. L. Peters, J. H. Gauthier, M. L. Wilson, M. S. Tierney, and E. A. Klavetter, Total system performance assessment code (TOSPAC) volume 1: physical and mathematical bases, SAND85-0002, Sandia National Laboratories, Albuquerque, NM, 1988.

Duguid, J. O., and P. C. Y. Lee, Flow in fractured porous media, USGS-73-WR-1, *Water Resources Res.*, 13, 558–566, 1977.

Eaton, R. R., D. K. Gartling, and D. E. Larson, SAGUARO—a finite element computer program for partially saturated porous flow problems, SAND86-2772, Sandia National Laboratories, Albuquerque, NM, 1983.

Eaton, R. R., and N. E. Bixler, Analysis of a multiphase, porous-flow imbibition experiment in fracture volcanic tuff, *Flow and Transport Through Unsaturated Fractured Rock*, Geophysical Monograph 42, eds. D. D. Evans and T. J. Nicholson, American Geophysical Union, Washington, DC, 91–98, 1987.

Eaton, R. R., N. E. Bixler, and D. C. Reda, Coupled hydrothermal flows of liquid and vapor in welded tuff: numerical modeling of proposed experiment, *Coupled Processes Associated with Nuclear Waste Repositories*, ed. C. F. Tsang, Academic Press, Orlando, FL, 409–420, 1987.

Eaton, R. R., and R. C. Dykhuizen, Effect of material nonhomogeneities on equivalent conductivities in unsaturated porous media flow, Proceedings of the International Conference and Workshop on the Validation of Flow and Transport Models for the Unsaturated Zone, New Mexico State University, Las Cruces, NM, 1988.

Evans, D. D., Unsaturated flow and transport through fractured rock related to high-level waste repositories, NUREG/CR-3206, 1983.

Evans, D. D., and T. J. Nicholson, Flow and transport through unsaturated fractured rock: an overview, *Flow and Transport Through Unsaturated Fractured Rock*, Geophysical Monograph 42, eds. D. D. Evans and T. J. Nicholson, American Geophysical Union, Washington, DC, 1–10, 1987.

Evans, D. D., Proceedings of workshop IV on *Flow and Transport Through Unsaturated Fractured Rock Related to High-level Radioactive Waste Disposal*, ed., D. Evans, Tucson, AZ., Dec. 12-15, 1988

Ewing, R. E., *The Mathematics of Reservoir Simulation*, ed. Richard E. Ewing, Soc. for Industrial and Applied Mathematics, Philadelphia, PA, 1983.

Fleming, J. F., J. Y. Parlange, and W. L. Hogarth, Scaling of flux and water content relations: comparison of optimal and exact results, *Soil Sci.*, 1137, 464–468, 1986.

Freeze, R. A., and J. A. Cherry, *Groundwater*, Prentice-Hall, Englewood Cliffs, NJ, 1979.

Gelhar, L. D., A. Mantoglou, C. Welty, and K. R. Rehfelft, A review of field-scale physical solute transport process in saturated and unsaturated porous media, final report, EA-4190, Electric Power Research Institute, Palo Alto, CA, 1985.

Glass, R. J., J.-Y. Parlange, and T. S. Steenhuis, Wetting front instability I: theoretical discussion and dimensional analysis, *Water Resources Res.*, 25, 1187–1294, 1989a.

Glass, R. J., T. S. Steenhuis, and J.-Y. Parlange, Wetting front instability II: experimental determination of relationships between system parameters and two-dimensional unstable flow field behavior in initially dry porous media, *Water Resources Res.*, 25, 1195–1207, 1989b.

Glass, R. J., T. S. Steenhuis, and J.-Y. Parlange, Mechanism for finger persistence in homogeneous unsaturated porous media: theory and verification, *Soil Science*, in press, 1989c.

Golder Associates, Numerical modeling capabilities to predict repository performance, UCRL-15176, Golder Associates Inc., Golden, CO, 1979.

Green, R. T., and D. D. Evans, Radionuclide transport as vapor through fractured rock, NUREG/CR-4654, 163, 1987.

Hadley, G. R., Theoretical treatment of evaporation front drying, *Int. J. Heat Mass Transfer*, 25, 1511, 1982.

Hadley, G. R., Numerical modeling of the drying of porous materials, Proceedings of the Fourth International Drying Symposium, 1, Tokyo, Japan, 1984.

Hadley, G. R., PETROS—A program for calculating transport of heat, water vapor, and air through a porous material, SAND84-0878, Sandia National Laboratories, Albuquerque, NM, 1985.

Haverkamp, R., M. Vauclin, J. Tovma, P. J. Wierenga, and G. Vachaud, A comparison of numerical simulation models for one-dimensional infiltration, *Soil Sci. Soc. Am. J.*, 41, 285–294, 1977.

Haverkamp, R. and M. Vauclin, A comparative study of three forms of the Richards equation for predicting one-dimensional infiltration in unsaturated soil, *Soil Sci. Soc. Am J.*, 45, 13–20, 1981.

Hills, R. G., I. Porro, D. B. Hudson, and P. J. Wierenga, Modeling one-dimensional infiltration into very dry soils: 1. Model development and evaluation, *Water Resources Res.*, 25, 1259–1269, 1989.

Hopkins, P. L., R. R. Eaton, and S. Sinnock, Effect of drift ventilation on repository hydrology and resulting solute transport implications, *Flow and Transport Through Unsaturated Fractured Rock*, Geophysical Monograph 42, eds. D. D. Evans and T. J. Nicholson, American Geophysical Union, Washington, DC, 99–106, 1987.

Hopkins P. L., and R. R. Eaton, LLUVIA: a program for one-dimensional, steady-state flow through partially saturated porous media, SAND88-0878, Sandia National Laboratories, Albuquerque, NM, 1989.

Huang, C., and D. D. Evans, A 3-dimensional computer model to simulate fluid flow and contaminant transport through a rock fracture system, NUREG/CR-4042, Nuclear Regulatory Commission, 1985.

Huyakorn, P. S., and G. E. Pinder, *Computational Methods in Subsurface Flow*, Academic Press, New York, 1983.

Jennings, J. D., The heat pipe effect in dual-permeability porous systems, M.S. Thesis, University of California, Berkeley, CA, 1984.

Jones, R. L., and P. S. C. Rao, Reflections on validation and applications of unsaturated zone models, Proceedings of the International Conference and Workshop on the Validation of Flow and Transport Models for the Unsaturated Zone, eds. P.J. Wierenga and D. Bachelet., 197–205, May 23–26, 1988.

Kipp, K. L., Effect of topography on gas flow in unsaturated fractured rock: numerical simulation, *Flow and Transport Through Unsaturated Fractured Rock*, Geophysical Monograph 42, eds. D. D. Evans and T. J. Nicholson, American Geophysical Union, Washington, DC, 11–22, 1987.

Lin, W., and W. Daily, Transport properties of Topopah Spring Tuff, UCRL-53602, Lawrence Livermore National Laboratory, Livermore, CA, 1984.

Mantoglou, A., and L. W. Gelhar, Effective hydraulic conductivities of transient unsaturated flow in stratified soils, *Water Resources Res.*, 23, 57–67, 1987.

Montazer, P., and W. E. Wilson, Conceptual hydrologic model of flow in the unsaturated zone, Yucca Mountain, Nevada, USGS-WRI-84-4345, U. S. Geological Survey, Lakewood, CO, 1984.

Montazer, P., E. P. Weeks, F. Thamir, S. N. Yard, and P. B. Hofrichter, Monitoring the vadose zone in fractured tuff, Yucca Mountain, Nevada, *Ground Water Monitoring Review*, 8, 72–88, 1988.

Mualem, Y., A new model for predicting the hydraulic conductivity of unsaturated porous materials, *Water Resources Res.*, 12, 513–522, 1976.

Narasimhan, T. N., and P. A. Witherspoon, Numerical model for saturated-unsaturated flow in deformable porous media, part 1, theory, *Water Resources Res.*, 13, 657–664, 1977.

Narasimhan, T. N., P. A. Witherspoon, and A. L. Edwards, Numerical model for saturated-unsaturated flow in deformable porous media, part 2, the algorithm, *Water Resources Res.*, 14, 255–261, 1978.

Neuman, A. P., Stochastic continuum representation of fractured rock permeability as an alternative to the REV and fracture network concepts, 28^{th} US Symposium on Rock Mechanics, Tucson, AZ, June 29-July 1, 1987.

Nicholson, T. J., T. J. McCartin, and P. A. Davis, International projects in validating groundwater flow and transport models, Proceedings of the International Conference and Workshop on the Validation of Flow and Transport Models for the Unsaturated Zone, eds. P. J. Wierenga and D. Bachelet, 292–299, May 23–26, 1988.

Nielsen, D. R., M. Th. van Genuchten, and J. W. Biggar, Water flow and solute transport processes in the unsaturated zone, *Water Resources Res.*, 22, 89–108, 1986.

Odeh, A. S., Unsteady behavior of mutually fractured reservoirs, *Soc. Pet. Eng. J.*, 5, 60–65, 1965.

Peters, R. R., A. Klavetter, I. J. Hall, S. C. Blair, P. R. Heller and G. W. Gee, Fracture and matrix hydrologic characteristics of tuffaceous materials from Yucca Mountain, Nye County, Nevada," SAND84-1471, Sandia National Laboratories Albuquerque, NM, 1984.

Peters, R. R., E. A. Klavetter, J. T. George, and J. H. Gauthier, Measuring and modeling water imbibition into tuff, in *Flow and Transport Through Unsaturated Fractured Rock*, Geophysical Monograph 42, eds. D. D. Evans and T. J. Nicholson, American Geophysical Union, Washington, DC, pp 99–106, 1987.

Peters, R. R., and E. A. Klavetter, A continuum model for water movement in an unsaturated fractured rock mass, *Water Resources Res.*, 24, 416–430, 1988.

Peterson, A. C., R. R. Eaton, A. J. Russo, and J. A. Lewin, Technical correspondence in support of an evaluation of the hydrologic effects of exploratory shaft construction at Yucca Mountain, SAND88-2936, Sandia National Laboratories, Albuquerque, NM, 1988.

Philip, J. R., and D. A. de Vries, Moisture movement in porous materials under temperature gradients, *Trans. Am. Geophys. Union,* 38, 222–232, 1957.

Philip, J. R., Theory of infiltration, *Adv. Hydrosci.,* 5, 215–296, 1969.

Prindle, R. W., and P. L. Hopkins, On conditions and parameters important to model sensitivity for unsaturated flow through layered, fractured tuff: results of analyses for HYDROCOIN level 3 case 2, SAND89-0652, Sandia National Laboratories, Albuquerque, NM, 1989.

Pruess, K., and J. S. Y. Wang, TOUGH—a numerical model for isothermal unsaturated flow to study waste canister heating effects, *Materials Research Symposia Proc.,* 26, Boston, MA, 1031–1038, 1983.

Pruess, K., TOUGH user's guide, NUREG/CR-4645, Nuclear Regulatory Commission, 1987.

Pruess, K., and J. S. Y. Wang, Numerical modeling of isothermal and nonisothermal flow in unsaturated fractured rock—a review, *Flow and Transport Through Unsaturated Fractured Rock,* Geophysical Monograph 42, eds. D. D. Evans and T. J. Nicholson, American Geophysical Union, Washington, DC, 11–22, 1987.

Rasmussen, T. C., and D. D. Evans, Unsaturated flow and transport through fractured rock related to high-level waste repositories, NUREG/CR-4655, Nuclear Regulatory Commission, 474, 1987.

Reda, D. C., Liquid permeability measurements on densely welded tuff over the temperature range 25°to 90°C, SAND85-2482, Sandia National Laboratories, Albuquerque, NM, 1985.

Reda, D. C., and G. R. Hadley, Saturated permeability measurements on pumice and welded-tuffaceous materials, *J. Env. Geol. and Water Sci.,* 8, 137–145, 1986.

Reda, D. C., Influence of transverse microfractures on the imbibition of water into initially dry tuffaceous rock, in *Flow and Transport Through Unsaturated Fractured Rock,* Geophysical Monograph 42, eds. D. D. Evans and T. J. Nicholson, American Geophysical Union, Washington, DC, 83–90, 1987a.

Reda, D. C., Slip-flow experiments in welded tuff: the Knudsen diffusion problem, *Coupled Processes Associated with Nuclear Waste Repositories,* ed. C. F. Tsang, Academic Press, Orlando, FL, 485–493, 1987b.

Reeves, M., and J. O. Duguid, Water movement through saturated-unsaturated porous media: a finite-element Galerkin model, ORNL-4927, Oak Ridge National Laboratory, Oak Ridge, TN, 1975.

Richards, L. A., Capillary conduction of liquids through porous mediums, *Physics,* 1, 318–333, 1931.

Ross, B., A conceptual model of deep unsaturated zones with negligible recharge, *Water Resources Res.,* 20, 1627–1629, 1984.

Russo, A. J., and D. C. Reda, Drying of an initially saturated fractured volcanic tuff, Proceedings of the Conference on Multiphase Transport in Porous Media, FED, 60, eds. R. R. Eaton, K. S. Udell, and M. Kaviany, 1987.

Schrauf, T. W., and D. D. Evans, Relationship between the gas conductivity and geometry of a natural fracture, NUREG/CR-3680, Nuclear Regulatory Commission, 1984.

Slattery, J. C., Two-phase flow through porous media, *AIChE Journal,* 16, 245–352, 1970.

Stephens, D. B., A. V. Parsons, E. D. Mattson, K. Black, K. Flanigan, R. S. Bowman, and W. B. Cox, A field experiment of three-dimensional flow and transport in a stratified soil, Proceedings of the International Conference and Workshop on the Validation of Flow and Transport Models for the Unsaturated Zone, eds. P. J. Wierenga and D. Bachelet, 401–413, May 23–26, 1988.

Travis, B. J., TRACR3D: a model of flow and transport in porous/fractured media, LA-9667-MS, Los Alamos National Laboratory, Los Alamos, NM, 1984.

Tsang, C. F., Comments on model validation. *Transport in Porous Media,* 2, 623–629, 1987.

Tsang, Y. W., and K. Pruess, A study of thermally induced convection near a high-level nuclear waste repository in partially saturated fractured tuff, LBL-21311, Lawrence Berkeley Laboratory, Berkeley, CA, 1987.

Udell, K. S., Heat and mass transfer in capillary porous media considering phase change and capillarity—the heat pipe effect, *Int. J. Heat Mass Transfer,* 28, 485–495, 1985.

Udell, K. S., and J. S. Fitch, Heat and mass transfer in capillary porous media considering evaporation, condensation, and noncondensable gas effects, *Heat Transfer in Porous Media and Particulate Flows,* ASME HTD, 46, 1986.

Updegraff, C. D., and E. J. Bonano, Comparison of strongly heat-driven flow codes for unsaturated media, NUREG/CR-5097, Nuclear Regulatory Commission, 1988.

van Genuchten, M. Th., Closed-form equation for predicting the hydraulic conductivity of unsaturated soils, *Soil Sci. Am. J.,* 44, 892–898, 1980.

Wang, J. S. Y., and T. N. Narasimhan, Hydrologic mechanisms governing fluid flow in a partially saturated, fractured, porous medium, *Water Resources Res.,* 21, 1861–1874, 1985.

Warren, J. E., and P. J. Root, Behavior of naturally fractured reservoirs, *Soc. Pet. Eng. J.,* 9, 245–255, 1963.

Weeks, E. P., and W. E. Wilson, Preliminary evaluation of hydrologic properties of cores of unsaturated tuff, test well USW H-1, Water-Resources Investigations Report 84-4193, USGS, Lakewood, CO, 1984.

Weeks, E. P., Effect of topography on gas flow in unsaturated fractured rock: concepts and observations, *Flow and Transport Through Unsaturated Fractured Rock,* Geophysical Monograph 42, eds. D. D. Evans and T. J. Nicholson, American Geophysical Union, Washington, DC, 11–22, 1987.

Whitaker, S., Diffusion and dispersion in porous media, *AIChE Journal*, 13, 420–427, 1967.

Whitaker, S., The transport equations for multi-phase systems, *Chem. Eng. Sci.*, 28, 139–147, 1973.

Whitaker, S., Moisture transport mechanisms during the drying of granular porous media, *Drying '85*, Hemisphere Publishing Corp., Washington, DC, 21–32, 1985.

Wierenga, P.J., Validation of flow and transport models at the Jornada test facility, Proceedings of the International Conference and Workshop on the Validation of Flow and Transport Models for the Unsaturated Zone, eds. P.J. Wierenga and D. Bachelet, 525–530, May 23–26, 1988.

Wierenga, P. J., and D. Bachelet, eds., Proceedings of the International Conference and Workshop on the Validation of Flow and Transport Models for the Unsaturated Zone, New Mexico State University, Las Cruces, NM, 1988.

Winograd, I. J., Radioactive waste storage in thick unsaturated zones, *Science*, 212 (4502), 1457–1464, 1981.

Yeh, T. C. J., T. C. Rasmussen, and D. D. Evans, Simulation of liquid and vapor movement in unsaturated fractured rock at the Apache Leap Tuff Site: models and strategies, NUREG/CR-5097, Nuclear Regulatory Commission, 1988.

Zanotti, F., and R. G. Carbonell, Development of transport equations for multiphase systems—I and II, *Chem. Eng. Sci.*, 39, 263–297, 1984.

Zimmerman, R. M., R. L. Schuch, D. S. Mason, M. L. Wilson, M. E. Hall. M. P. Board, R. P. Bellman, and M. L. Banford, Final report: G-tunnel heated block experiment, SAND84-2620, Sandia National Laboratories, Albuquerque, NM, 1986.

Table 1: EFFECT OF OBSTRUCTION ON PARTICLE TRANSPORT TIME

Pathline	Particle Transport Times (yr) x_o=3.8 m	x_o=1.0 m
1	544	184
2	542	206
3	536	228
4	530	270
5	—	647

Figure 1: Yucca Mountain, plan view.

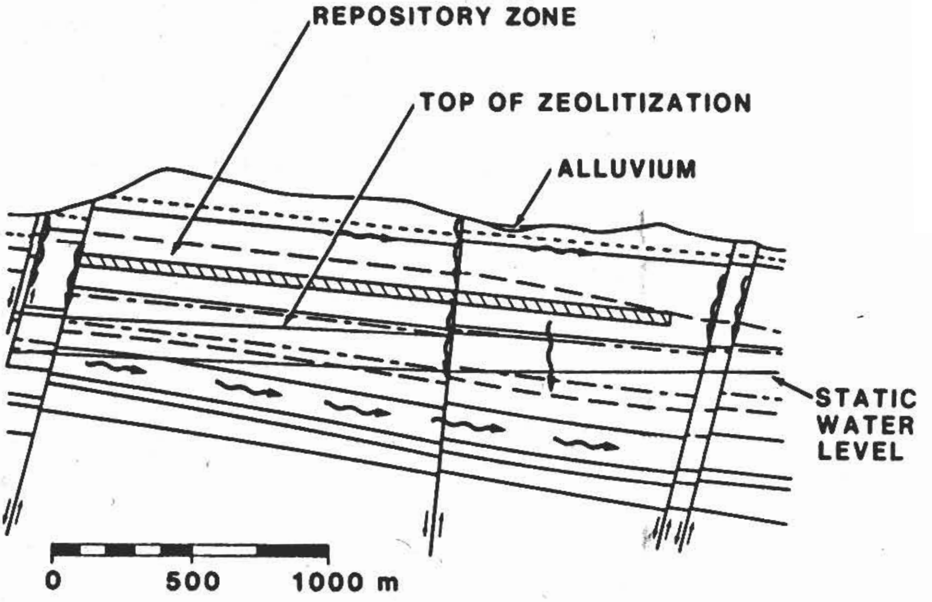

Figure 2: Yucca Mountain.

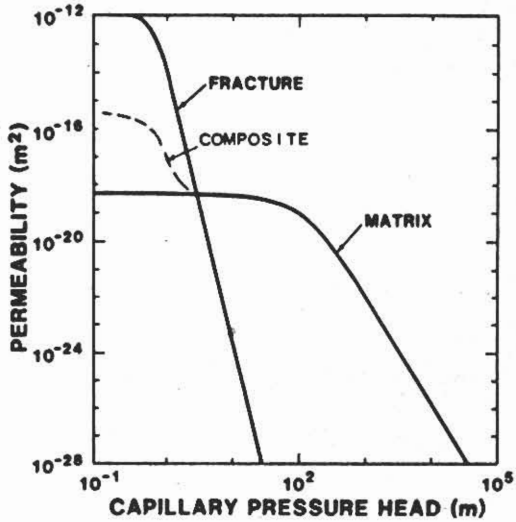

Figure 3: Characteristic curves for permeability.

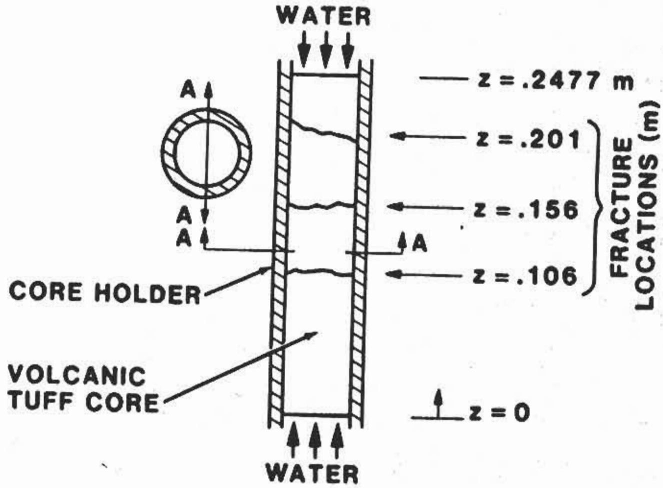

Figure 4: Imbibition and drying experiment geometry.

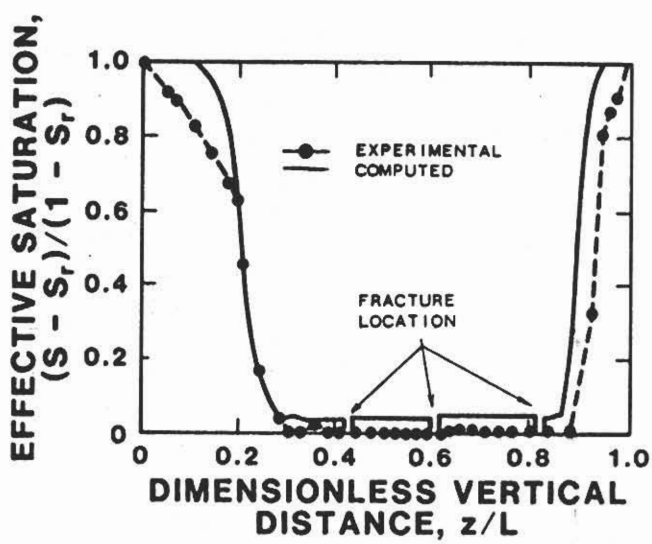

Figure 5: Comparison of predicted effective saturation profile with imbibition experimental data, 1.2 days.

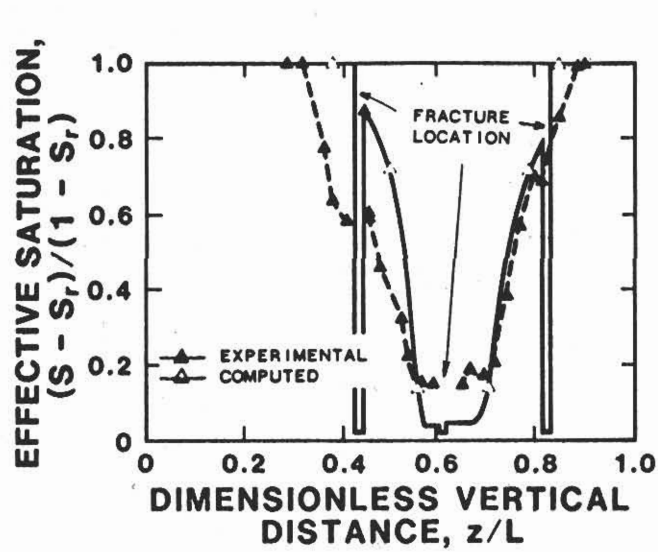

Figure 6: Comparison of predicted effective saturation profile with imbibition experimental data, 12.5 days.

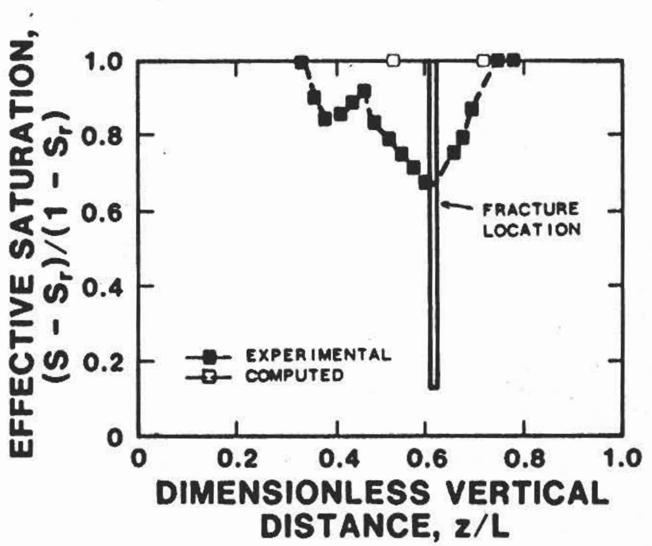

Figure 7: Comparison of predicted effective saturation profile with imbibition experimental data, 26 days.

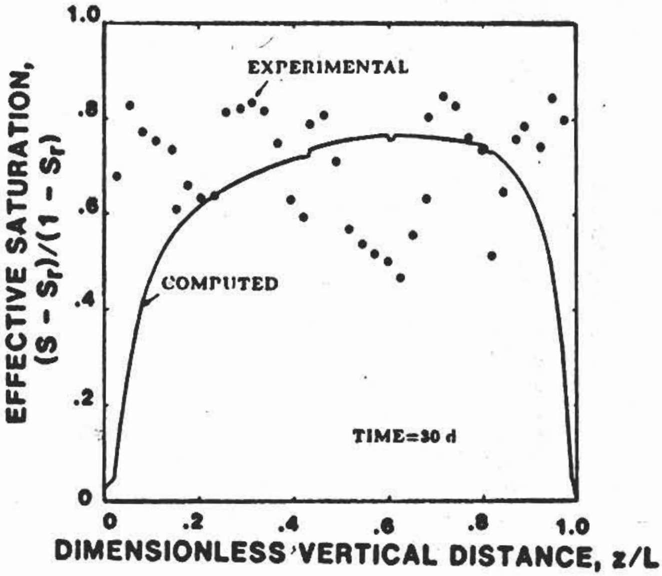

Figure 8: Comparison of predicted effective saturation profile with drying experimental data.

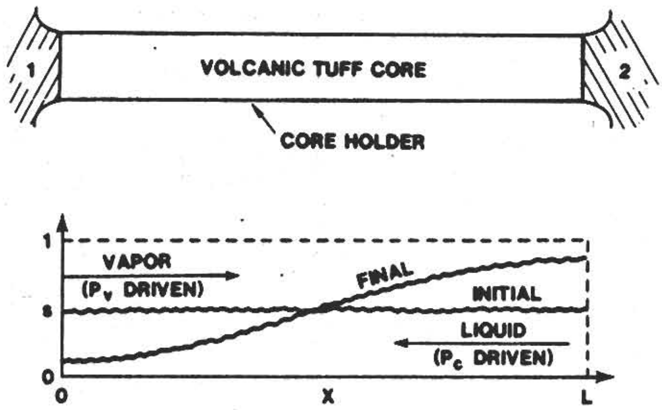

Figure 9: Proposed approach for countercurrent liquid/vapor laboratory experiment. (Top) Schematic of volcanic tuff in core holder. (Bottom) Schematic of closed-system heat pipe.

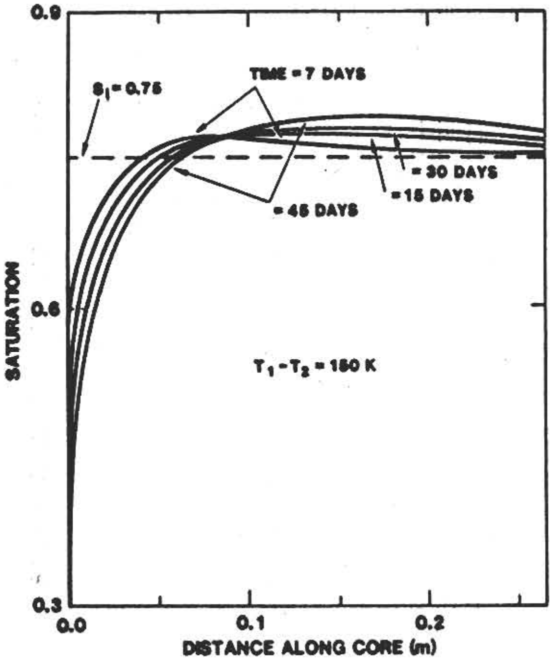

Figure 10: Liquid saturation profiles for applied temperature difference of 150 K at times 7, 15, 30, and 45 days, s_i=0.75.

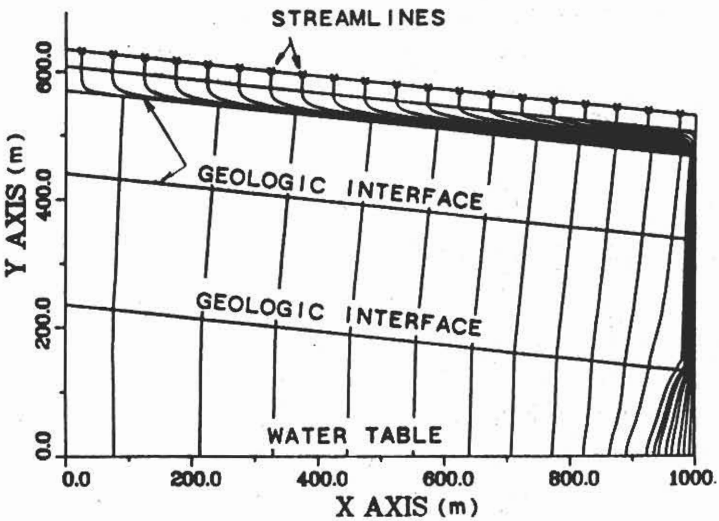

Figure 11: Redistribution of infiltrating water resulting from unit down dip.

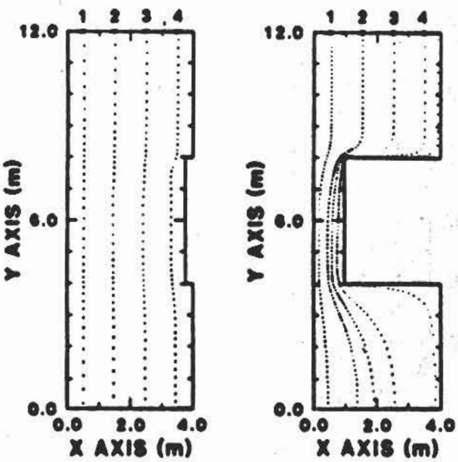

Figure 12: Particle pathlines for two obstruction sizes.

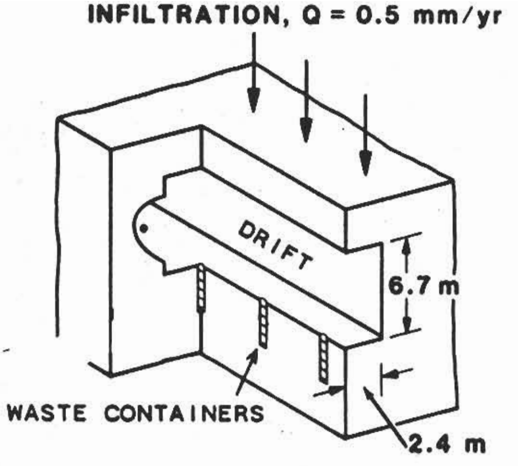

Figure 13: Geometry of drift ventilation investigation.

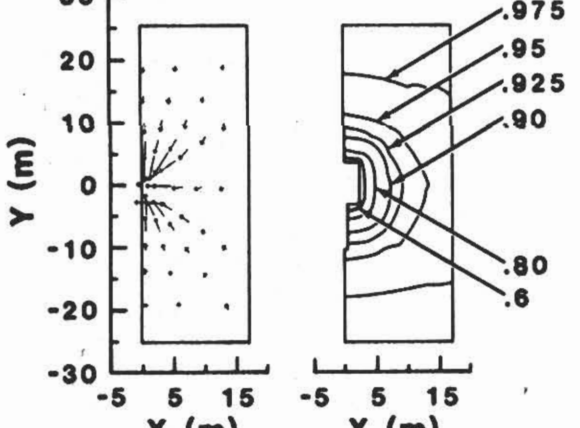

Figure 14: Calculated motion of liquid resulting from drift ventilation, (a) velocity vectors and (b) saturation contours.