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 relatively permeable rocks such as sandstone has received considerable attention for many years. The treatment of flow (excluding 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 make it a challenging and unique problem from a computational and experimental viewpoint.
INTRODUCTION.

Mathematical description of flow through porous media has 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 (1911) 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. (1996), 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 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 escarp 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 600 m above the water table and greater than 200 m below the ground surface, where the water saturation has been measured at 47 to 80% (Wells 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^-12 m/s, and high unsaturated fracture conductivities (Peters and Klawitter, 1948). Matrix porosity ranges from 0.03 to 0.30. Fracture porosity ranges from 10^-4 to 10^-2. The nonwelded, vitric tuffs have few fractures and relatively high saturated matrix conductivities in the range of 10^-6 to 10^-5. 

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7.5 × 10⁻⁹ m/s. The nonwelded chertified tuffs have low saturated matric conductivities, 10⁻⁶ to 10⁻⁴ cm/s or less. Permeability ranges from about 0.20 to 0.40. Additional heterogeneity and anisotropy exist within each of the units as a result of such processes as microcrack-rg, fracturing, inclusion of fragments and air pockets, cross-bed verticalization, 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 Tuff Canyon welded unit (Montaser 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 tuff 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. Noninfiltration 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 solute toward the waste containers may occur in the near field (Evans et al., 1987). Vapor transport resulting from geothermal gradients may 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. Furthermore, 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 permeability of the welded units usually require very long elapsed times for experiments and extreme boundary conditions pressures or initial conditions, far from the in situ conditions in Yucca Mountain. An underground laboratory for field-scale testing (experimental staff 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 Calder Associates (1979). They focused primarily on saturated flow. Evans (1983) gave a status of modeling capabilities which included unsaturated flow. He addressed 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 ongoing research programs. Additional aspects of the progress in numerical modeling through 1986 were given by Freeze 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 tools 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 fluid flow in such media. The simplest and most direct approach is to treat the fractures discretely. Each fracture is described by 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 the fractures. Dual porosity models (e.g., Barenblatt et al., 1960; Warren and Root, 1963; Odeh, 1965; Dugaid 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 effective property that represents 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 (Freeze, 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 (Binder, 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. Keurden diffusion may also be important because average pore diameters are only on the order of 100 A, and the mean free path of a molecule is about 1000 A at standard conditions (Reda, 1987b). Binary diffusion often controls the motion of the gaseous components where temperatures are less than 100°C. Thermo diffusion 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 Czegléde 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 Whithaker (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 Chiew (1984). Hadley (1984) and Whithaker (1985) have shown that their models describe well the drying experiment performed by Czegléde 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 the requirement of accurate code tend to be linear 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 VMP 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-state 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, 1983). 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 full 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, TUSPACE (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 VMP 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. TRAC91D (Travis, 1984) uses finite differences to solve two or three-dimensional problems. NORMA (Nassimian and Witherspoon, 1977; Nassimian et al., 1978) uses integrated finite differences and can also handle either two or three-dimensional problems. Four codes, PEMWATER (Reeves and Duguid, 1975), SAGUARO (Eaton et al., 1983), NAMMU (Atkinson et al., 1983), and NORMA (Bailer, 1985), are based on Galerkin/finite elements and are written to treat two-dimensional problem configurations. The single-phase version of NORMA is an offspring 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 VMP performance assessment. NORMA is based on finite elements and is written for two dimensions, as mentioned above. The WAFPE code, which was developed by Travis of Los Alamos National Laboratory, is based on standard finite differences and is written for three dimensions. TOUGH (Pruss and Wang, 1983, and Pruss, 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 vapor models can be used in multiphase flow codes. The chief advantage of an equilibrium model is that a 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 exist,
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 Bider (1985) for a more complete description of this model].

The extremely nonlinear property behavior needed to represent Yucca Mountain tufts 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 multidimensional, 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 so
ations 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 the actual 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 isotothermal flow, numerical codes have traditionally been compared with Philip's (1969) perturbation water solution for one-dimensional, transient infiltration into a semi-infinite porous medium at a uniform initial moisture content (see, e.g., Haverkamp et al., 1971; Haverkamp and Vassilin, 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 Vassilin demonstrate that a large error can occur (on the order of 50% 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. (Weish has found good agreement between this solution and results using TOUCH, the four hydrology codes were compared extensively under the auspices of CVE-2A (Code Verification Exercise), (Seabold and Prindle, 1991). 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 (Nasarinhm and Witherspoon, 1977; Nasarinhm et al., 1978); NODIA (Bleder, 1985); TOSOPAC (Dudley et al., 1988); and TRACCRD (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 (Anderson 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 95 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. Upcraft 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 systems 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 them with 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 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 unconsolidated 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 low pore pressures expected to occur within these formations. Experimental difficulties arise because of the extremely low pore pressures that exist in the unsaturated rock (about 100 bar for a saturation of 0.3 in the welded unit) and the large 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 sites present at Yucca Mountain (Poteat et al., 1984). Hydraulic property data are also being measured on similarly sized samples at a site in the Apache Leap Tuff of Arizona (Veh et al., 1988). Additional experiments at the Apache Leap Tuff site are currently being conducted as part of INTRAVEL 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. Computed 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 unstructured matrix liquid permeability (Reda 1985; Reda and Hadley, 1986) and gas permeability as a function of core pressure (Reda, 1987b). Under a confining pressure of 5.5 MPa, water was applied at a pressure of 6.46 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 transverse liquid transport. A schematic of the core showing the locations of the transverse fractures is given in Figure 6. Etoot and Bixler (1987) applied the finite element code NORIA (Bixler, 1985) to model Reda's experiment. Their computational mesh consisted of 83 eight-node, sub-parametric, quadrilateral elements. The measured dependence of saturation on capillary pressure was fit to a van Genuchten (1980) functional form. Using the theory of Musalem (1976), the fitted saturation-capillary pressure curve yields the preserved 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 100 hr. period during which the water profile was monitored. Fractures were found to be regions of rapid drying 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 3% 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 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 to these simulations. Monsters et al. (1987) measured and modeled water in an un- 

fractured, non-welded, highly porous (48%), relatively permeable (21.9 × 10⁻⁶ m/s) Paint- 
brush 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 mi- 
crometer 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 character- 

istic curves to obtain better agreement between modeled 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 permeabil- 

ities of 2.54 m and 6 cm diameter × 10 cm long cores of both fractured and unfractured 

Poyogah Spring welded tuff subjected to several wetting and dehydration cycles at a 

constant 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/imbibition 

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 sealing of 

fractures by the redistribution of silica within the fracture apparently occurring only 

above 90°C. Permeability of the unfractured sample did not decrease under similar 

circumstances. It should be noted, however, that the fractures were initially "sealed" 

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 drying of 

fractures followed by slow drying of the matrix. During imbibition, a uniform wet- 

ting 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 non- 

fractured 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 rough- 

ness 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. 

Davis (1987) conducted a transient nonthermal moisture and solute flow ex- 

periment 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 cold 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. In the other 

direction, water flux in the opposite direction. Soluble tracer in the water conducted on 

the dry end of the core as is expected in heat-driven, two-phase transport. Appar- 

ently 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 1. The saturation distribution along the core was modeled 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.
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 evacuation 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 site boreholes inclined at angles of 45° were drilled in tuff 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. (1986c). 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 fractured 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 on experimental design should be placed on developing and applying the concepts of non-dimensionalization, 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.

Both the results of 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 50°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 fingerling within unsaturated fractures should be addressed systematically under realistic boundary conditions. We are currently exploring the various causes of such channelled 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 assuming 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 Klawetter (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 recrystallized, 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 and Yucca Mountain hypothesis that the low-water 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 seems to be most significant with distance from the fracture plane 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 confinement 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 confinement and armoring could cause the formation of sealed saturated conduits or "wells" 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 Dougherty and Press (1985), Eaton et al. (1987), Jennings (1986), and Tsang and Press (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 Narasingam (1985) investigated the effect of cyclic climatic changes on the subsurface variations in moisture content. They found that most variations were dampened out at depths well above the proposed repository elevation. Kuchlis investigated the effect of dissolution of elements within the rock pore and its effect on the material properties (Evans, 1989). Peterson et al. (1988) investigated the effect of residual drilling water and 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. Now (1986) predicted that for infiltration rates of less than 0.00 mm/yr the upward movement of vapor is equivalent to the downward flow 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 steep 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 sites 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 tuft 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 low 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

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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, $e_i=0.75$. 
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.