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Publication Date
1986-12-01

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December 1986

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Prepared for the U.S. Department of Energy under Contract Number DE-AC03-76SF00098.
Numerical Modeling of Isothermal and Nonisothermal Flow in Unsaturated Fractured Rock – A Review

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NUMERICAL MODELING OF ISOTHERMAL AND NONISOTHERMAL FLOW IN UNSATURATED FRACTURED ROCK - A REVIEW

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Abstract. In recent years, considerable efforts have been made to study the feasibility of geologic disposal of high-level nuclear wastes in deep unsaturated zones in desert environments. The tuff formations at and near the Nevada Test Site, which are under consideration for this purpose, are comprised of fractured-porous material, with hydrologic properties quite different from those encountered in most previous unsaturated flow studies dealing with soils. Another difference from "conventional" unsaturated flow is that in the vicinity of the waste packages, flow is driven by high temperatures (exceeding 100 °C) and large temperature gradients. The approximations developed in soil science for weakly nonisothermal flow are not applicable to this situation, and a multiphase description of flow is required, similar to approaches used in modeling of geothermal reservoirs and thermally enhanced oil recovery. The conventional approach to unsaturated flow is applicable, however, to a variety of problems relating to natural (undisturbed) and far-field flow conditions. This paper reviews recent work on numerical modeling of unsaturated flow undertaken in the context of nuclear waste isolation studies. Concepts and applications of broader interest are summarized, including the role of fractures in partially saturated flow, the response of a fractured medium to infiltration events, and a simplified description of flow based on an effective continuum approximation. It is pointed out that the heat released from the waste packages gives rise to multi-phase flow with heat pipe effects, which may have a dramatic impact on thermal and hydrologic conditions. A number of important issues are identified which have not been adequately explored. These include the possibility that liquid water may flow along the rough walls of fractures the bulk of which is drained. Pre-existing or induced fracture coatings may have significant hydrologic effects. Large-scale moisture movement may be important to describe natural (nearly isothermal) hydrologic conditions as well as waste-induced gas phase convection far beyond the thermally disturbed zone. The importance of model validation and calibration with laboratory and field measurements of unsaturated flow in fractured rock is emphasized.

Introduction

The Nevada Nuclear Waste Storage Investigations project (NNWSI) of the Department of Energy is studying the suitability of tuff formations near the Nevada Test Site (NTS) as a host medium for geologic disposal of high-level nuclear wastes. The potential repository horizon is located in the Topopah Spring unit of the Yucca Mountain tuffs at a depth of approximately 350 m beneath the ground surface and 225 m above the water table [U.S. DOE, 1986]. At this horizon, approximately 80% of the formation pore volume contains water, held in the smaller pores by capillary suction. The remaining voids contain air and a small amount of water vapor at ambient pressures and temperatures.

The possibility of disposing of high-level nuclear wastes in unsaturated zones in desert environments was first suggested in a report by the National Academy of Sciences [1966]. A detailed and persuasive case for unsaturated disposal was presented by Winograd [1974, 1981]. The chief asset of thick unsaturated zones is that there may be no effective mechanism to dissolve and transport radionuclides to a deep water table or to the land surface under arid climatic conditions.

High-level nuclear wastes need to be isolated from the accessible environment for long time periods (>10^5 years) [U.S. NRC, 1981]. A large volume of rock, of the order of 1 km^3 or more, will be impacted by thermal and hydrologic change from a repository. The time- and space-scales involved limit the possibility for direct verification of disposal system performance. Therefore, repository design and performance assessment must to a large extent be based on extrapolations of known effects and trends. The chief means by which such extrapolation can be accomplished is mathematical modeling (computer simulation).

A review of modeling capabilities relevant to the disposal of high-level nuclear wastes in unsaturated formations has been given by Evans [1983]. The present paper addresses some recent developments in modeling of fluid and heat flow in partially saturated, fractured-porous media that were undertaken to help quantify the option of unsaturated disposal. Chemical composition and transport effects are outside the scope of this paper [see e.g., Travis et al., 1984; Nielsen et al., 1986]. Our emphasis is on concepts, applications, and issues relevant to thermohydrologic aspects of nuclear waste isolation. The reader seeking specific information on the mathematical and numerical formulation of multiphase flow problems is referred to a recent review by Allen [1985]. We begin with a brief summary of (nearly) isothermal flow in the "far field," away from the heat-generating waste packages. Much of the modeling capabilities needed for this problem can be readily adopted from soil science. More complex flow processes are encountered for the strongly nonisothermal conditions in the vicinity of the waste packages. Modeling techniques for this problem borrow heavily from methods developed in the context of geothermal reservoir analysis and enhanced oil recovery.

Isothermal Flow

The conventional description of saturated-unsaturated flow, as recently reviewed by Narasimhan [1982], was developed primarily...
by soil physicists. It assumes isothermal conditions and treats the

gas phase as a passive spectator that remains at constant pressure

(1 atm) at all times. Water transport is accounted for only in the

liquid phase and is driven by gravity and capillary forces, as
described by Richards' equation [1931]. The capillary force, arising

from cohesive forces among the water molecules and adhesive

forces between the water and rock solid surfaces, is inversely

proportional to the effective radii of the pores. In an unsaturated

porous medium, the pressure in the liquid phase is less than atmos-

pheric pressure because of capillarity, and the liquid saturation is a

strong function of liquid-phase pressure. As the liquid-phase pres-

sure in the porous medium is decreased below atmospheric pres-

sure, or equivalently the pressure head (liquid pressure - atmos-

erpheric pressure) becomes negative, the largest pores will desaturate

first, followed by the desaturation of successively smaller pores.

The nonlinear pressure-saturation characteristic curve for a porous

medium depends on details of pore geometry (pore sizes, shapes,
connectivity).

Fracture Effects

Since the welded tuff in the Topopah Spring unit is extensively

fractured [Scott et al., 1982; Sinnock et al., 1984], many recent stu-

dies have generalized the conventional description of unsaturated

soils to fractured media with pervasive fractures partitioning the
tight rock matrix [Evans and Huang, 1982; Evans, 1983; Peters et

al., 1984; Montazer and Wilson, 1984; Wang and Narasimhan,

1985; Klawetter and Peters, 1986]. Due to large differences in pore

size and geometry, the desaturation behavior of planar fractures

with apertures of tens to hundreds of micrometers is expected to be

very different from that of cemented volcanic ash flow tuff with

pore sizes in the micrometer to submicrometer ranges. For tuff

matrix, although different methods (psychrometer, mercury intru-
sion) have often given inconsistent results, data for intact rock

have been obtained on small core samples [Peters et al., 1984]. At

the present time, no measurement techniques or data are available

for the capillary behavior of realistic rough-walled fractures.

Without experimental measurements, the alternative approach to
understanding the behavior of partially-saturated fractures is to

derive the characteristic curves based on fracture geometry and

capillary theory. This approach is sometimes also used in soil phy-
sicists to derive the pressure-permeability data from pressure-sa-

turation data with the use of theoretical models such as the

capillary tube models [e.g., Mualem, 1976; van Genuchten, 1980].

Before we summarize the recent developments in unsaturated

fracture flow, let us briefly review the theoretical studies and

experimental evidence of the unsaturated flow behavior of hetero-
genous soils containing large root channels and worm holes in

response to infiltration of rains and injection of tracers [Beven and

German, 1982; Edwards et al., 1979; Hoogmoed and Bouma,

1980; Scotter and Kanchanasut, 1981; Davidson, 1985]. If the rain-

fall arriving at a soil surface is low, all the water at the surface is

absorbed by the micropores in the soil matrix. Vertical flow of

water into large cracks or tubular channels occurs when the rainfall

exceeds the infiltration rate into the soil matrix. When tracers

dyes and anions) were used to study soil core samples containing

macropores under both unsaturated flow and saturated flow condi-
tions, the tracers distributed over the small pores in the soil matrix

under unsaturated conditions and stayed around the macropores

under saturated flow conditions [Scotter and Kanchanasut, 1981].

Although the macropores in shallow soil are very different from the

fractures in deep, welded tuff rock, the physical insight from these

observations in soil physics may substantiate the theoretical and

modeling approaches of the studies of unsaturated flow in fractured

rocks. These considerations are tentative and need to be substan-
tiated with experimental data on flow in unsaturated fractured

rocks.

In most early saturated fracture flow studies, fractures were
idealized as parallel-plate, smooth-wall openings with a constant
aperture. When the capillary theory is applied to this model, the

saturation-pressure relationship is a step function with $S = 1$ (fully

saturated) when the suction pressure is weak and $S = 0$ (com-
pletely drained) when the suction pressure is strong enough to

overcome the capillary force holding the water in the fracture

between the parallel plates. The step change occurs at a capillary

pressure inversely proportional to the aperture. A real fracture has

rough walls and variable apertures, with part of the walls in con-
tact. The sections with large aperture will drain first as the magni-

tude of the suction pressure increases (or the pressure head

becomes more negative). The step function is replaced with a

smooth but steep function determined by the aperture distribution.

Within a partially saturated fracture, the remaining water will be

held in sections with small apertures near the contacts, and the

liquid phase may be surrounded by air. The presence of a rela-

tively continuous air phase will produce an almost infinite resis-
tance to liquid flow parallel to the fracture plane. Therefore, as a

fracture begins to desaturate, its effective permeability will decline

abruptly by many orders of magnitude as the pressure head

decreases.

However, even under conditions where the bulk volume of a

fracture has been drained, liquid will still be present on the frac-
ture walls (as an adsorbed film or held in fracture roughness; Phi-
lip, 1978). From considerations of idealized parallel-plate fractures,

it was concluded by Evans [1983] that film flow effects should be

detectable, but no data are available for realistic rough-walled frac-
tures.

Relative Permeability

If the effective permeability of fractures to liquid declines

abruptly as pressure head becomes more negative, the transport of

water through the rock matrix can no longer be ignored. Although

the saturated permeability of the rock matrix is several orders of

magnitude smaller than the saturated permeability of the fractures,
it is likely that during desaturation, the effective permeability of

fractures will become smaller than that of the matrix. An interest-
ing consequence of this role reversal between fractures and matrix

in transporting liquid is that water will tend to flow across the

fractures at asperity contacts from one matrix block to another

instead of flowing along the fractures. The flow lines may be

expected to circumvent drained portions of the fractures. Figure 1

illustrates schematically the distribution of liquid water held in the

finer pores in the matrix and near the fracture contacts. The flow

lines bypass the drained portions of the fractures, going from one

matrix block to another normal to the fracture planes. Figure 2

describes the changes of liquid- phase configuration in the

fracture plane from continuous at high saturation (low suction)
to discontinuous at low saturation (high suction) with liquid form-
ing rings around contact areas. Figure 3 shows a theoretical pred-
icion of the abrupt decline of fracture permeability and the cross-

over of the fracture curves below the measured matrix curve of a

welded tuff matrix sample at large negative pressure head [Wang

and Narasimhan, 1985, 1986].

The fracture permeability curves shown in Figure 3 were
derived from fracture aperture distribution functions based on

limited data on fracture spacings, orientations and equivalent fracture

continuum permeabilities [Winograd and Thordarson, 1975; Tor-
darson, 1983; Spengler and Chornack, 1984]. Recent measurements

and analyses of rock surface roughness profiles should lead to

better quantification of the aperture distributions. Fourier spectral
analyses of low-resolution roughness profiles of tuff samples indicate that the tuff surfaces may be of a wavy nature with a well-defined periodicity [Harrold et al., 1985]. If the tuff rock surfaces are composed of parallel features of hills and valleys along a given direction, the fracture permeability will be highly anisotropic, and liquid will flow preferentially along the periodic contact strips. The periodic strip pattern is unusual since rock surfaces are typically more irregular and less anisotropic. Brown and Scholz's [1985] spectral analyses of different rock samples over different spatial scales indicate that the roughness profiles have a nearly featureless spectrum, and the rock surfaces can be described by scale-invariant fractal geometry [Mandelbrot, 1983]. Wang et al. [1987] constructed a fractal model that provides a more realistic description of fracture geometry than the schematic models used in Wang and Narasimhan [1985].

Fractured-Porous Flow

Characteristic curves of fractures and porous matrix, such as illustrated in Figure 3, have been used to simulate the desaturation of a small fractured tuff column with discrete vertical and horizontal fractures [Wang and Narasimhan, 1985]. It was observed that the early transient changes from fully saturated conditions to partially saturated conditions are sensitive to fracture properties. However, subsequent to the initial transient, fluid flow in the fractured tuff column was nearly identical to simulation results for the same column without taking the fractures into account. As soon as the fractures are drained, the transport of fluid will be through the matrix and will be controlled by the characteristic curves of the matrix. At a given elevation, the pressure values in the fractures are nearly equal to the pressure values inside the matrix blocks. If the fracture pressures are the same as the matrix pressures, there is no need to model separately the fractures and the matrix. The local pressure equilibrium is one of the key assumptions in the development of an "effective continuum" approximation [Montazer and Wilson, 1984; Klaavetter and Peters, 1986; Peters et al., 1986; Pruess et al., 1986]. With equal pressures and parallel flow directions between fractures and matrix, the effective permeability of a fractured-porous medium is the sum of the fracture and matrix permeability, weighted by the cross-sectional areas of the flow channels. It generally has a double-hump structure with fracture-dominated shape at low suction and matrix-dominated shape at high suction. The fractures also dominate the capacitance coefficients at low suction, while at higher suctions most water release occurs from the matrix [Peters et al., 1986; Klaavetter and Peters, 1986].

For isothermal conditions, applications of the effective continuum approximation have been made to vertical infiltration problems [Peters et al. 1986, Wang and Narasimhan, 1986]. Nonisothermal flow studies with the equivalent continuum approximations will be discussed in later sections.

On the scale of distance between the ground surface to the water table (500 to 600 m at Yucca Mountain), another heterogeneity of concern for the simulation of water movement through the unsaturated zone is the layered structure with alternating highly-fractured welded units and porous nonwelded units. The contrasts in the characteristics of the alternating layers require careful consideration of space discretization for numerical modeling, especially near the interfaces between different units. Large saturation gradients may develop near the contact between...
Most of the simulations to date assume that material properties are uniform within each stratigraphic unit. However, in reality there is additional spatial variability within each unit that may introduce local changes and transitions [Peters et al., 1984]. Sillcock et al. [1984] take into account the statistical variations of some of the hydrological properties by Monte Carlo simulation techniques in calculating the groundwater travel times using a unit gradient approximation. The unit gradient approximation [Weeks and Wilson, 1984] is approximately valid in the interior of a thick unit away from the interfaces where the saturation becomes uniform and the hydraulic gradient is solely determined by gravity. Certainly the effects of the spatial variability and spatial correlation of geostatistical analyses need to be addressed in future studies of steady and transient simulations. The scale dependence of material properties, as evident in the differences observed between laboratory data [Peters et al., 1984] and field scale data [Montazer et al., 1985], should also be addressed.

**Additional Issues**

In addition to fluid flow studies, chemical transport studies will be of great interest for performance assessment of an unsaturated repository. Some of the unresolved fluid flow issues have impacts on the transport of radionuclides through an unsaturated, fractured medium. Returning to the small spatial scale of a matrix block surrounded by discrete rough-walled fractures as shown in Figure 1, it is clear that constriction of flows between matrix blocks across the small contact areas will distort the flow lines in converging-diverging patterns, thereby increasing tortuosity.

Another issue affecting the role reversal of fractures and matrix in unsaturated flow is the presence of fracture surface coatings that may diminish the hydraulic communication between the fractures and matrix through the contact areas. Tuff fracture surface data show that some coatings exist [Spengler and Chornack, 1984] from which it is possible to estimate the contact areas [Wang and Narasimhan, 1985]. We have performed simulation studies to investigate how easily the water in the fractures can overcome the low-permeability coating resistance to attain local equilibrium with the matrix. Figure 4 shows results of a simple one-dimensional flow simulation of a fracture in contact with a partially saturated

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**Fig. 3.** Permeabilities of partially saturated discrete fractures and tuff matrix with parameters derived from Topopah Spring Member data.

**Fig. 4.** Simulated saturation in a fracture, as it is being drained by capillary action from a matrix block with skin.
(80%) tuff matrix of permeability $k_m = 1.9 \mu m$. A layer with thickness equal to average fracture aperture (0.6 mm) is sandwiched between the fracture and the matrix interior to represent coating. The permeability of the coating is assigned orders of magnitude lower values than the tuff matrix. At time $t = 0$, the fracture is assumed filled with water ($S = 1$), and the transient change in fracture saturation is simulated as water is being sucked across the coating into the matrix. Figure 4 shows that the desaturation of the fracture occurs rather rapidly even with extremely low coating permeability. However, relative changes in time scale due to fracture skin can be large. If fracture skin becomes the dominant flow resistance, the times required to achieve a given saturation change will increase proportional to the inverse of skin permeability. In our example this occurs when skin permeability is as low as 1% of matrix permeability or less (see Figure 4). If the effective fracture-matrix area is reduced instead of the coating permeability, similar results are obtained. The parameters in these simulations are identical to those used in Pruess et al. [1986].

In isothermal unsaturated flow studies, it is usually assumed that the gas phase behaves as a passive spectator at constant pressure, so that the liquid flow does not experience any resistance or drag from the gas phase. However, it is well known that during transient infiltration events, the pressurization of air ahead of a wetting front can produce significant flow effects, especially in low-permeability systems [Wilson and Luthin, 1983; Youngs and Peck, 1984; Bianchi and Haskell, 1986; Green et al., 1970]. One may envision a situation in which a matrix block is suddenly surrounded by liquid water on all sides. As the liquid rushes into the matrix, the gas phase that initially occupies the matrix pores will become pressurized and begin to flow outward. This will create additional resistance to the advance of wetting fronts. The pressurization and associated relative permeability effects as gas flows opposite an advancing infiltration front need to be evaluated for the conditions expected at the Yucca Mountain site.

The purpose of most of the recent isothermal simulations of the unsaturated fractured flow systems is to develop a better understanding of the ambient conditions and to assist in the design of a site characterization program. Certainly in the modeling of ambient conditions, other effects from multiphase flow and mild geothermal gradients should be taken into account. Ross [1984] and Montazer and Wilson [1984] discussed moisture movement driven by vapor diffusion under an ambient geothermal gradient in low-infiltration systems. Weeks [1986] reported observations of strong seasonal air flow in boreholes at Yucca Mountain, driven by thermal buoyancy effects. The recent simulation studies by Tsang and Pruess [1986] have indicated that thermal buoyancy effects from a waste repository can cause strong gas phase convection in a large region, extending far beyond the thermally disturbed zone, right up to the ground surface. In site characterization, the regions between the repository level and the ground surface are at least equal in importance to the regions between the repository level and the water table. Even though the prereplacement ambient conditions are characterized by dominant net downward infiltration to the water table, the postclosure groundwater transport through an unsaturated, fractured medium may be quite different from the ambient flow paths.

**Strongly Heat-driven Flow**

The conventional description of saturated-unsaturated flow has been extended to "weakly" nonisothermal systems (temperatures below 50° C) by Philip and de Vries [1967], Jury [1973], Sophocleous [1979], Milly [1982], and others. These authors allow for water migration in the form of liquid or vapor. The only mechanism considered for vapor transport is molecular (binary) diffusion; no overall movement of the gas phase is taken into account. The subject of "weakly" nonisothermal unsaturated flow has been recently reviewed by Walker, Sabey, and Hampton [1981], and Childs and Malstaff [1982].

The emplacement of high-level nuclear wastes in a partially saturated, permeable medium will give rise to strongly heat-driven flow, for which the approaches mentioned above are not applicable. As temperatures near the waste packages approach or exceed the boiling point of water, vaporization will take place with associated increases in vapor partial pressure and overall gas-phase pressure. Substantial redistribution of water accompanied by large latent heat effects will then occur from gas-phase flow. In a fractured- porous medium, conditions will be favorable for the development of vapor-liquid counterflow, which provides a very efficient heat transfer mechanism known as "heat pipe" [Eastman, 1968; Jennings, 1984; Doughty and Pruess, 1985]. In a heat pipe, a volatile liquid is vaporized in response to heat injection (Figure 5). The vapor flows away from the heat source and condenses in cooler regions, depositing its latent heat of vaporization there. This sets up a saturation profile, with liquid-phase saturation increasing away from the heat source. The corresponding gradient in capillary pressure will cause liquid to flow back toward the heat source, where it can again vaporize. Engineered heat pipes are usually closed systems, which operate in steady-state mode where liquid and vapor flow balance each other so that there is no net mass transport. In the nuclear waste isolation problem, heat pipe conditions are of a transient nature, because the flow system is open and essentially infinite; furthermore, heat input varies with time.

To describe the hydrologic and thermal conditions near the waste packages, it is necessary to employ a multiphase approach to fluid and heat flow, that fully accounts for the movement of gaseous and liquid phases, their transport of latent and sensible heat, and phase transitions between liquid and vapor. The gas phase will in general consist of a mixture of water vapor and air, and both these components must be kept track of separately.

**Numerical Models**

Recently developed modeling capabilities for strongly heat-driven problems borrow heavily from techniques used in the simulation of geothermal reservoirs and enhanced oil recovery operations [Travis, 1983; Eaton, 1983; Eaton et al., 1983; Pruess and Wang, 1984; Hadley, 1985; Bixler, 1985; Pruess, 1986; Pollock, 1986]. Table 1 summarizes the various physical processes con-
**TABLE 1. Physical Processes in Strongly Heat-Driven Flow in Partially Saturated Rocks**

<table>
<thead>
<tr>
<th>Process</th>
<th>Mechanism</th>
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<tbody>
<tr>
<td><strong>1. Fluid Flow</strong></td>
<td>pressure forces</td>
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<td>viscous forces</td>
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<td></td>
<td>inertial forces</td>
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<td></td>
<td>gravity</td>
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<td></td>
<td>interference between liquid and gas</td>
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<td>dissolution of air in liquid</td>
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<td></td>
<td>capillarity and adsorption</td>
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<tr>
<td></td>
<td>hysteresis</td>
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<td></td>
<td>differential heat of wetting</td>
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<td></td>
<td>chemical potential gradients</td>
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<td>mixing of vapor and air</td>
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<td>vapor pressure lowering</td>
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<td>binary diffusion</td>
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<td></td>
<td>Knudsen diffusion</td>
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<td></td>
<td>thermodiffusion</td>
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<td><strong>2. Heat Flow</strong></td>
<td>conduction</td>
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<td></td>
<td>flow of latent and sensible heat</td>
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<td></td>
<td>radiation</td>
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<td></td>
<td>viscous dissipation</td>
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<tr>
<td></td>
<td>mechanical work</td>
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<tr>
<td><strong>3. Vaporization and Condensation</strong></td>
<td>temperature and pressure effects</td>
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<tr>
<td></td>
<td>capillarity and adsorption</td>
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<tr>
<td><strong>4. Changes in Rock Mass</strong></td>
<td>thermal expansion</td>
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<td></td>
<td>compression under stress</td>
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<tr>
<td></td>
<td>thermal stress cracking</td>
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<tr>
<td></td>
<td>mineral redistribution</td>
</tr>
</tbody>
</table>

sidered in these models. Nearly all effects deemed potentially important have been modeled; however, all of the presently available models are incomplete in that they only account for a subset of the relevant processes.

The mathematical and numerical methods used in the different variably-saturated nonisothermal flow codes are generally similar, with some variations in the handling of space and time discretization and solution of the coupled non-linear equations. Discretization methods used include finite differences, integral finite differences, and finite elements for spatial variables, and first- and higher-order schemes for time. The time scale over which "significant" changes occur can vary tremendously over the course of a flow problem, related to phase transitions, onset or cessation of fracture flow, reversals in flow direction, and other transient phenomena. Therefore, most numerical simulators provide some form of automatic time step control to achieve efficient yet accurate computation. Mass- and energy-balance equations have sometimes been solved sequentially rather than fully coupled. Some authors have written the basic governing equations in terms of phases rather than components, including appropriate sink- and source terms to allow for phase transitions. Different sets of primary variables have been used (e.g., pressure, temperature, saturation, capillary pressure, air partial pressure). The governing equations are highly non-linear and are solved by means of Newton-Raphson iteration. The linear equations arising at each iteration step have been solved with direct as well as iterative methods. While each of the different methods offers certain advantages for specific kinds of problems, it appears that the diversity of nonisothermal, partially saturated flow problems is such that no single set of methods is superior to all the others.

**Applications**

Several authors have modeled strongly heat-driven flow under conditions representative of those expected near buried high-level waste packages. Model applications have included the study of heat pipe effects [Pruess and Wang, 1984; Eaton et al., 1985]; fluid and heat flow on a small spatial scale in and near fractures [Evans, 1983; Pruess et al., 1985, 1986]; nonisothermal flow on a repository scale [Travis, 1984; Pollock, 1986; Tsang and Pruess, 1987]; and the design of laboratory experiments [Eaton et al., 1985]. In this paper, we will limit ourselves to summarizing some illustrative
examples, that address basic issues in strongly heat-driven flow in a fractured-porous medium.

Thermohydrological Conditions Near Waste Packages

Pruess and coworkers [1985, 1986] attempted to resolve in detail the interplay between fractures and matrix in the flow field near the waste packages. They studied a highly idealized emplacement configuration (see Figure 6), the symmetry of which made it possible to model a small region in which individual fractures could be represented explicitly. Using parameters believed to be relevant to the conditions at the potential repository horizon [Hayden et al., 1983], they observed the following general behavior (see Figure 7). After waste emplacement, temperatures rise in both rock matrix and fractures. Initially, this causes evaporation of a modest amount of water, but boiling becomes vigorous as temperatures approach 100°C. Most of the vapor generated in the rock matrix flows toward the fractures and then radially outward, where it soon condenses on the cooler fracture walls. The behavior of the liquid condensate depends critically upon whether or not the liquid initially present on the fracture walls has a significant mobility. Note that even in fractures whose bulk volume is drained liquid can be held on the rough walls by capillary and phase adsorption forces [Philip, 1978]; it is not known whether such liquid is mobile. In our modeling work [Pruess et al., 1985], we considered two cases, one without and the other with significant liquid mobility in the fractures at ambient suction conditions (estimated at -10.93 bars). If liquid is immobile in the fractures, the condensate is sucked back into the matrix, where it migrates down the saturation profile toward the boiling region near the waste package. Due to small matrix permeability, the inflow of liquid to the heated region is less than the outflow of vapor in the fractures, so that the vicinity of the waste packages will dry up. This will create a zone with predominantly conductive heat transfer near the waste packages, giving rise to large temperature gradients and temperatures (see Figure 8). System behavior is completely different when liquid is assumed mobile in the fractures. In that case, the backflow of condensate toward the heat source takes place along the fracture walls, and after a rapid initial transient, a balanced counterflow is established, in which outflow of vapor is balanced by backflow of condensate. Thus, the vicinity of the waste package will not dry up, and therefore temperatures in the vicinity of the waste package remain constrained to near 100°C, the saturation temperature at ambient pressure. The different thermal regimes are illustrated in Figure 8, which shows simulated temperatures just outside the waste emplacement hole for parameters and conditions believed representative of the Topopah Spring unit of Yucca Mountain tuffs [Hayden et al., 1983; Pruess et al., 1985].

Effective Continuum Approximation

Detailed modeling of individual fractures can provide some interesting insight into fluid and heat flow patterns near the waste packages, but it does not offer a practical way for studying realistic emplacement configurations and overall repository performance. Based on the thermohydrological behavior observed in the explicit-fracture studies, Pruess et al. [1985] proposed an 'effective continuum' approximation, in which fracture effects are approximately accounted for by a suitable modification of the matrix hydrologic properties. Specifically, it was suggested that fractures would provide high-permeability pathways for gas-phase flow (and perhaps also for liquid flow, if film flow effects are significant). By suitably adjusting gas and liquid relative permeabilities, Pruess et al. [1985] were able to match the simulated thermohydrological behavior of fractured porous media with single-effective continuum calculations (see Figure 8). Subsequently, they derived an effective...
Here \( k \) depends, generally speaking, not only on the thermohydrological properties of the medium, but also on the nature of the flow processes considered. The approximation will be valid when the characteristic time for achieving local thermodynamic equilibrium between matrix and fractures is short compared to the time required for "significant" global propagation of thermal and hydrologic perturbations. More specifically, in the thermally disturbed zone, an effective continuum approximation will be applicable when the propagation of temperature changes radially (away from the waste packages) is slow in comparison to the propagation of (gas and liquid) pressure changes between fractures and matrix at a given radial distance. The effective continuum approximation will break down for very rapid transients (at early times near the waste packages) or for very low matrix permeability or large fracture spacing [Pruess et al., 1986].

We believe that for most problems relating to thermohydrologic conditions in an actual waste repository, the effective continuum approximation will be satisfactory. For some cases where it is not, it will be necessary to resort to double- or multiple-porosity techniques [Barenblatt et al., 1960; Warren and Root, 1963; Duguid and Lee, 1977; Pruess and Narasimhan, 1985]. A multiple-porosity approach may generally be necessary for the description of chemical transport, because equilibration of species concentrations between matrix and fractures is a much slower process than hydraulic (pressure) equilibration [Neterticks and Rasmuson, 1984; Wilson and Dudley, 1986].

### Discussion and Conclusions

Recently developed techniques for modeling fluid and heat flow in partially saturated, fractured-porous media are quite powerful and sophisticated. A number of computer programs are available that are capable of solving the severely nonlinear equations arising in these flow processes and whose accuracy has been verified by comparison with a variety of known solutions. Applications to "realistic" repository problems, including actual waste emplacement configurations, loading schedules, and long-term thermohydrological conditions, are now possible and should be pursued vigorously. Such studies can be valuable for waste package and repository design, as well as for the development of techniques for monitoring repository performance. The chief limitation of numerical modeling applications at this point appears to be that important data are either unavailable or have a large range of variability [Peters et al., 1984; Guzowski et al., 1983; Tien et al. 1985]. It should also be pointed out that the presently available numerical simulators have been constructed on the basis of general principles of fluid and heat flow. Well-designed and carefully controlled laboratory and field experiments are needed to more completely define the physical systems to be modeled [see e.g., Eaton et al., 1985; Bixler et al. 1986; Zimmerman and Blanford, 1986]. Most important are those parameters and processes that could significantly affect the thermohydrologic conditions near the waste packages, and the large-scale movement of liquid, gas, and chemical species. This includes the mobility (or lack thereof) of liquid films on fracture walls, and the porosity and tortuosity of the fracture network on a field scale. Sensitivity studies can help in the design of laboratory experiments and in the development of site characterization and field test efforts.

We wish to point out that additional advances in numerical modeling techniques are possible and desirable. The composite characteristic curves applicable for an effective continuum description of flow in fractured-porous media lead to extreme nonlinearities in the governing equations. These tax the capabilities of present simulators, and it is not clear that calculations for "large" space- and time-scales can be made without compromising to some extent the realism of hydrologic parameters. Three-dimensional calculations remain a challenge, because the computational work required is very much larger than for one- and two-dimensional calculations. Usually some trade-off is required between dimensionality of the flow problem, attainable space- and time-resolution, and realism of problem parameters. As had been pointed out before, all presently available simulators are limited to a subset of the physical and chemical processes considered relevant for fluid and heat flow. Of the various coupled processes that need to be studied, perhaps the most important is redistribution of silica and the associated changes in porosity and permeability. Fracture aperture changes from thermal expansion and associated stress could also have significant permeability effects [Barton et al., 1984].

Braithwaite and Nimick [1984] made an approximate evaluation of host rock dissolution and precipitation on a large spatial scale (several hundred meters), and found the effects to be insignificant. However, in the vicinity of the waste packages, significant effects appear possible. silica will precipitate out near the waste packages as liquid water boils into steam. Our numerical simulations show that boiling rates are largest at the fracture walls, where pressures jump from somewhat elevated levels in the rock matrix to the nearly ambient levels in the fractures. From simulated mass fluxes, and the known dependence of quartz solubility on temperature [Fournier and Potter, 1982], it is possible to estimate the rate of silica deposition. Using results of our explicit-fracture simulations [Pruess et al., 1986], we estimate the rate of deposition on the frac-
ture walls at approximately $10^{-4}$ m$^3$/year/m$^2$ at 5 years after waste emplacement. Typical fracture volumes per unit area are probably of the order of $10^{-4}$ m$^3$/m$^2$ (Weber and Bakker, 1981; Pruess et al., 1985; Zimmerman and Blanford, 1986), so that it appears that effects of deposition on fracture porosity will be small. However, recent experimental work has indicated that small porosity changes can cause very large permeability effects (Vaughan, 1985), which has been attributed to the converging-diverging nature of flow channels in "real" permeable media (Verma and Pruess, 1986), as opposed to flow channels of uniform cross-sectional area that are often employed in idealized model studies. The most important development of a fracture is of the order of 1985; the effect of mineral deposition on fracture walls at approximately $10^{-6}$ m$^3$/year/m$^2$ at 5 years after waste emplacement. Typical fracture volumes per unit area probably $10^{-4}$ m$^3$/m$^2$ (Weber and Bakker, 1981; Pruess et al., 1985; Zimmerman and Blanford, 1986), so that it appears that effects of deposition on fracture porosity will be small. However, recent experimental work has indicated that small porosity changes can cause very large permeability effects (Vaughan, 1985), which has been attributed to the converging-diverging nature of flow channels in "real" permeable media (Verma and Pruess, 1986), as opposed to flow channels of uniform cross-sectional area that are often employed in idealized model studies. The most important development of a fracture "skin" (Moench, 1983), which may severely diminish the permeability for matrix-fracture crossflow.

An important issue in the application of numerical models is validation, i.e., the demonstration that a model adequately represents the important physical (and chemical) processes encountered in a real-world system. This is to be distinguished from the much simpler, more straightforward problem of verification, which involves nothing more than a demonstration that a computer program will in fact provide an approximate solution to the governing equations it was designed to solve. Verification is usually accomplished by comparing numerical results with analytical or semi-analytical solutions or with calculations made with a different previously verified computer program. To validate a computer model, it must first be calibrated against a real-world (laboratory or field) system and subsequently be used in predictive mode to evaluate the level of agreement with measured data. A "double-blind" approach, in which the experiment and the modeling prediction are done independently, is preferable to obtain an unbiased comparison (Tsang and Doughty, 1985). Model calibration requires that the relevant system parameters be properly identified, which in practice can be an exceedingly difficult task, because system identification usually remains incomplete and nonunique (Yeh, 1986). Thus, even if a model has been successfully calibrated against certain data, subjecting the system to be modeled to a different process for validation purposes will often result in the need to re-calibrate the model. Instead of verifying model predictions outright, therefore, one then ends up adjusting model parameters until experimental data can be matched. As modeling applications go, obtaining a good match to experimental data can be rather difficult, yet it falls far short of a model validation. Despite all of these difficulties, strong efforts at model validation need to continue, since there is no substitute by which credibility in model predictions can be established.

Acknowledgement. This work was supported by the NNWSI Performance Assessment Division, Sandia National Laboratories, and the U.S. Department of Energy under Contract No. DE-AC03-76SF00098. The authors are indebted to B. S. Langkof, R. Peters and P. Hopkins of Sandia and C. Doughty and Y. Tsang of LBL for careful reviews of the manuscript, and for suggesting improvements. Technical editing by Sandia is appreciated. L. Fairbanks and E. Klahn cheerfully assisted in the word processing.

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