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Simulation of Liquid and Vapor Movement in Unsaturated Fractured Rock at the Apache Leap Tuff Site

Models and Strategies

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ABSTRACT

The physical, hydraulic and pneumatic properties of variably saturated, fractured tuff are currently being evaluated at the Apache Leap Tuff Site, located near Superior, Arizona. Nine inclined boreholes, the deepest of which penetrate to a depth of thirty meters, have yielded over 270 m of oriented core. Field and laboratory data with regard to matrix and fracture properties are being collected which will be used to characterize the site. A description of the characterization parameters as well as field and laboratory techniques used to collect the parameters is presented. To extend the characterization to larger scales, as well as to interpret collected data, computer simulation modeling will be performed. A review and description of available computer models is presented. Recommendations for site characterization includes the use of analytic stochastic models, equivalent porous media models, and discrete fracture network models. Such models may accurately reproduce the expected dual porosity, three-dimensional characteristics of fluid flow at the Apache Leap Tuff Site. Also, the variable saturation which exists within fractures and the matrix at the site will also be reproduced. Simulation scenarios including constant head and flux surface boundary conditions, as well as slug and cyclic surface boundary conditions are recommended.

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EXECUTIVE SUMMARY

Characterization of fluid flow and solute transport through unsaturated fractured rock requires that site-specific conceptual models be defined, parameters for the models be estimated using field and laboratory data, and validation of the conceptual models be performed. This document reviews data collection and interpretation strategies, along with available numerical models which can be used to formulate and test conceptual models. The document focuses on data collected with the purpose of interpreting and predicting flow and transport processes within unsaturated fractured volcanic tuff at the Apache Leap Tuff Site located near Superior, Arizona. Inclined boreholes have been drilled at the site with the intent of obtaining core samples for laboratory analysis. The boreholes are also being used to collect hydraulic, pneumatic, and transport parameters.

Rock matrix flow and transport parameters of interest include, but are not limited to:

- o Bulk density, porosity, and pore size distribution;
- o Moisture characteristic curve;
- o Saturated and unsaturated hydraulic conductivity;
- o Dry and unsaturated pneumatic conductivity;
- o Effective matrix diffusivity; and
- o Matrix retardation coefficients.

Laboratory experiments on unfractured segments of oriented cores obtained from the inclined boreholes are now underway. Over one hundred samples are to be analyzed to determine the spatial distribution of the rock matrix flow and transport parameters at a sampling frequency of every three meters.

Rock fracture flow and transport parameters of interest include, but are not limited to:

- o Number of fracture sets;
- o Fracture center locations;
- o Fracture orientations;
- o Fracture areal extents and shapes;
- o Fracture density and spacing;
- o Fracture porosities;
- o Fracture aperture;
- o Fracture-surface characterization;
- o Fracture connectivity;
- o Fracture moisture release curves; and
- o Saturated and unsaturated fracture transmissivities.

Fracture parameters are estimated from inspection of oriented cores and from in situ borehole tests and measurements. Over two hundred discrete fractures have been identified along the borehole walls, many of which do not contribute to flow and transport. Field tests are currently underway to identify the spatial distribution of hydraulically active fractures at a wide range of fluid potentials.

Once characterization parameters have been collected, inferences about fluid flow and solute transport properties for distances larger than the scale at which the parameters were collected must be provided. Various models have been developed to provide such inferences, including stochastic analytic, discrete fracture network, numerical continuum, and dual porosity models. Stochastic analytic models such as those developed by Gelhar and Axeness (1983) and Yeh et al. (1985a,b,c) will be examined. Also, numerical models will also be examined, including:

- o TRUST;
- o TOUGH;
- o UNSAT2;
- o FEMWATER;
- o SATURN;
- o TRACER3D;
- o HUYAKORN-3D;
- o BIM2D; and
- o BIM3D.

The relative merits and disadvantages of each of these models are presented with regard to their respective capabilities to simulate three dimensional flow and transport through unsaturated fractured rock

Simulation scenarios include the initial assessment of flow and transport through an unsaturated rock matrix with heterogeneous physical, hydraulic, pneumatic and transport parameters and with no embedded fractures, subject to constant, pulsed and cyclic boundary conditions at an upper surface which represents the atmosphere-earth interface. The resulting fluid fluxes will be assessed along with the distribution of travel times.

Once the capability to model flow and transport through an unfractured rock matrix has been demonstrated, three types of models which explicitly incorporate fracture flow will be examined. The models include analytic stochastic, effective continuum, and discrete fracture network approaches. Comparisons between models will be used to develop strategies for model validation.

CHAPTER 1

INTRODUCTION

To simulate and model the movement of fluid and solutes in unsaturated fractured media, it is necessary to establish a conceptual model. The conceptual model generally takes the form of laws and concepts, such as Darcy's law, Fick's law and the conservation of mass. Once the conceptual model has been defined, it is translated into mathematical expressions, usually partial differential equations with boundary and initial conditions. Analytical and numerical methods are employed to solve these equations for the behavior of the flow system subjected to any input stresses.

The laws and principles in the conceptual model are generally established for a certain size volume of media. For example, Darcy's law and classic governing ground water flow equations for porous media are developed for the size of the representative elementary volume, REV, which is a size corresponding to a large collection of pores. Laboratory and field measurements of the hydraulic properties of the media represent averages over many pores. Such an REV representation essentially replaces a complex spatial distribution of pore channels in the media at the microscopic level with a continuum at a macroscopic level.

1.1 Flow in Saturated Fractured Rocks

In fractured rocks, the size of fractures is much larger than the size of pores. Also, the density of fractures at the macroscopic level is much lower than the density of pores. As a result, one has to enlarge the size of the REV in order to visualize the fractured rocks as an equivalent porous continua at large-scale. The implication of this assumption is that the detailed spatial distribution of individual fractures within the REV is ignored.

Alternately, if knowledge of the detailed spatial distribution of the fracture network is available, and the behavior of flow in each fracture is of interest, one may treat the fractures as distinct flow channels embedded within a porous medium. The individual fracture is then visualized as a continuum with a smaller REV which ignores much smaller scale discontinued flow channels within the fracture. In general, the size of the REV for fractures is not the same as that for the rock matrix.

These approaches for modeling flow and transport in fractured rocks are classified into continuum approaches and discrete approaches, respectively. The continuum approach assumes that one enlarges the REV so that the flow behavior in both fractures and the porous matrix are conceptualized as flow in an equivalent homogeneous medium. This assumption implies that the hydraulic properties of such an REV represents the averages of the properties of fractures and rock matrix within the REV. The continuum approach can be further divided into single network approach and double network (dual porosity) approaches.

In the single network approach, a fractured medium is represented by a single network of which the hydraulic properties is the average of both the fracture and the rock matrix. Thus, the governing flow equation is written as:

$$(1.1) \qquad \nabla \cdot (K \cdot \nabla h) = S_s \, \delta h / \delta t$$

where

- K hydraulic conductivity, m/s;
- h hydraulic head, m; and
- S_s specific storage, 1/m.

The coefficients in Equation (1.1) represent average values in both the fracture and rock matrix within the volume of the REV. The hydraulic properties of such an REV are the averages over both fracture and rock matrix. Due to the simplicity of this formulation, many works (Long et al., 1982; Schwartz and Smith, 1985; Endo and Witherspoon, 1985) have used this representation to study flow in saturated, fractured rocks.

For saturated rock the coefficients are dominated by the properties of fractures and the influence of the porous matrix is negligible, while for rocks of low saturation the coefficients are dominated by the properties of the matrix. The REV approach also assumes that flow equilibrium exists between the fractures and the rock matrix which may not be valid for most cases, especially when the response within, say the fractures, is more rapid than within the matrix. Under these conditions it becomes necessary to define two separated networks within the REV: one representing the fracture network and the other representing rock matrix. Each network is considered as a homogenous continuum. Spatial distribution of fractures or rock matrix is not required to be specified within the REV. This conceptualization is called a double network or dual porosity model.

Generally, the double network approach (Barenblatt et al.,1960; Warren and Root, 1963; Kazemi, 1969; Huyakorn et al., 1983; and Moench, 1984) assumes that the hydraulic responses of an REV result from two flow systems where each network is represented by a separate differential equation. The influences of fractures on the flow regime in the rock matrix or vice versa are then entered as a sink or a source term in the governing equations. More specifically, the controlling differential equation for flow in the fracture network is assumed to be described by the classic groundwater flow equation with a source term to account for contributions from the matrix rock:

$$(1.2) \qquad \nabla \cdot (K_f \cdot \nabla h_f) = S_{sf} \, \delta h / \delta t + q$$

where

- K_f fracture hydraulic conductivity, m/s;
- S_{sf} fracture specific storage, 1/m;
- h_f hydraulic head in the fracture network, m; and
- q flow contribution from the rock matrix, 1/s.

Similarly, for the matrix rock the governing flow equation is given as:

$$(1.3) \qquad \nabla \cdot (K_m \cdot \nabla h_m) = S_{sm} \, \delta h / \delta t - q$$

where

K_m matrix hydraulic conductivity, m/s;
S_{sm} matrix specific storage, 1/m; and
h_m hydraulic head in the rock matrix, m;

In general, the dual porosity approach better depicts the flow system than the single network approach because the non-equilibrium interaction between the rock matrix and the fracture is considered in the formulation of the governing equations. Both single and double network approach assume the medium is homogeneous within the REV. This assumption implies that the predicted flow behavior represents an average over the REV. For small scale problems, these averaging approaches may be of limited practical use and the discrete fracture network approach may be necessary.

Several discrete fracture network (DFN) models for flow in saturated fractured media have been developed in the past few years (e.g., Huyakorn et al., 1983; Andersson and Thurnvik, 1986, Elsworth, 1987; and Rasmussen et al., 1987). The DFN approach is similar to the dual porosity approach in that both approaches treat the flow in fractures and rock matrix as separate flow regimes with the exception that the DFN assumes that an explicit knowledge of all fractures in the rock formation is available at all scale levels. Individual fractures are treated as a continuum in the same sense that a porous medium is a continuum representation of the interconnecting pore space. Generally, the parallel plate analogue is used to simulate flow within individual fractures. The flow regime in the host rock is represented by the classic equations for flow in porous media. Because flow in the fracture and porous matrix may interact, these two flow regimes are not independent. Interaction is entered through the coupling of the two equations, i.e. the flow term in Equations (1.2) and (1.3) are coupled.

An equation is also used to relate the flow term to the heads in both rock matrix and fracture. In order to apply the DFN approach, the site of interest is discretized into many rock matrix zones and fracture zones which are represented by either Equations (1.2) or (1.3). As the number of zones increases, the number of Equations increases accordingly. Solving such a large set of differential equations becomes a formidable task. This is the major difficulty of the DFN approach. However, if the matrix water content is constant and flow is steady, one may focus on the flow in the fracture system only. In this case only the equation for flow through the fracture network has to be solved.

Finally, one can also conceptualize the fracture/rock matrix system as heterogeneous continuum or stochastic continuum (Neuman, 1987). This approach is similar to the single network approach discussed earlier. A major difference is that in the stochastic continuum approach any volume can be used to define the hydraulic properties of the fracture and the rock matrix. Because the volume over which the averaging takes place contains several fractures and the rock matrix, the spatial distribution of the hydraulic properties becomes smooth and differentiable and the classic partial differential equations for flow in heterogeneous porous media are again appropriate. In summary, the continuum approach predicts the hydraulic behavior with the volume which is an average of that

of fractures and rock matrix, instead of detailed hydraulic behavior within fractures. Additionally, the transient interaction between the fractures and rock matrix in the volume is omitted.

1.2 Flow in Unsaturated Fractured Rocks

As mentioned previously, many flow and transport models based on the single or double network continuum approach, and discrete fracture network approach have been developed for saturated fracture rocks in the past few years. However, models for flow and transport through unsaturated fractured rocks are rare. The existing models are based on the single continuum or discrete fracture network conceptualization. No dual porosity models have been developed. Available discrete fracture models for unsaturated fractured rock generally use the single network approach without considering the interaction between the fracture and the rock matrix or assumes some simplified flow system. This is mainly attributed to the inherent difficulty in the discrete fracture network approach as discussed above, the complexity of unsaturated flow, and difficulties in determining unsaturated hydraulic properties in fractured rocks. The complexity stems from the fact that unsaturated flow systems are generally nonlinear. The nonlinearity of the systems become even more severe due to the occurrence of fractures, and the high contrast in hydraulic conductivity between the rock matrix and fractures.

Wang and Narasimhan (1985) used the single heterogeneous continuum approach to simulate flow in a hypothetical, unsaturated fractured rock. A formula for calculating fracture conductivity under partially saturated conditions was developed. The effects of distortion of flow paths by the air pockets are taken into account by a phase-separation constriction factor in a generalized cubic law for fracture flow under a partially saturated condition. The reduction of matrix-fracture flow area is taken into account by summing the aperture distribution function to a saturation cutoff aperture, which is inversely proportional to the suction head as prescribed by capillary theory. Based on the statistical theory, they generated fracture hydraulic conductivity curves as a function of saturation, saturation-suction curves, and matrix hydraulic characteristics curves for the densely welded tuff of the Topopah Spring Member at Yucca Mountain, southern Nevada. These characteristic curves of fractures and porous matrix are then used to simulate the desaturation of a small fracture tuff column with discrete vertical and horizontal fractures with the aid of a computer model, TRUST. They concluded that the early transient changes from fully saturated conditions to partially saturated conditions are sensitive to fracture properties. However, the quasi-steady changes of the fluid flow of a partially saturated, fractured, porous system could be approximately simulated without taking the fractures into account. Peters et al. (1986) and Wang and Narasimhan (1986) derived the effective permeability of a fractured-porous medium as the sum of the fracture and matrix permeability weighted by the cross-sectional areas of the flow channels. They applied this effective continuum approximation to vertical infiltration problems.

Huang and Evans (1985) proposed a discrete fracture network model to simulate flow and transport processes in three-dimensional fractured media. The model was developed to provide estimates of global hydraulic conductivity within a rock mass for specified distributions of fracture

orientations, apertures, and densities. The model is also able to calculate solute travel times and breakthrough curves. However, the model assumes steady, saturated flow conditions, and uses a piston flow approximation for simulating mass transport. The model later was extended with some simplified assumptions by Rasmussen (1987) for applications to variably-saturated fractured media. This is accomplished by defining a characteristic curve which relates the total head within the fracture to a capillary aperture using capillary theory. Also, an integrated air/water flow formulation is developed to explain hysteretic effects within the fracture rock network as the fluid potential changes. Finally, the capacity to account for matrix diffusion of solutes into the walls of the fractures has been added.

Other conceptual models using stochastic analytic approaches (Yeh et al. 1985a,b,c) may be developed to improve our predictive ability of flow through unsaturated fractured rocks. The stochastic approach uses estimates of spatial auto-correlation functions of hydraulic properties over local scales to determine hydraulic properties at larger scales. By incorporating random variations of hydraulic properties, improved accuracy in predicting flow and transport characteristics over large regions can be obtained.

Neither the continuum, discrete fracture network, nor the stochastic analytic models have been verified with either laboratory or field experiments. The ongoing laboratory and field characterization of unsaturated flow in natural fractured rocks at the Department of Hydrology and Water Resources at the University of Arizona thus plays a vital role in the understanding of flow through unsaturated, fractured rocks. The results of this study may provide a means to verify the conceptual models discussed above.

CHAPTER 2

SITE DESCRIPTION

The Apache Leap Test Site is located in central Arizona near the extreme western edge of the Pinal mountains, which rise to over 2100 m in elevation. Lying immediately east of Superior, Arizona is the Apache Leap which forms a 600 m west-facing escarpment that exposes a volcanic, zoned ash-flow tuff sheet and an underlying carbonate. The Apache Leap Tuff Site is approximately one km to the east of the escarpment at an approximate elevation of 1200 m. Nine inclined boreholes have been installed at the site in three sets (Figure 1). Each set consists of three boreholes drilled in a plane at an angle of 45° and with spacings of 10 m. The boreholes are not of the same length, with the lengths of the boreholes being 15, 30, and 45 m. This design results in the bottom of each borehole lying below the same point on the surface. The three borehole sets are parallel to each other, except that one set is oriented 180° opposite of the other two sets. A synthetic plastic cover has been placed over the rock surface to cover an area of approximately 50 m x 30 m. The cover is designed to prevent evaporation from the rock to the atmosphere as well as to prevent precipitation from infiltrating into the rock.

2.1 Geologic Setting

The rocks exposed at the Apache Leap Tuff Site are the uppermost unit of a sequence of ash-flow tuff sheets. The tuff is a consolidated deposit of volcanic ash, with particle diameters less than 0.4 mm, resulting from a turbulent mixture of gas and pyroclastic materials of high temperature. In addition to the volcanic ash groundmass, the tuff also contains various mixtures of phenocrysts, pumice fragments, and entrained foreign rocks, principally diabase. Figure 2 summarizes the elemental and mineralogical composition of the groundmass and the phenocrysts. The groundmass and the phenocrysts were ejected from a cauldera which was possibly located some distance to the north of the field site. The other materials were entrained by the ejected materials during the eruption event or as the tuff traveled rapidly downslope as a nuee ardente.

The ash-flow deposits at one time covered an area of approximately 1000 km^2 with a maximum thickness of 600 m but have been subsequently eroded in some places to about 150 m. The structure of the ash-flow tuff sheets consists of jointed, layered planar deposits. Near-horizontal joints, parallel to the plane of the flattening of the pumice fragments, are distinct to indistinct with dips to about 30°, but in some places to as much as 60°. Near-vertical parallel joint sets are also present with spacings from 1.5 to 4.5 m. Such sets intersect at angles between 60° and 90°. Identified faults generally trend north to northwest, with the west or southwest side being downthrown. Figure 3 summarizes strike and dip data at the Apache Leap Tuff site.

According to Peterson (1968), the mid-Miocene (19 m.y.) ash-flow sheet is composed of five units, (1) a basal unit with little to no welding, (2) an overlying vitrophyre composed of a matrix of black glass and the

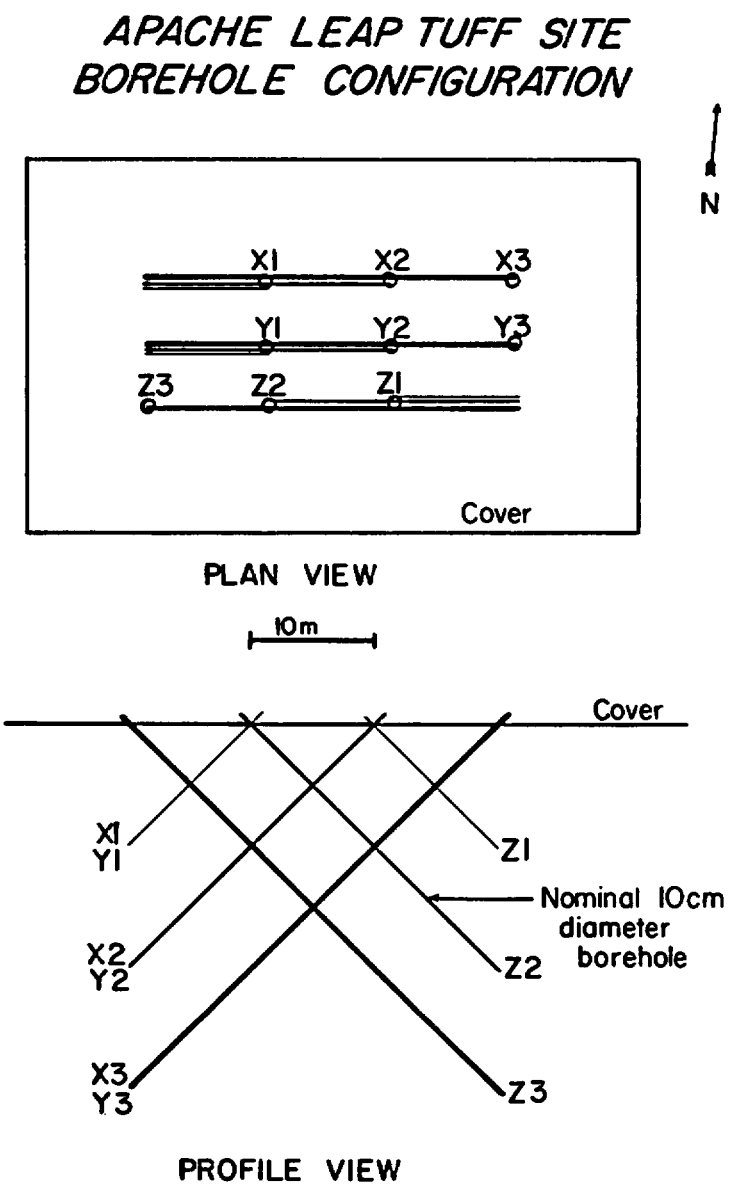

Figure 1: Borehole configuration at the Apache Leap Tuff Site showing inclined boreholes and 30 x 50 m plastic cover.

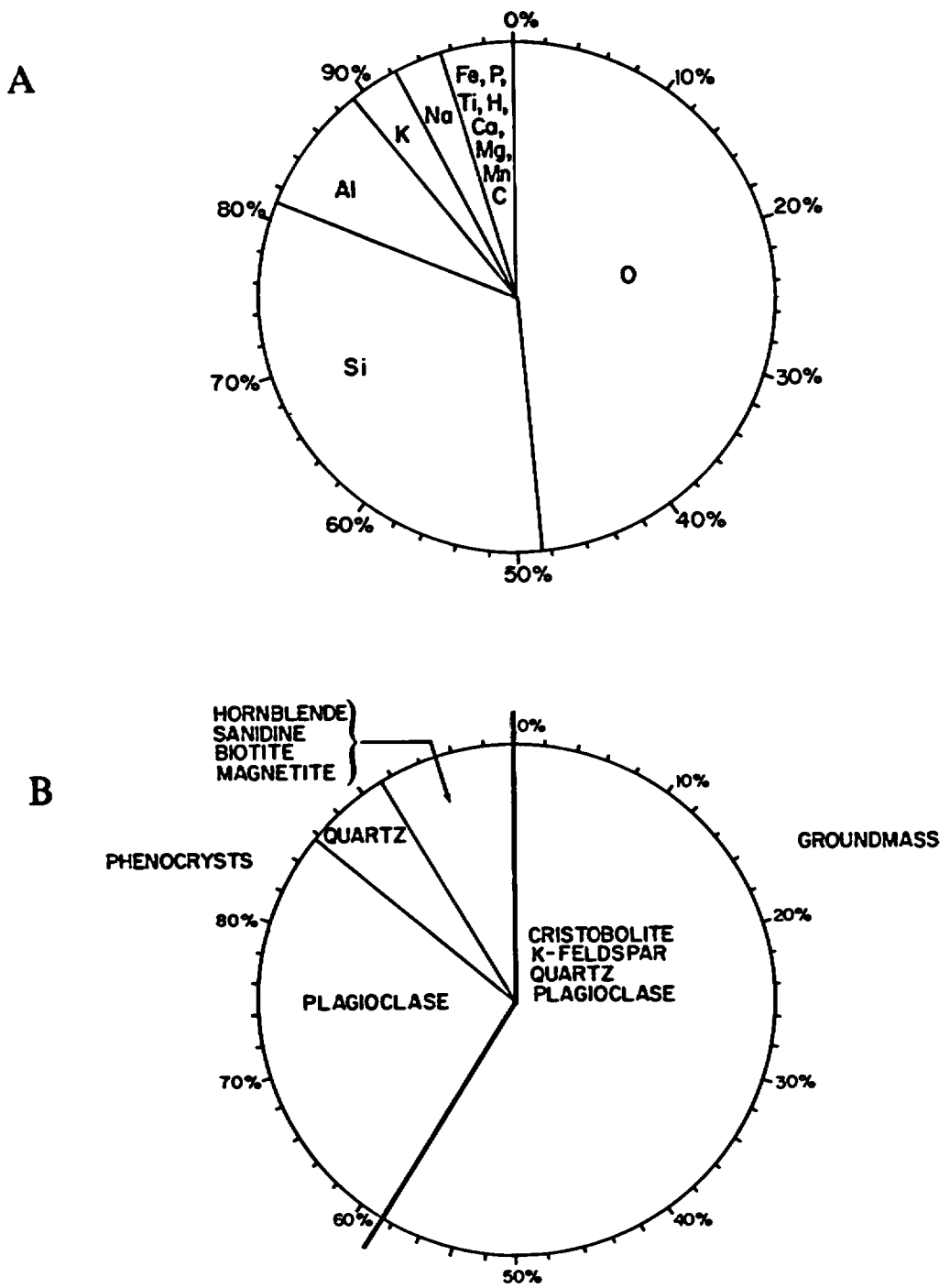

Figure 2: Whole rock elemental composition (A) and mineralogic composition of tuff groundmass and phenocrysts (B) at the Apache Leap Tuff Site.

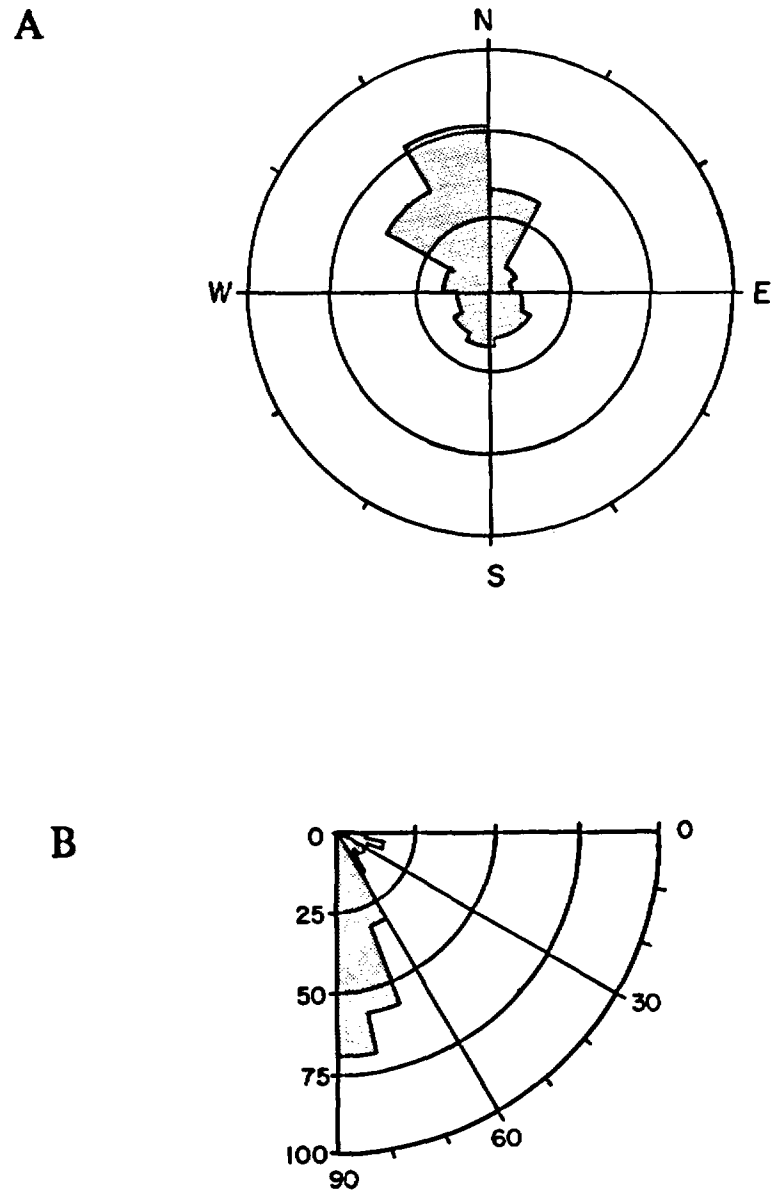

Figure 3: Distribution of fracture strikes (A) and dips (B) at the Apache Leap Tuff Site.

normal assemblage of phenocrysts and sparse to abundant lithic inclusions, (3) a brown, densely welded unit upon which has been superimposed a zone of devitrification, (4) a gray zone in which the original welded tuff has been obscured by the superimposed crystallization, and (5) a white unit with crystallization so intense that the original vitroclastic textures have been completely obliterated. The tuff is called a dacite due to the numerous quartz and feldspar phenocrysts, the feldspar phenocrysts being mostly plagioclase. The tuff can also be called a quartz latite due to its chemical composition. It is noted by Peterson that SiO_2 and ferric iron decrease with depth, while ferrous iron, magnesium and calcium increase with depth. The iron trends indicate that greater interaction with the atmosphere has occurred in shallower rocks, while the other trends are attributed to gases escaping during cooling of the ash-flow sheet.

2.2 Hydrologic Setting

Precipitation has been recorded within one km of the Apache Leap Tuff Site (Magma Number 9 Shaft at an elevation of 1270 m) for the period from 1974 to 1984. During this period the average annual total was 640 mm. A longer term average at the Apache Leap Tuff Site can be estimating by using data from a station at the nearby town of Superior (elevation 910 m) with a 61 year period of record. During the same 11 year record (i.e., 1974-1984) the average annual precipitation was 539 mm, compared to 453 mm for the entire record. Using the same ratio of precipitation for the two time periods, the longer term average at the site is estimated to be 538 mm. Most of the precipitation at the Apache Leap Tuff Site occurs during two periods, from mid-July to late-September, and from mid-November to late-March. The summer storms are characterized by high-intensity, short-duration thunderstorms during periods of high temperature and evapotranspiration demand. The winter storms are of longer duration and lower intensity during cooler periods with much lower evapotranspiration demand.

A large number of ephemeral streams are present near the Apache Leap Tuff Site which respond to seasonal precipitation. Because evapotranspiration is lowest during the winter, most of the streamflow occurs during the winter months. Infiltration from the ephemeral streams into fractures exposed on the bottom of the channel is possible during flow events, and a vortex above a fracture in the Queen Creek channel near the Apache Leap Tuff Site during periods of runoff has been noted. In some places the stream channels are formed along regional faults and fractures, providing enhanced infiltration potential during flow events. No perennial surface water is present in the vicinity of the Apache Leap Tuff Site except for a few stock ponds which are able to maintain their water supply during long drought periods. These ponds are underlain by accumulations of clay which inhibit recharge. It can be concluded from these field observations that the most probable infiltration mechanism is from intermittent winter streamflow in channels which intersect open fractures.

Regional ground water levels below the Apache Leap Tuff Site have been substantially modified by dewatering activities at the Magma mine which extends to a depth of 1500 m below the Apache Leap Tuff Site. The water levels have been drawn down to levels below the lowest tuff unit.

Perched water has been observed at several locations near the Apache Leap Tuff Site, notably in shallow alluvial aquifers along major washes, and at the interface between the base of the tuff deposit and the underlying carbonate unit. Noticeable increases in inflows to the main haulage tunnel for the Magma mine are observed within days following streamflow in Queen Creek, which is located approximately 100 m above the haulage tunnel. Deeper levels observe increased inflows up to several weeks following streamflow events.

CHAPTER 3

MATRIX CHARACTERIZATION PROCEDURES

The development of a conceptual model for flow and transport of fluids and solutes through the fractured tuff observed at the Apache Leap Tuff Site requires that relevant physical and geologic parameters be characterized. In particular, rock matrix and rock fracture characterization parameters are determined using field and laboratory data. Matrix parameters are obtained from field data for 90 samples located at depths varying from 3 to 30 m (Figure 4). The rock samples are collected from 5 cm diameter, oriented cores which were extracted at the time of borehole construction. The samples are removed from unfractured core sections at roughly three meter intervals along the core.

For saturated fluid flow and solute transport through the rock matrix the task is to estimate the spatial distributions of the saturated hydraulic conductivity as well as the effective porosity of the medium. For unsaturated flow through the rock matrix the parameter estimation task is complicated by the rapidly changing nature of the unsaturated hydraulic conductivity, which is a function of the water content of the medium. Required matrix characterization parameters include the unsaturated hydraulic conductivity for the rock matrix, as well as the rock matrix moisture characteristic curve. Because the relationships between the degree of saturation, the moisture potential, and the hydraulic conductivity tensor may be determinable using capillary theory, the distribution of pore sizes within the rock matrix is another important characterization parameter. The spatial variability of flow and transport parameters directly affects estimates of large scale flow behavior. To examine the importance of spatial variability it is first necessary to obtain data at more than one point. Data collection activities must incorporate sufficient detail so that trends and correlation scales can be identified.

3.1 Porosity, Pore Size Distribution, and Bulk Density

The total water holding capacity of the rock matrix is limited by the porosity of the geologic medium. The matrix porosity is the amount of pore space within a rock mass, exclusive of fractures and sizable solution openings. The total matrix porosity includes pores which are isolated from other pores, or which dead-end. The effective matrix porosity refers only to the pores which are interconnected, and is less than or equal to the total matrix porosity.

The pore size distribution is a quantification of the porosity in terms of a distribution of pores with an assumed right cylindrical shape. The pore size distribution can be obtained using a mercury porosimeter (Klavetter and Peters, 1987) or the nitrogen gas adsorption technique (Rasmussen and Evans, 1987). The mercury porosimeter relies on a negative wetting coefficient resulting from a contact angle of about 140°. The mercury porosimetry technique is appropriate for pores with a radius in excess of 3.5 nm. Pores smaller than 0.1 nm can also be measured using nitrogen gas adsorption techniques.

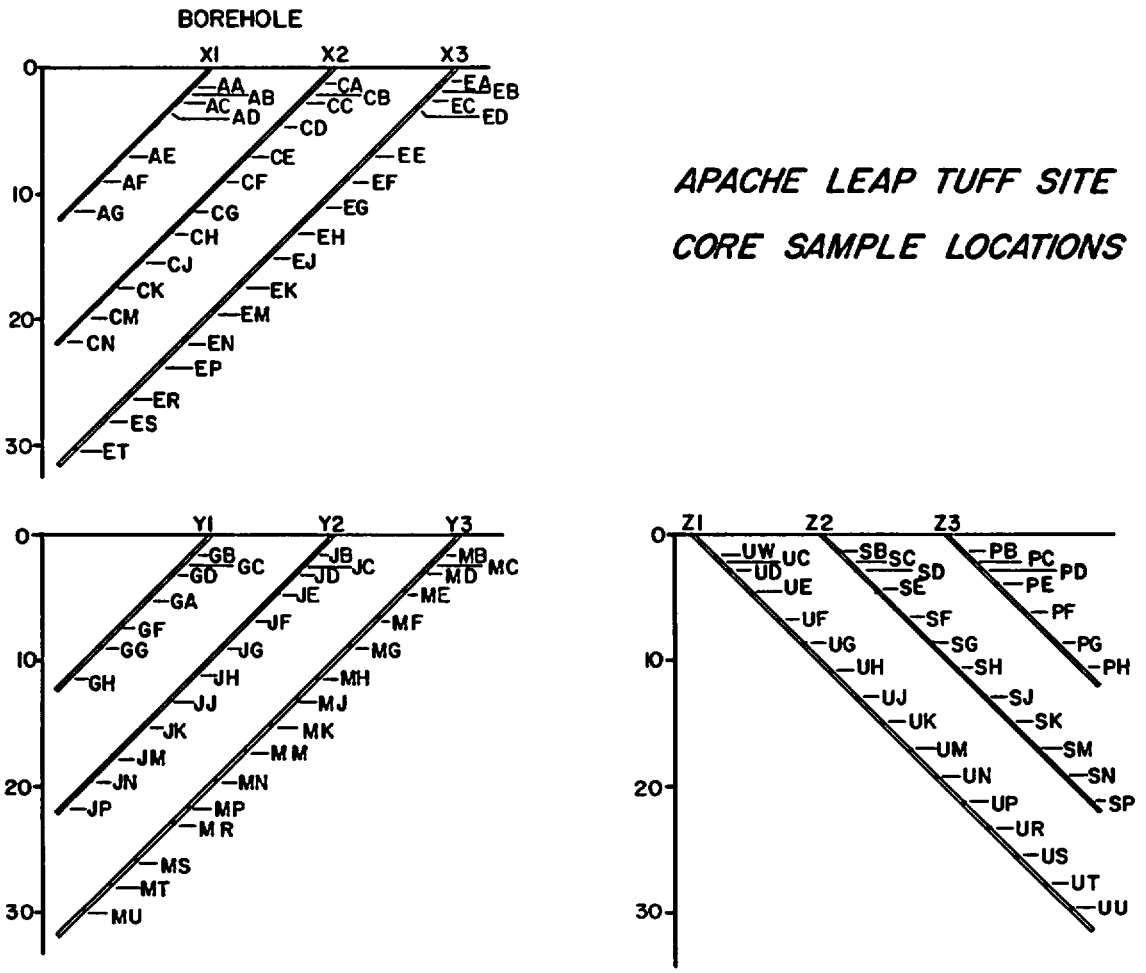

Figure 4: Core sample locations in inclined boreholes at the Apache Leap Tuff Site.

The bulk density and porosity of a rock sample are determinable using the paraffin, water saturation, gravimetric and gamma ray attenuation methods (Rasmussen and Evans, 1986). Caliper measurements of rock volume with gravimetric determination of rock weight can also be used to determine rock bulk density. In general, the bulk density is defined as:

$$(3.1) \qquad \rho_b = M_{dry} / V$$

where

ρ_b bulk density of the sample, kg/m^3;
M_{dry} mass of oven dried sample, kg; and
V volume of the sample, m^3.

If the sample is a regular solid, then the volume can be found by measuring the physical dimensions of the sample. If the sample is not regular, the sample must first be saturated under a vacuum and added to a beaker of water. The difference in the weight of the beaker with and without the sample is the weight of the saturated sample. The sample is then suspended by a fine wire under water within the beaker and the difference in weight between the beaker with the sample and without the sample is recorded. The volume of the sample is determined using:

$$(3.2) \qquad V = M_{sus} / \rho$$

where

M_{sus} difference in mass of suspended, saturated sample and beaker, kg; and
ρ density of water, kg/m^3.

The effective porosity, n_e (dimensionless), of the sample is estimated using:

$$(3.3) \qquad n_e = (M_{sat} - M_{dry}) / (\rho V)$$

The residual rock density, ρ_g (kg/m^3), which includes rock grains and isolated pores, is found using:

$$(3.4) \qquad \rho_g = \rho_b / (1 - n_e)$$

The pore size distribution is determined using mercury intrusion. A cylindrical rock sample with dimensions of 2.5 cm x 2.5 cm is examined by subjecting the sample to pressures of 0 to 2000 bars. Because mercury is lithophobic, increasingly higher pressures are required to force mercury into smaller pores. By measuring the volume of mercury intruded into the sample as a function of pressure, a relationship between pore size and frequency can be determined. Mercury intrusion can also be used to determine the rock core segment volume, total effective porosity, and residual rock density.

3.2 Saturated Hydraulic Conductivity

The saturated hydraulic conductivity is estimated using six centimeter diameter core segments cut to a five centimeter length. The core seg-

ment is saturated under a vacuum and placed inside of a permeameter (Figure 5). An inflatable packer within the permeameter is then pressurized to at least three bars to prevent bypassing of water between the core and the permeameter wall. A known pressure head of nitrogen gas, approximately one bar, is applied to the upper surface of a column of water which is in contact with the upper surface of the rock core. The outflow is measured by collecting water from the bottom of the permeameter. The saturated hydraulic conductivity is determined using:

$$K = Q L / A H \quad (3.5)$$

where

- K hydraulic conductivity, m/s;
- Q volumetric flow through the core segment, m^3/s;
- L length of the core segment, m;
- A area of the core segment, m^2; and
- H hydraulic head across the core segment, m.

The hydraulic head is computed from:

$$H = p + (z_1 - z_2) \quad (3.6)$$

where

- p pressure head applied to the water surface, m;
- z_1 elevation of water surface above core, m; and
- z_2 elevation of the outlet point, m.

In addition to the hydraulic conductivity, the intrinsic permeability can also be computed:

$$k = K \mu / \rho g \quad (3.7)$$

where

- k intrinsic permeability, m^2;
- μ dynamic viscosity, Pa s;
- ρ fluid density, kg/m^3; and
- g gravitational constant, m/s^2.

3.3 Moisture Characteristic Curve

The matrix moisture characteristic curve relates the fluid content of a rock sample to the ambient fluid potential within the matrix. This relationship can be generated by applying capillary theory to the pore size distribution or by using a pressure plate extractor or a Tempe pressure cell. Both the pressure plate extractor and the Tempe pressure cell are used to apply a known positive pressure to the sample and to measure the resulting liquid displacement.

The rock matrix moisture characteristic curve between zero and one bar suction is obtained using the outflow method for the core segments. The outflow method uses a Tempe pressure cell with a one bar porous plate to provide an enclosed chamber within which an air pressure greater than atmospheric is applied (Figure 6). The excess air pressure is used to drive water from the sample through the porous plate, the rate of water

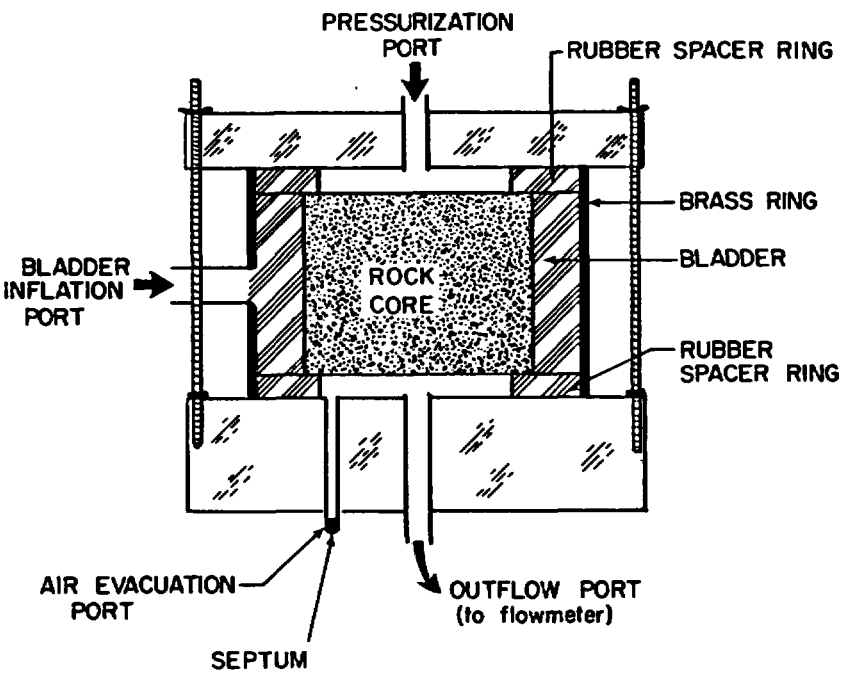

Figure 5: Permeameter used to obtain saturated hydraulic conductivity and unsaturated pneumatic permeabilities for rock core samples obtained from the Apache Leap Tuff Site.

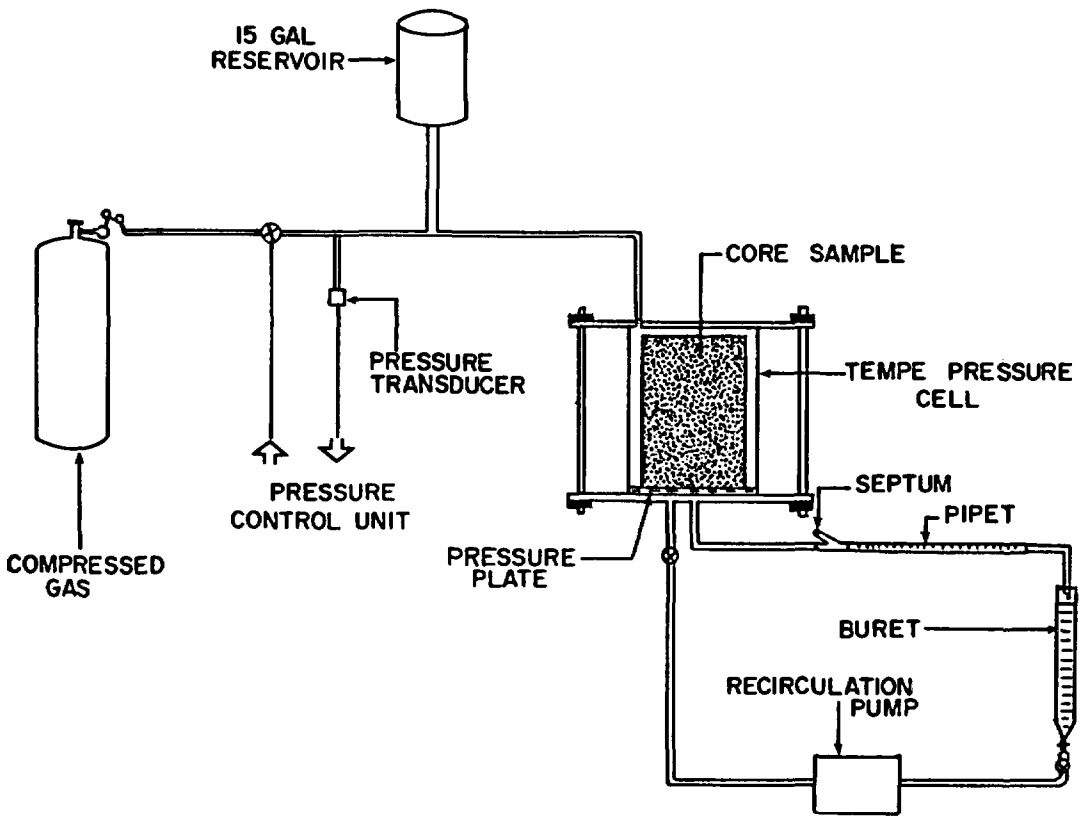

Figure 6: Outflow method experimental setup for determining unsaturated hydraulic conductivity and characteristic curves for rock core samples obtained from the Apache Leap Tuff Site.

flow and the total volume being used to determine the hydraulic diffusivity, moisture content, and the unsaturated hydraulic conductivity. Rahi (1986) provides a description of the apparatus and procedure used.

Between one and ten bars suction, the matrix moisture characteristic curve is determined using a pressure extractor vessel. The interior of the chamber is maintained at the desired pressure and a rock sample is placed on the pressure plate until an equilibrium water content is achieved. The weight before and after the pressure is applied is used to determine the rock water content. For suctions greater than approximately ten bars, a thermocouple psychrometer (Rasmussen and Evans, 1986) is used to measure the moisture characteristic curve. The thermocouple psychrometer measures the wet-bulb depression of air that immediately surrounds a 1 x 1 cm rock cylinder. The wet-bulb depression is obtained by observing the temperature difference between a dry thermocouple and a thermocouple which has been immersed and removed from de-ionized water. The wet-bulb depression can be related to the water potential using tables calibrated from osmotic solutions. The water potential at various water contents is measured by allowing the rock sample to desaturate by evaporation in the atmosphere. The water content is determined using gravimetric procedures.

3.4 Unsaturated Hydraulic Conductivity

Laboratory estimates of the unsaturated matrix hydraulic conductivity within the range of zero to one bar suction are obtained using the outflow method, previously described. A field technique is also available for estimating the unsaturated rock matrix hydraulic conductivity using changes in rock matrix water content. This technique requires that a vertical unit hydraulic gradient be present in the rock, that no evaporation or vapor transport be present, and that a means to measure changes in water content is also available. Neutron probes provide a means for monitoring rock water content. Neutron probes incorporate a fast neutron source and a thermal neutron counter. Because the hydrogen atoms within the water molecule efficiently convert fast neutrons to thermal neutrons, the number of thermal neutrons counted can be directly related to rock water content within approximately 0.5 m of the source. The change in rock water content over time can also be related to the rock water drainage rate, which is related to the unsaturated hydraulic conductivity. Stephens (1985) also presents a method using flow nets derived from field data for determining the unsaturated hydraulic conductivity. Wierenga et al., (1986) also present a methodology for estimating unsaturated hydraulic conductivity from field tests. These field estimates of matrix unsaturated hydraulic conductivity can then be compared with laboratory estimates obtained from core samples to evaluate procedures and assumptions.

3.5 Unsaturated Pneumatic Conductivity

Unsaturated pneumatic conductivity is obtained by employing the permeameter previously illustrated in Figure 5 for rock core segments. The water content of core segments is lowered to a prescribed suction or water content and then placed inside of the permeameter with the packer inflated to prevent bypassing of air around the outside of the core. A known pressure gradient is applied longitudinally across the core

segment and the air flow is measured using a soap bubble flow meter. The unsaturated pneumatic conductivity is determined using the measured air flow, cross sectional area and core segment length. Because the air is compressible, the ideal gas law can be employed with the assumption of isothermal flow:

$$(3.8) \qquad P = 2\ Q\ L\ H_o\ /\ A\ (H^2 - H_o^2)$$

where

- P pneumatic conductivity, a function of water content, m/s;
- H_o ambient atmospheric pressure head, m; and
- H absolute pressure pressure head applied to the upper rock surface, m.

The pneumatic permeability can be computed from air flow measurements using Equation (3.7). The permeability of a dry sample computed using air flow measurements should be similar to the permeability of a wet sample computed using water measurements.

3.6 Effective Matrix Diffusivity

Rasmussen (1982) presents equations for estimating the effective matrix diffusivity from estimates of matrix tortuosity, matrix porosity, and the diffusivity of the solute in water. Laboratory determination of matrix porosity are presented above. Estimates of matrix tortuosity are more difficult to obtain. A direct estimate of the effective matrix diffusion can be obtained from diffusion studies using twin reservoirs of water separated by a thin slice of the rock matrix. A known concentration of solute is maintained within one reservoir, and the change in concentration of the solute in the second reservoir is used to obtain an estimate of the effective matrix diffusion coefficient.

3.7 Matrix Retardation Coefficient

Retardation coefficients can be obtained using crushed samples of the matrix rock of interest. A known concentration of solute is mixed with the rock until an equilibrium concentration of the solute is observed. The mass of solute on the solid phase per unit mass of solid phase divided by the concentration of solute in solution is used to obtain the distribution coefficient. The retardation coefficient is calculated from the distribution coefficient using:

$$(3.9) \qquad R = 1 + \rho_b / n_e\ K_d$$

where

- R retardation coefficient, dimensionless;
- K_d distribution coefficient, m^3/kg.

CHAPTER 4

FRACTURE CHARACTERIZATION REQUIREMENTS

Fractures provide pathways for increased water flow and solute transport as well as obstructions to flow when the fractures are desaturated or filled with geochemical precipitates. Water flow from boreholes at the Apache Leap Tuff Site is highly variable, dependent upon the presence of a few isolated high permeability zones. In some cases these zones can be related to individual fractures, but no good general agreement can be found between fracture density and water loss. In addition, the amount of flow through fractures under unsaturated conditions is not known quantitatively.

The ability to directly or indirectly collect information about specific fracture parameters is dependent upon the capability to sample or observe parameter values. This capability is limited to openings large enough to enable the entry of humans or data-gathering equipment. Such access can be gained by using natural rock exposures, such as bare ground and caves, or by creating exposed surfaces such as boreholes, trenches, and mine shafts. The surfaces are then used to provide information about parameters of interest. Additional information can be obtained using bulk samples of the underground material. Rock analyses can be performed on cores obtained from drilled boreholes, from rock slabs obtained from quarrying, and from boulders obtained from surface exposures. Data obtained directly from rock surfaces and bulk samples are limited due to both the cost and destructive effects of sampling. Indirect measurements must often be used to replace or to supplement direct measurements, especially when only a small sample is available for inferring the total system. Inferences about flow parameters can be obtained from hydraulic and pneumatic testing. Fluid samples are injected or recovered to obtain information which is then used to infer system parameters.

While major geologic structures (such as dikes, faults, bedding planes, and large shear zones) can often be observed because of their continuity and visibility, the minor structures (such as shrinkage joints, tectonic joints, stress-release joints, and cooling joints near margins of igneous bodies) usually cannot be mapped individually from one borehole or exposure to another. In the latter case, statistical data about the parameters must also be obtained.

The following discussion is related to the description of characterization data and data collection procedures for fractures within geologic media. In particular, such parameters as orientation, size, density, number of fracture sets, connectivity between fractures, and transmissivity are described.

4.1 Number of Fracture Sets

A network of fractures can generally be separated into distinct fracture sets whose parameters are more uniform when compared to parameters obtained from all fractures. Each fracture set can be attributed to

different formation histories, and relevant fracture parameters are stratified according to membership in a particular fracture set (Zanback, 1977). Data about the number of fracture sets is usually obtained from a stereonet plot of fracture orientations (Jones, 1983). The orientation parameters provide the most discriminating evidence for stratification of fracture parameters into distinct fracture sets. Techniques for estimating the number of fracture sets from stereonets are usually based on ocular interpretations rather than on rigorous statistical tests.

Bles and Feuga (1986) describe four types of fractures: joints, tension gashes or fractures, stylolites, and faults (Figure 7). Joints are defined as discontinuities with contiguous sides showing no relative movement between the sides. Joints can be divided into sets, or into networks having two or more related orientations, but are normally perpendicular or at an angle to the stratification or schistosity. The joints can vary from tens of centimeters in length to tens of meters on occasion. While the aperture of joints is generally very small, they can open to a few millimeters. The joints may also be lined with quartz or calcite precipitates.

The second type of fracture is described as either tension gashes or tension fractures. These fractures demonstrate displacement perpendicular to the plane of the original fissure. This displacement may be centimeters to tens of centimeters thick. Tension fractures usually extend tens of centimeters, but range from a few centimeters to several tens of meters. The fractures are usually aligned en echelon, with the longitudinal length being much greater than the transverse continuity (i.e., much taller than wider). Tension fractures are almost always filled with calcite, quartz or other crystals.

A third type of fracture is an irregular discontinuity, termed a stylolite. This type of fracture is extremely rough and far from planar, showing alternating peaks and hollows, with either a cylindrical or conical shape. Stylolites extend from a few tenths of millimeters to a few centimeters in length, rarely extending to several tens of centimeters. This type of fracture can be coated with a thin film of clay or with clay residues and insoluble iron oxides.

The final type of fracture is a fault, described as having a displacement relative to two surfaces in a direction parallel to the plane of the fracture. Evidence of displacement is the presence of polished surfaces, striations, and conjugate sets. The conjugate sets arise from two fracture sets which intersect either horizontally, resulting from normal faulting, or vertically, resulting from strike-slip faulting. Faults can be from tens of centimeters to hundreds of kilometers in length. This type of fracture is filled with recrystallized quartz and calcite, or cataclastic and crushed infillings.

4.2 Fracture Center Location

The location of a fracture can be characterized by its central tendency, or center location. For centers located randomly (i.e., as an independent and identically distributed, IID, random variable), a Poisson process can be assumed. Such a process is based on (Law and Kelton, 1982):

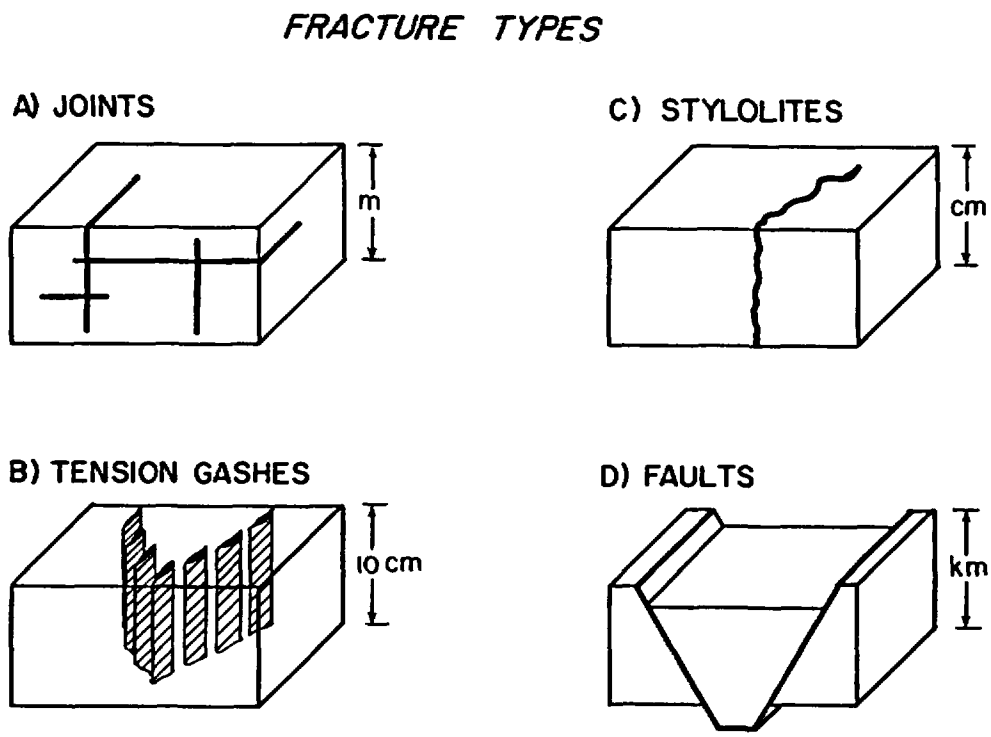

Figure 7: Fracture types common in fractured rock. Notice difference in scale between fracture types.

- o The probability of two fracture centers occupying the same position is zero;

- o The number of fracture centers in any volume is independent of location; and

- o The number of fracture centers in any volume is independent of the number of fracture centers in any other volume.

For a Poisson process, the locations of fracture centers can be described using a uniform probability distribution. The observed distance between fracture centers for a Poisson process is also an IID random variable, with an exponential probability distribution. Snow (1968) indicates that observed fracture spacings along a sample line are, in fact, exponentially distributed. The number of fracture centers per unit volume, another IID random variable, can be described using a Poisson probability distribution.

For a medium within which fractures appear to occur at uniform intervals, such as in bedded sedimentary deposits, the distances between fractures will be normally distributed in the direction perpendicular to the fracture planes. Priest and Hudson (1976) demonstrated that an evenly-spaced set of centroids results in a distribution which cannot be described by the negative exponential distribution. They observed that a mix of random, clustered, and evenly-spaced centroids results in a distribution which can be statistically described by the negative exponential distribution. The reader is referred to Law and Kelton (1982) for the condition when fracture centers are not generated using stationary parameters, or when fracture centers are present in clusters.

4.3 Fracture Orientation

Fracture orientation is determined from either surface or subsurface exposures of fracture traces. At the Apache Leap Tuff Site fracture orientations are obtained from oriented cores collected during the drilling of inclined boreholes at the site. Orientation was provided by placing a mark every 3 m on the core. The orientation mark was made on the end of each core segment by dropping a drilling tool with a sharp point protruding from the lower end of the tool down the borehole. Because the borehole was slanted and the sharp point was offset and heavily weighted, a mark was made on the lower edge of the end of each core.

Once the oriented core has been collected, a goniometer is used to obtain the geometric information needed to determine the relative and absolute strike and dip of the fractures (McClellan, 1948). The data indicate the presence of many fractures which dip steeply to the southwest and northwest, as well as a fewer number of flat to shallow lying fractures (Figure 8). The existence of these sets is supported by fracture surface exposures in surrounding outcrops of the study area. Because the orientation of the dominant set is generally perpendicular to the bedding of the ash flow sheet, the dominant fractures are termed joints. Many of the joints are lined with quartz and calcite precipitates.

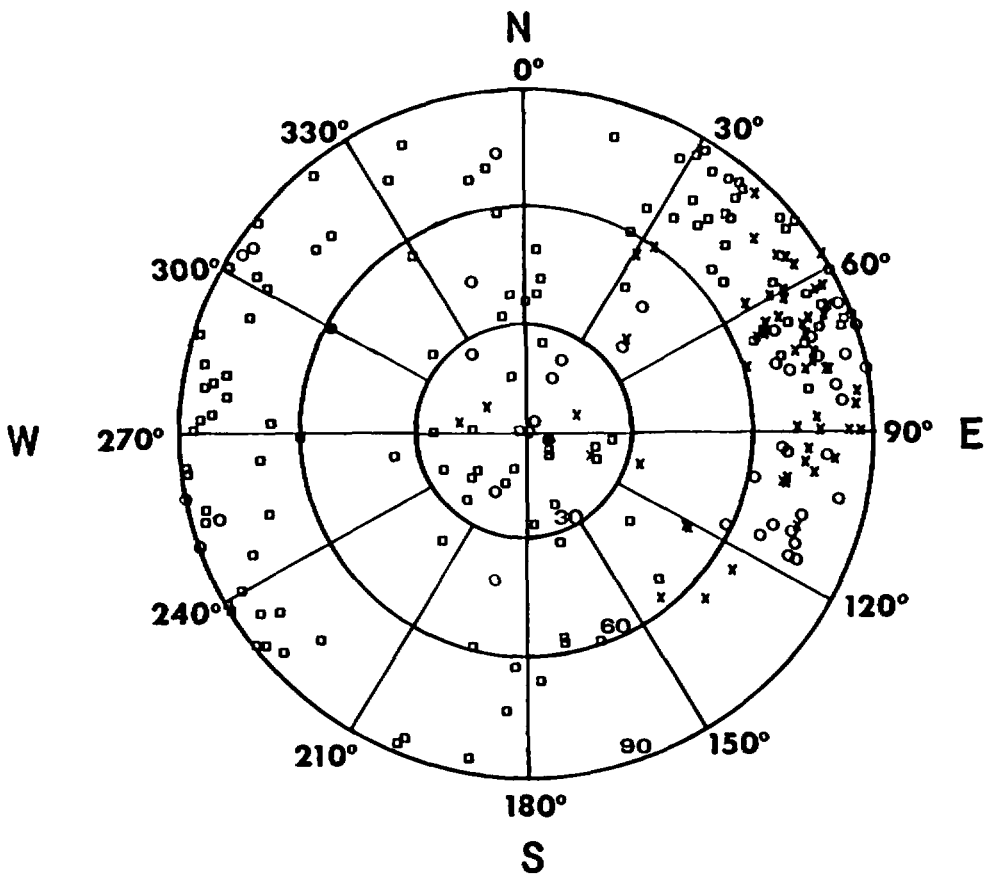

Figure 8: Lower stereonet projection of fracture orientations observed at Apache Leap Tuff Site, from X-series boreholes (crosses), Y-series boreholes (circles) and Z-series boreholes (squares).

4.4 Fracture Areal Extent and Shape

Fracture areal extent is a measure of the two-dimensional length of each fracture. The measure is difficult to obtain because length cannot be measured from individual cores. Also, lengths measured from surface exposures or within mine shafts are chords between two endpoints of a fracture and underestimate of fracture lengths. The only method for obtaining accurate estimates of fracture lengths is through repeated corings and/or slicings along lines perpendicular to the plane of each fracture set.

The areal extent of fractures is difficult to measure chiefly due to the limited rock surface exposures available. No standardized methods have been developed as a result. While fracture surfaces could be delineated from surface exposures or by correlation between borehole-fracture logs, neither method is entirely successful. Most exposed rock surfaces are of limited extent and generally smaller than the linear fracture traces being measured.

The fracture shape is a means for establishing the relationship between the areal extent of a fracture and its orientation. If a known relationship between fracture length and orientation can be estimated, then the fracture shape can be defined. When fracture length is constant with respect to the orientation of the fracture the fracture assumes a circular shape. For a square fracture the expected length of any side is required along with the orientation of the sides. The lengths and orientations of the major and minor axes are required for fractures with elliptic or rectangular shapes.

Robertson (1970) showed that fracture shape (plan view) is equidimensional (which results in the major axes being uncorrelated). For assumed circular fractures, fracture lengths have been described by a lognormal distribution (Baecher et al., 1977). The gamma distribution did not provide as good a fit as the lognormal, while the exponential and normal distributions performed poorly. Baecher et al., (1977) cite MacMahon (1974), Bridges (1976), and Barton (1977) to support their observations. Other authors (Robertson, 1970; Stetten, 1970; Call, 1976), however, report obtaining better results using the exponential distribution to describe fracture lengths.

Because borehole fracture logs suffer from the limited ability to correlate fracture intercepts between all but closely spaced boreholes, a large number of boreholes are required to delineate the areal extent of fractures. The analysis of fracture extent from fracture trace measurements is possible if certain simplifications can be made:

- o The distribution of fracture centroids is assumed, usually random;
- o Fractures have an assumed shape, usually circular; and
- o The distribution of fracture lengths is assumed, usually lognormal or exponential.

Using these simplifications, the distribution of trace lengths along any sampling line can be predicted. Field measurements of trace length

represent a censored and truncated sample of this distribution, because larger trace lengths exceed the exposed measurement surface and very small trace lengths are often ignored during mapping. To account for the limited sample, the parameters of the complete trace distribution are first calculated. The parameters of the true size distribution are obtained from this distribution.

4.5 Fracture Density and Spacing

The density of fractures is a measure of the number of fractures in a rock body. The measure can be refined to estimate the density for individual fracture sets (Priest and Hudson, 1976). Such a measure should provide information about the number of fracture centers within the rock mass, as well as the total fracture porosity. The common method for measuring fracture density is to use a line measure, such as a drill core. This technique requires that a line orthogonal to the orientation of the fractures be used for each fracture set. The number of fractures intersecting the line are counted and the sum is divided by the length of the line. The reciprocal of the number per unit length is used as the estimate of the fracture density. It is important that intersections from other fracture sets are not included in this measure.

A second method for determining fracture density uses a plane surface, such as a mine shaft wall or surface exposure, to obtain measurements of the length of fractures intersecting the wall surface. The total length of fractures in each fracture set is divided by the surface area to obtain the density measure. A third method employs a volumetric measure. This measure is formulated in terms of the fracture-matrix surface area contained within a volume of rock for each fracture set. If only one wall of the fracture is considered, then the density measure is estimated as the fracture surface area divided by the volume of the rock examined.

The first two techniques fail to incorporate fracture length into the measure. For example, a single long fracture can provide the same total length of fracture on a planar surface as many shorter fractures. To determine the number of fractures per unit volume requires that the density measures estimated above be normalized by the areal extent of the fractures.

4.6 Porosity

Fracture porosity is the ratio of the volume of fracture openings to the volume of whole rock. One way to calculate the fracture porosity is to find the product of the mean fracture aperture and the mean fracture density. The second measure is the effective fracture porosity which is the percentage volume of fracture openings which are interconnected to each other and to an exterior surface. The effective fracture porosity can be calculated using solute breakthrough curves by noting the amount of fluid discharged before half of the solute volume is discharged following a step input of tracer. Because the effective fracture porosity will always be smaller than the calculated fracture porosity, the lower limit of the product of the mean aperture and the mean fracture density can be established.

It is important to emphasize that while the fracture porosity may be small, the fracture porosity can play an important role in determining the hydraulic conductivity of a geologic medium. To demonstrate that the fracture porosity is normally small, a core taken from the densely-welded unit of the Apache Leap tuff is presented as an example. Using an estimated fracture density of three fractures per meter and assuming an extreme mean aperture to be 300 mm, the fracture porosity is not more than 0.001. The effective porosity depends to a large extent on fracture continuity. Gordon (1986) presents a simulation study which demonstrates that the fracture effective porosity is both a function of the scale of analysis and fracture continuity. The difference between the effective porosities as calculated at different scales may differ by several orders of magnitude. Methods to estimate the porosity of the fractures as well as the rock fracture unsaturated hydraulic conductivity are still in the development stage. Laboratory and field techniques will require the isolation of individual fractures and the use of tracer tests to establish flow velocities.

4.7 Aperture

Aperture refers to the perpendicular distance between adjacent walls of a fracture in which the intervening space is filled with air or water. This definition excludes fractures which have been closed by mineral deposits. Fracture aperture is not a constant but varies from zero aperture at points of contact (which may exist to transmit stress), to some maximum value (Billaux, 1984; Kilbury et al., 1986; Neuzil and Tracy, 1981). Fractures with apertures greater than 200 mm can be crudely measured along exposed rock surfaces using a millimeter scale, while narrower apertures can be accurately measured with a feeler gauge. A very accurate method (<10 um absolute error) has been developed (Snow, 1969) using a penetrant dye and camera. The difficulty with measurements at surface exposures is that stress relief, weathering, and blast damage tend to alter fracture apertures from those in undisturbed rock.

Boreholes provide another means for directly measuring fracture apertures. A grouted rod may be overcored and removed to preserve fracture apertures in the core. More commonly, borehole surfaces are inspected directly using borescopes or borehole television cameras. As an example, a small diameter (32 mm) TV logging camera provided by the U.S. Office of Mine Safety has been used to observe drillholes for the purpose of investigating nominal aperture widths. These estimates are qualitative and provide no absolute measure of fracture apertures.

While measurements of 256 fractures on surface outcrops indicate that individual fracture apertures can be lognormally distributed (Bianchi and Snow, 1969), the measurement of intra-fracture aperture variation has not been performed. Field measurements have been limited to direct measurement of fracture apertures along exposed rock surfaces where measurements give an estimate of aperture variability. Direct measurements of fracture aperture have also been made on large laboratory samples containing rough natural fractures (Sharp and Maini, 1972). Fracture contact areas as a function of stress were measured by Iwai (1976) using pressure sensitive plastic on lab samples containing rough, induced fractures.

Indirect methods of measuring fracture apertures have been developed based on hydraulic and pneumatic properties of fractures. Liquid and gas injection tests in both saturated and unsaturated rock have been used to measure changes in individual fracture apertures (Pratt et al., 1977; Hardin et al., 1981), to assess fracture aperture changes associated with blast damages (Montazer, 1982) and to assess fracture porosity and aperture distribution (Snow, 1968, 1969). A new technique developed by Kilbury et al. (1986) uses a fractured rock infiltrometer to estimate the fracture aperture on the earth-atmosphere interface. The infiltrometer can be used to measure both water or air intake rates at the interface. Analytic solutions were developed for both air and water flow, which use different flow equations and boundary conditions to estimate fracture aperture. Estimates using the two fluids are in close agreement.

The principal advantage of indirect methods is that the aperture over greater fracture surface areas are measured. The principal disadvantage is their reliance upon a physical relationship between the quantity being measured and the parameter of interest. Indirect methods for measuring intra-fracture aperture variability can only be suggested. Tracer dispersion may represent one possible method if diffusion and dispersion due to other factors can be separated or ignored. Another possible method is based on the relationship between stress and fracture aperture, which can be measured either in situ or on large laboratory samples (Schrauf and Evans, 1986).

4.8 Fracture-Surface Characterization

While fracture apertures are often idealized as smooth parallel plates, natural fractures are more likely to:

- Deviate from a planar surface (fracture waviness);
- Deviate from parallel sides (aperture variation); and
- Have reduced flow cross sections (increased contact area).

Schrauf and Evans (1986) show that existing numerical and experimental data for fracture apertures under approximately 0.2 to 0.3 mm suggest that the magnitude of roughness and waviness effects of fracture surfaces are secondary in comparison with the effect of contact area between fracture surfaces. Iwai (1976), in a comprehensive study of water flow through a single fracture, demonstrated that the reduction of flow cross section as a result of increasing contact area significantly affected observed water flow. In fact, Iwai showed that the expected flow rate decreased hyperbolically as the fracture surface contact area increased. However, roughness and waviness of the fractures become more significant as apertures increase due to increased effects of turbulence and inertial forces.

Tsang (1984) investigated the effect of fracture aperture variability on path tortuosity and channeling of fracture flow using an electrical resistivity analog. The analysis performed by Tsang indicates that as the number of small fracture apertures and contact regions increases, the larger the effect of tortuosity becomes. In addition to Tsang's

work, Montazer and Wilson (1984) and also Wang and Narasimhan (1985) evaluated the effect of fracture aperture variability on the unsaturated hydraulic conductivity.

The fracture specific surface of a rock is defined as the total fracture surface area per bulk volume of rock. Specific surface resulting from fractures may be obtained by multiplying the number of fractures per square meter by two (the number of fracture sides), and dividing by a unit depth of one meter. For the densely-welded Apache Leap Tuff Site, the fracture specific surface may be obtained by using an average fracture density of three fractures per square meter. The fracture specific surface is calculated to be 6 m^2 per cubic meter.

4.9 Fracture Connectivity

Fracture connectivity corresponds to an occupied bond in the context of percolation theory. Fracture connectivity is used to evaluate field and computer estimates of fracture parameters. Field estimates of fracture connectivity are critical not only for determining the effective fracture porosity, but also for estimating fracture lengths and apparent hydraulic apertures. The use of a tracer to identify fractures which are continuous between two boreholes, or groups of intersecting fractures which provide continuous air-phase passageways, has been tested at the Apache Leap Tuff Site. The method has been developed for locating connecting fractures by injecting a helium tracer gas into one borehole and monitoring its appearance in adjacent boreholes. Helium is an non-sorbing, inert air-phase tracer which is only slightly soluble in water. Detection of the gas is made possible by the use of a thermal conductivity meter. Because the thermal conductivity of helium is substantially less than the atmosphere, it can be detected at levels above 1×10^{-6} cc/sec.

The helium detection system includes a downhole probe for obtaining the gas sample from a specific point within the formation, a sampling pump to draw the gas sample from the downhole probe, and a detector unit for monitoring the gas concentration (Figure 9). The downhole probe used at the Apache Leap Tuff Field Site was specially constructed for application in the 10 cm nominal diameter boreholes located there. The probe consists of a hollow cylinder 45 cm long and approximately 8 cm in diameter, allowing an approximate 1 cm gap between the borehole wall and the probe. The space exterior to the probe is isolated from the rest of the borehole by using a 7.5 cm wide collar at either end of the cylinder. The collar provides a sealed volume of approximately 850 cm^3.

Leading to the volume through the interior of the probe are four sampling tubes which are placed radially near the upper end of the isolated volume. In addition, two return air ports are located opposite each other near the base of the isolated volume. The return air ports are used to flush out the sampling volume and to provide make-up air during a recirculation test. Because of the tight fit between the collar and the borehole wall, a weight is attached to the unit to allow it to slide down the hole. A 0.5 cm (3/16") steel cable is used to control the vertical location of the unit within the borehole. The lower end of the cable is attached to the upper end of the probe, while the upper end of the cable is coiled on a garden hose reel.

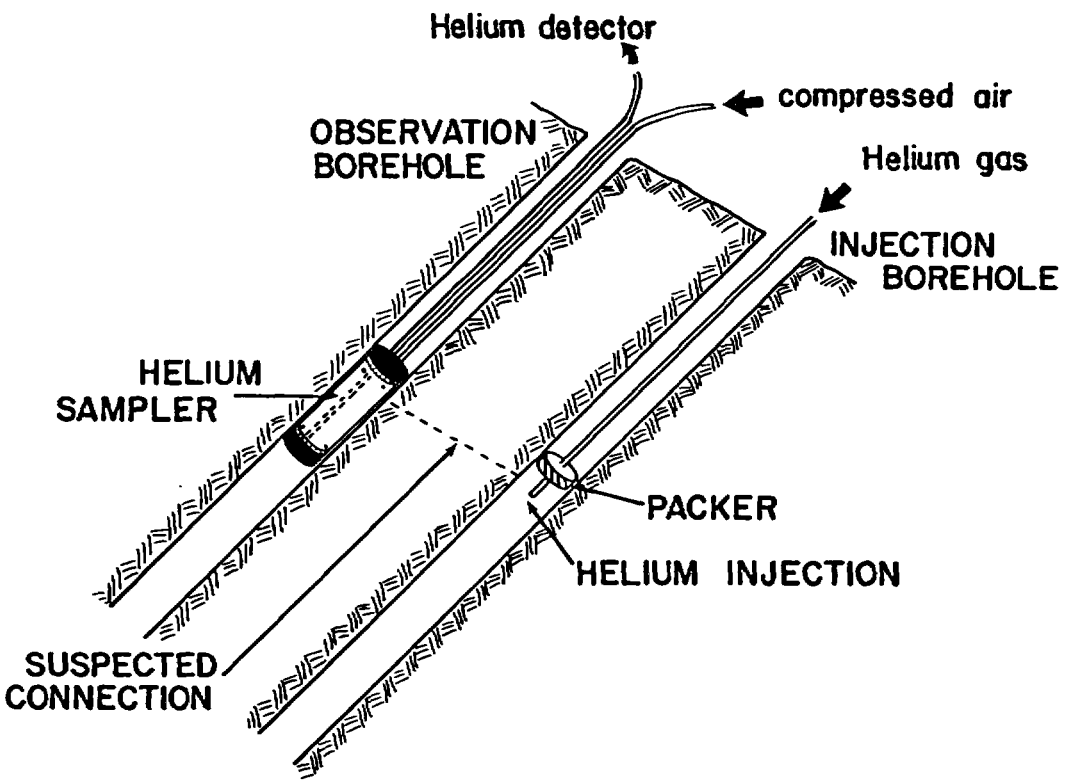

Figure 9: Cross-borehole helium tracer detection setup used at the Apache Leap Tuff Site.

Air samples are brought to the surface using a low volume air pump connected to the probe using a 0.6 cm (1/4") outside diameter (O.D.) polyethylene or nylon tubing. Valves are used to switch between recirculation and sampling modes. In the recirculation mode, output from the pump is returned downhole using a second tube of similar construction which is connected to the lower set of ports on the downhole probe. A portable thermal conductivity meter is used to detect helium arriving from an injection test. Because the thermal conductivity of helium is substantially less than that of standard atmosphere, any concentration of helium above the lower limit will be detected. The meter compares the thermal conductivity of a reference atmosphere, obtained from a port on the front panel of the unit, with the sampled gas via a connection between the downhole sampling tube and a probe attached to the meter. Both the detector unit and the sampling pump are powered using a voltage inverter connected to a twelve volt truck battery.

One drawback associated with using a non-specific detector is that the detector responds to the humidity and temperature differences between the ambient air in the boreholes and the surface air which is used as a reference resulting in difficulties with zeroing the detector. If the detector is zeroed with the probe at the surface, the humidity in the borehole air changes the reading after the probe is in the hole. This effect becomes more pronounced as a test progresses resulting a loss in sensitivity. Zeroing the probe in the hole prevents this problem.

A test performed between Boreholes X-2 and X-1 was successful in locating a fracture connection between the two boreholes. During the experiment, 2834 liters (100 ft^3) of helium gas was injected from a tank using a regulating valve which maintained a constant pressure of 1.4 bars (20 psi). The gas was injected into Borehole X-2 below a packer gland set at an inclined depth of 19.8 m and inflated to 3.4 bars (50 psi). The tank of helium was exhausted in approximately 2.9 hours at which time compressed air was injected into the interval to maintain the imposed pressure field. The pressure was also increased to 1.7 bars (25 psi) to provide faster travel times. After 7.35 hours the injection pressure was reduced to 1.0 bars (15 psi).

The first indication of a helium breakthrough occurred at around 9 m inclined depth in Borehole X-1 about four hours after the start of the test. By five hours into the test helium concentrations in this area were high enough to exceed the detection limit of the detector and after 6 hours helium had started to fill the hole and mask the exact location of inflow. At this time the hole was flushed with a large volume of air from a 1 cm (3/8") line inserted into the bottom of the hole and connected to an air compressor. After the flushing was completed, helium was first encountered at 10 m when moving upwards from the bottom of the hole. This procedure was repeated and the probe was moved downward from 7.5 m. Helium was first encountered at 10 m.

Several repetitions of this procedure gave consistent evidence that the primary source of helium inflow was located at an inclined depth of between 9.5 and 10 m. Within this interval there is a fracture which is closely aligned with a fracture located near the injection interval in Borehole X-2. A similar analysis in Borehole X-3 provided no detectable quantities of helium gas. The data are presented in Figure 10. The

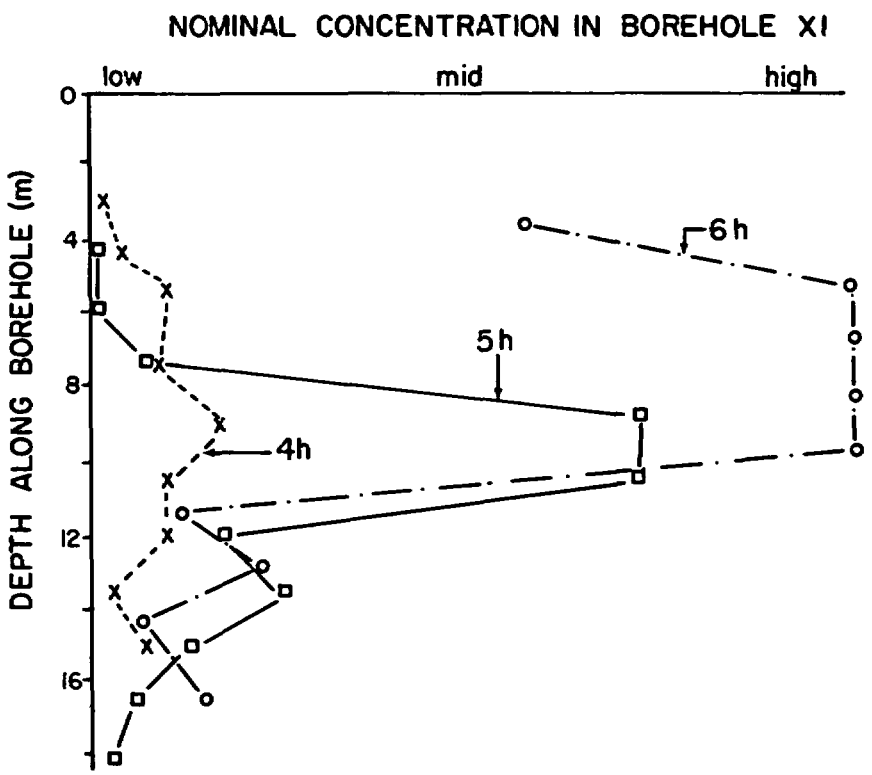

Figure 10: Cross-borehole helium tracer test data obtained from Apache Leap Tuff Site.

above evidence supports the conclusion that field measurements of fracture connectivity can be obtained using helium gas. The technique is reliable and easily applied in unsaturated, fractured media. Applications to unfractured rock and to more highly saturated media have not yet been made.

4.10 Saturated Fracture Transmissivity

The fluid flow properties of fractures within the saturated zone can be determined using single hole and cross hole hydraulic testing procedures as described by Hsieh and Neuman (1985) and Hsieh et al. (1985). Within the unsaturated zone no procedures are yet available. Kilbury et al. (1986) present a method for estimating fracture transmissivity on rock surfaces. Testing strategies must be developed to determine the transmissivity of individual fractures within boreholes where the near and far field boundary conditions are poorly known. The characterization of flow within a locally saturated borehole is a subject of considerable investigation (Stephens, 1979).

Estimation of fracture transmissivity begins with the measurement of intake rates from isolated borehole intervals with known borehole pressure heads. Messer (1986) presents a technique based on a device developed by Skibitzke (1955) which uses a downhole heat flowmeter to determine fluid losses into an isolated borehole interval. The precalibrated flowmeter is introduced at a known depth below the water surface to measure the downhole or uphole flow velocity. The velocity is obtained by measuring the time difference between when an electric heating grid is pulsed and the arrival time of the thermal pulse at a thermistor located a known distance above or below the heating grid. An estimate of the volumetric flow rate can be obtained by multiplying the measured velocity by the known cross-sectional area. Calibration trials performed by Messer indicated an ability to measure flows within the range of 0.04 to 1.9 l/min. The downhole heat flowmeter has been subsequently evaluated by Tidwell (in preparation) and shown to be inaccurate under a wide range of flow conditions.

An alternate technique developed by Tidwell (in preparation) using near-constant head piezometers with variable radii has been used with substantially improved reliability to obtain flow loss estimates at three meter intervals within the nine boreholes at the Apache Leap Tuff Site. The measured rate of water loss into the borehole can be obtained by locating a packer at multiple positions within the borehole. The difference in measured flow rates can be used to estimate flow losses to the formation. Estimates of fracture transmissivity using measured flow losses are being made by calibrating a computer simulation model, TRACER3D (Travis, 1984) with the observed flow losses (Tidwell, in preparation).

Crosshole tests can also be used to estimate fracture transmissivities in the unsaturated zone. Trautz (1984) injected air into one borehole and monitored the pressure in a borehole offset by 0.89 m. By analytically solving the flow problem in radial coordinates he was able to calculate an apparent hydraulic aperture.

4.11 Characteristic Curve and Unsaturated Transmissivity

Both the moisture characteristic and unsaturated transmissivity curves for individual fractures have not been obtained due to the difficulty in monitoring both fracture water content and fracture potential. Experimental laboratory procedures are being developed (Haldeman, in preparation) to determine the moisture characteristic curve and the unsaturated hydraulic conductivity for an individual fracture within a 20 x 20 x 50 cm block of tuff. Porous plates will be affixed to the upper and lower surfaces with individual plates aligned along the fracture trace. The rock and plates will be contained within a pressure chamber which can be maintained at a pressure of up to one bar above atmospheric (Figure 11). The water content of the fracture will be monitored using mass balance calculations. The fluid potential will be determined by the pressure maintained within the pressure chamber. The flow rate between the upper and lower plates (each maintained at a constant potential) will be used to calculate the unsaturated transmissivity.

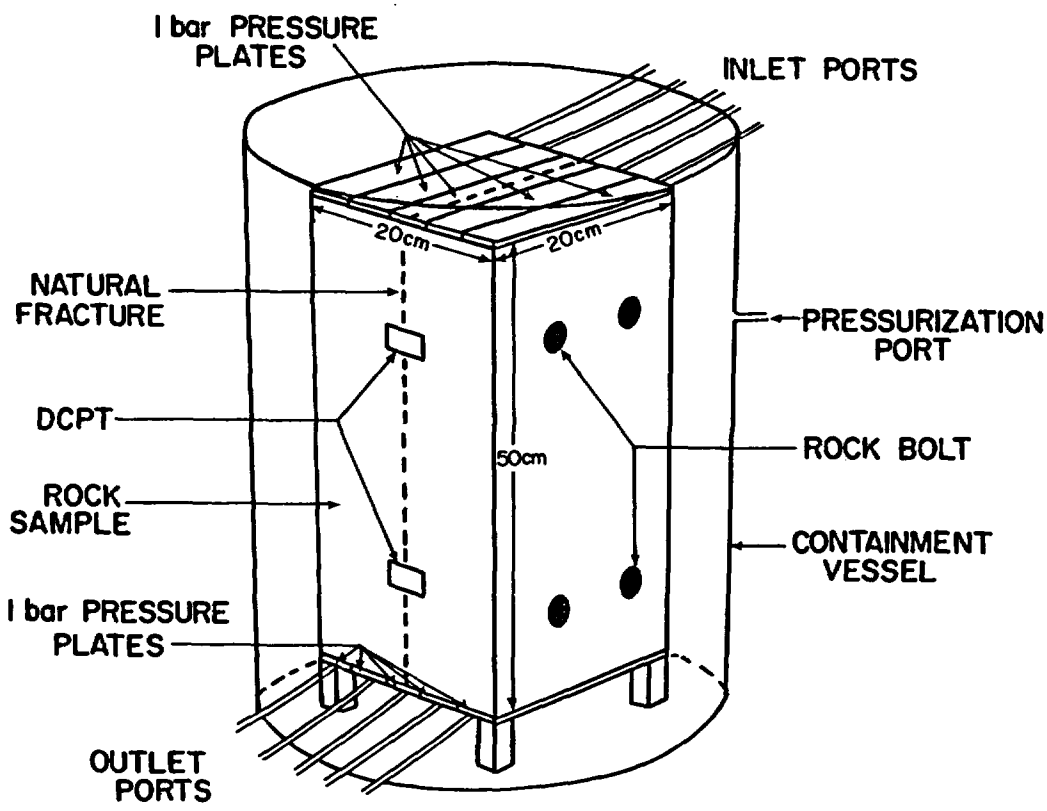

Figure 11: Experimental setup for unsaturated fracture-matrix flow studies.

CHAPTER 5

REVIEW OF NUMERICAL MODELS

The classical unsaturated model based on Richard's equation may be suitable for describing flow in unsaturated fractured rocks if one chooses the single network continuum or single network discrete fracture representation. Here, we will review some of well-known and widely used unsaturated porous media models, and discuss their advantages and disadvantages. This may shed light on the selection of appropriate numerical models for simulating flow and transport in unsaturated fractured rocks at the Apache Leap Tuff site. Ten computer models are discussed in this section. Peterson (1987) has an in-depth review of some of the models. The discussion of some of the models are condensed from his dissertation. The computer models to be examined are: TRUST, TOUGH, SUTRA, UNSAT2, FEMWATER, SATURN, TRACER3D, HUY3D, BIM2D, and BIM3D.

5.1 TRUST

The TRUST simulator is based on the integrated finite difference method (IFDM). The code, written in FORTRAN IV, evolved from an earlier model (TRUMP) authored by Edwards (1968) and designed to accommodate heat transport. TRUST was initially used for partially saturated, porous medium flow problems by Narasimhan (1975). Published information concerning the code, including its underlying theory, details of the model algorithm and code applications were later presented in a series of Water Resources Research (WRR) articles (Narasimhan and Witherspoon, 1976, 1977, 1978; Narasimhan, Witherspoon and Edwards, 1978). Later documentation of the code was provided by Reisenauer et al. (1982), along with a systematic description of data input organization.

Theory

Because TRUST is based on the IFDM, the fundamental equation from which the simulator is formulated is not the same as the differential equation (Richard's Equation) for variably saturated flow. Instead, as the name of this method infers, an integral form of the governing equation is first developed, and can be written as:

$$G + \int_{\rho} K(\psi)\, V(z + \psi)\cdot n \, d\Gamma = M \, D\psi/Dt \qquad (5.1)$$

where

G	source term, kg/s;
ρ	density of water, kg/m^3;
$K(\psi)$	unsaturated hydraulic conductivity, m/s;
z	elevation head, m;
ψ	pressure head, m;
n	unit vector directed outward normal to surface;
Γ	closed surface of the domain of interest in the flow region;
M	fluid mass capacity, kg/m; and
$D-/Dt$	total time derivative, 1/s;

The fluid mass capacity coefficient, M, represents the mass of fluid which the volume can absorb due to a unit change in the average value of pressure head, ψ. Following the mathematical reasoning of Reisenauer et al. (1982), the fluid mass capacity coefficient can be expanded into three separate components such that:

$$(5.2) \qquad M = \rho V_s (b S e \rho_o g + x'a S \rho g + e \, dS/d\psi)$$

where

- V_s volume of solids, m^3;
- b coefficient of compressibility of water, 1/Pa;
- S fluid saturation, dimensionless;
- e void ratio, dimensionless;
- ρ_o density of water at atmospheric pressure, kg/m^3;
- a coefficient of compressibility of medium, 1/Pa;
- x' parameter correlating change in effective stress and change in pore pressure, dimensionless.

The three terms on the right-hand side of Equation (5.2) represent, respectively, the compressibility of water, deformability of soil skeleton and desaturability of pores. By taking into account the second of these terms, TRUST simulates changes in available pore space in a deformable porous medium skeleton. The underpinnings of the deformable medium formulation stem largely from one-dimensional soil consolidation with some adjustments for unsaturated conditions. Deformation of the skeleton may be nonelastic.

TRUST was originally developed with the idea of providing a versatile flow simulation tool. Besides its previously mentioned ability to account for soil deformation, two other features distinguish this code (Reisenauer et al., 1982) from comparable simulators:

- o The mathematical model, along with its computational form, considers pressure-dependent density variations of water; and
- o The physical parameters in the governing equation are used in their primitive forms.

By the latter, it is meant that, rather than explicitly reading in hydraulic conductivity values and storage parameters, hydraulic conductivities and fluid mass capacities are calculated within the model itself after data for "primitive" parameters such as intrinsic permeability, fluid viscosity, fluid density, gravitational constants, void ratio, and compressibilities have been read. Thus, the mathematical foundation of TRUST is largely based on fundamental physical concepts rather than secondarily developed parameters evolved from simplified porous medium analysis. TRUST also attempts to represent soil moisture properties as realistically as possible by accounting for hysteresis.

Computational Algorithm

TRUST uses a mixed explicit-implicit approach in setting up and ultimately solving the equations that describe flow between subregions of the flow domain. This equation solving scheme recognizes that in a flow region with volume elements having widely varying time constants, iso-

lated groups of elements possessing relatively small time constants are only weakly coupled to each other through other elements possessing larger time constants. As a consequence, it is necessary to solve simultaneous equations only for the isolated groups of elements with time constants less than a specified time interval. The outcome of this observation is that the conductance matrix, which results from the formulation of Equation (5.1), can be partitioned into one or more submatrices, with iterative computations only being necessary on some of the submatrices. Thus the solution scheme is ostensibly more efficient than other algorithms requiring extensive simultaneous solution of all equations developed by the model.

The mixed explicit-implicit scheme assumes that the variation of pressure head over subregions is not rapid, and that the average properties within a subregion are associated with a representative nodal point, i. Assume also that the subregion is chosen so that lines joining nodal point i to its neighbor are normal to the interfaces that define the boundary between subregions. Furthermore, let the average properties associated with each nodal point be functions only of time, and assume that there is a spatially linear variation of these average properties between adjacent nodal points. Upon these premises, we can then apply Equation (5.1) to develop an explicit equation describing flow between two adjacent nodes:

$$(5.3) \qquad G_i \sum_j p\, K(\psi)\ r_{i,j} [(z_j+\psi_j) - (z_i+\psi_i)]/(d_{i,j}+d_{j,i}) = M_i\, \Delta\psi i/\Delta t$$

where the subscripts i and j are used to denote properties associated with elements i and j, respectively. Note that $r_{i,j}$ represents the area of the interface situated midway between elements and $d_{i,j}$ are the distances between elements. Inspection of Equation (5.3) shows that the quantity within the summation sign is equivalent to the flux across the interface separating elements i and j. In this sense, the unsaturated hydraulic conductivity, $K(\psi)$, in Equation (5.3) represents an interelement average at the interface between subregions. In heterogeneous domains, where elements i and j are composed of different materials, TRUST calculates a harmonic mean of the hydraulic conductivity in order to preserve continuity of flux at the interface. If we let $U_{i,j}$ represent the rate of flux across $r_{i,j}$ due to a unit difference between $(z_j+\psi_j)$ and $(z_i+\psi_i)$, Equation (5.3) can be rewritten as:

$$(5.4) \qquad G_i \sum_j U_{i,j} [(z_j+\psi_j) - (z_i+\psi_i)] = M_i\, \Delta\psi i/\Delta t$$

Equation (5.4) can be solved explicitly (Reisenauer, et al., 1982) for $\Delta\psi_i$. The resulting equation is:

$$(5.5) \qquad \Delta\psi_{i,exp} = \Delta t/M_i \quad (G_i + \Sigma U_{i,j} [(z_j+\psi_j) - (z_i+\psi_i)])$$

where the subscript, exp, denotes the explicit nature of the equation. Equation (5.5) is used to solve for changes in ψ at each time step, only for those elements where a local stability criterion is met (Reisenauer et al., 1982). The criterion is stated in terms of a maximum allowable time step for each node. If the model time step is greater than the

critical value for a given element, the node associated with the element is termed an implicit node, to which Equation (5.5) cannot be applied. Instead, an augmented form of the equation that includes an implicit correction is used; the implicit equation can be written:

$$(5.6) \qquad \Delta\Psi_i = \Delta\Psi_{i,exp} + f\,\Delta t/M_i\,[G_i + \sum_j U_{i,j}\,(\Psi_j - \Psi_i)]$$

where the coefficient, f, is an interpolation (stability) parameter, whose values can range from 0 (forward differencing) to 1 (backward differencing). The local nature of stability and the form of Equation (5.6) suggest that in order to carry out the solution process over the entire simulation domain, one must first compute $\Delta\Psi_{i,exp}$ for all nodal points in the flow region. The implicit correction must also be computed for only those elements whose stability limit is exceeded by the time step duration. Indeed, this is the approach taken in TRUST, with a Point-Jacobi type iterative scheme used for evaluating implicit equations.

All boundaries of a flow domain are handled in TRUST by a general head (see for example, McDonald and Harbaugh, 1984) boundary algorithm. That is, the entire domain boundary is formulated as if it were head dependent. Correspondingly, any boundary type, whether first (Dirichlet), second (Neumann), or third (Cauchy) type, is developed by manipulating a conductance term that comprises the coefficient of the head differential between an interior and exterior node (Reisenauer et al., 1982) located on the boundary. It naturally follows that system mass balance calculations also utilize the general head boundary algorithm.

Advantages

It is apparent from the foregoing discussion that TRUST has been designed to be versatile. Incorporation of the IFDM, along with a generalized means of inputting geometric data, broaden the code's capabilities in the sense that it does not intrinsically differentiate between a one-, two-, or three-dimensional problem. In accordance with this philosophy, the variety of polygonal shapes one may use for subregions is apparently endless.

TRUST'S ability to simulate skeleton deformation is an advantageous feature that many other flow simulators do not possess. The benefit to studies involving settlement and consolidation of soils is clear. Pressure dependent fluid density, and the opportunity to input matrix and water compressibilities separately rather than combining them in the form of a specific storage parameter, are also features that some modelers may find to their liking.

Another benefit of the TRUST algorithm is derived from the general head boundary condition that is used universally along all boundary segments. This approach, when specifically applied to Cauchy conditions, allows boundary influxes and effluxes to vary depending on computed head conditions. In contrast, other simulators frequently permit third-type (Cauchy) boundary conditions only for specialized forms of external flux (e.g. Davis and Neuman, 1983), such as evaporation and or infiltration. Also included in TRUST is a means of handling seepage face boundaries.

Because possible instability of the numerical solution is a crucial issue in any variably saturated flow simulation, TRUST includes an algorithm for automatically generating successive time step durations (Reisenauer et al., 1982). In the event that convergence within a specified number of iterations is not achieved during a time step, the results of the time step are discarded, and a new time step with a duration of half the previous one is used in succeeding calculations. The interpolation parameter used in Equation (5.6) is also updated at each time step (Reisenauer et al, 1982). The scheme for choosing an optimum makes use of rates of changes in pressure head during preceding time steps.

Difficulties and Potential Drawbacks

Because steady state simulations are considered to be crucial for modeling flow and transport in unsaturated fractured rocks, it is important to be able to obtain steady state results with relative ease. The TRUST code was written to only solve transient flow problems. Attempts using two different approaches for achieving equilibrium solutions in two-dimensional flow cases were unsuccessful (Peterson, 1987). In one of the approaches, the code was allowed to simulate large periods of time. The intent of this scheme was to extend the total simulation time to the point where a steady state would ultimately be reached. This tactic, however, proved impossible because the computing time became inordinately large, primarily due to the stability criteria severely limiting time step durations. Problems with system geometry and discretization were related to more inherent difficulties with the mixed explicit-implicit solver. A second approach used to achieve a steady state solution was to set the fluid moisture capacity, M, to a very low value with the intent of constructing numerical equations very similar to those that might result should a direct steady state solver be applied. This scheme was reported unsuccessful due to problems with numerical stability.

A second difficulty associated with the TRUST program appears to be related to the fundamental numerical scheme upon which it is formulated, namely the IFDM. Inter-element averages of flow rate controlling parameters are a necessary part of the IFDM. In the interest of preserving flux continuity, the original TRUST code uses a harmonic average (Reisenauer, et al., 1982) to compute the mean conductances. However, as reported by Siegel (1980), the harmonic mean conductance can lead to inaccurate solutions, especially near wetting fronts. Reisenauer et al. (1982, p. 2.12) have also pointed out this potential problem.

By virtue of the fact that the mixed explicit-implicit scheme, TRUST is a point iterative solver and therefore falls short of being a direct solver. As a consequence, the effects of hydraulic stress in one part of a domain to be passed on to another portion of the flow system is diminished, and the transmission of distinct properties at one element to contiguous elements is not performed in a direct manner. The same kind of problem is commonly observed with similar pointwise "relaxation" schemes such as successive over relaxation (SOR), in which computational times for problems involving a moderate number of nodes may far exceed those needed for a direct solution.

The inherent problems with the mixed explicit-implicit approach, as with any pointwise iterative solver, is that convergence to an accurate solution is sometimes inachievable. Reisenauer et al. (1982, p. 2.12) make mention of this sometimes troublesome aspect of TRUST, and go on to suggest the use of a direct solver in the code if needed. This drawback becomes compounded when working with domains of large size and containing large elements. Once again, by failing to solve all model equations simultaneously, as in a direct solver, stresses in an active part of the system cannot be directly felt (in a numerical sense) in less active areas lying some distance away. The problem becomes even more acute for elements with large aspect ratios, and especially when the longest axis of an element lies parallel to the flow direction.

5.2 TOUGH

The TOUGH program code (Pruess, 1987) simulates fluid flow in both liquid and gaseous phases due to pressure, viscous and gravity forces in accordance with Darcy's law, and with interference between phases as represented by relative permeability functions. Binary diffusion in the gas phase is also considered. Not considered are Knudsen diffusion, hysteresis in either capillary pressure or relative permeability, or for vapor pressure lowering even though capillary and phase adsorption effects are taken into account in the liquid phase. Thermophysical properties of liquid water and vapor are obtained within experimental accuracy from steam table equations. Air is treated as an ideal gas, and additivity of partial pressures is assumed for air/vapor mixtures. Air dissolution in water is described by Henry's law, but the temperature dependence of Henry's constant is neglected. Heat transport by means of conduction, with moisture dependent thermal conductivity, and by binary diffusion, which incorporates both sensible and heat transfer. The governing equations in TOUGH are applicable to one-, two-, and three-dimensional anisotropic porous and fractured media. TOUGH does not perform stress calculations for the solid skeleton, but does allow for porosity changes in response to changes in pore pressure and temperature using compressibility and expansivity coefficients, respectively.

Comments

Like TRUST, TOUGH uses the integral difference method to discretize continuum equations in space. Time is discretized fully implicitly as a first order finite difference to obtain the stability needed for performing efficient calculations. The resulting equations are strongly coupled because of interdependence of mass and heat flow, and are highly nonlinear because of orders of magnitude changes in parameters during phase transitions and because of non-linear material properties such as the relative permeabilities. To overcome these complexities introduced by coupled equations, TOUGH uses a completely simultaneous solution scheme to solve the discretized mass and energy balance equations, taking into account all coupling terms. Newton-Raphson iteration is used to solve the difficulties introduced by the nonlinear coefficients. Program TOUGH has been designed to reduce the numerical difficulties associated with TRUST. The accuracy of solutions depends upon the accuracy with which the various interface parameters in the continuum equations can be expressed in terms of average conditions in grid

blocks. A necessary condition for this to be possible is that there exists approximate thermodynamic equilibrium in almost all grid blocks at almost all times.

5.3 SUTRA

SUTRA (Saturated-Unsaturated Transport) is a computer program, developed by Voss (1984), which simulates fluid movement and the transport of either energy or dissolved substances in a subsurface environment. The model employs a two-dimensional hybrid finite-element and integrated-finite-difference method to approximate the governing equations that describe the two interdependent processes which are simulated:

- o Fluid density dependent saturated or unsaturated ground water flow and either:
  - † Transport of a solute in the ground water, in which the solute may be subject to equilibrium adsorption on the porous matrix, and both first-order and zero-order production or decay, or
  - † Transport of thermal energy in the ground water and solid matrix of the aquifer.

Disadvantage

As indicated in the SUTRA manual, the program is primarily intended for two-dimensional simulation of flow and either solute or energy transport in saturated variable-density systems. Although general unsaturated capability is implemented in SUTRA, it requires fine spatial and temporal discretization for unsaturated flow, and is therefore not an economical tool for extensive unsaturated flow modeling. In addition, test runs of the model for unsaturated flow problems have not been performed. However, the procedure used in the model to solve the nonlinear Richard's equation is a Picard type iteration. As illustrated in a later section, this type of iteration may not be suitable for highly nonlinear problem such as flow through fractured unsaturated rock.

5.4 UNSAT2

UNSAT2 is a two-dimensional finite element model based on Richard's equation. The underlying theory and computational scheme for this code was first developed by Neuman (1973). Further documentation and a user's guide for UNSAT2, which is written in FORTRAN IV, are found in Davis and Neuman (1983). The type of boundaries handled by UNSAT2 include first type (Dirichlet), second type (Neumann), and seepage face. In addition, algorithms are incorporated to simulate flux processes observed in partially saturated areas of the domain bounded by atmospheric conditions (Davis and Neuman, 1983). These latter boundary types include evaporation as well as infiltration from rainfall. Both are head-dependent in the sense that neither evaporation nor infiltration fluxes can be determined until the soil moisture level has been calculated. Unlike TRUST, hysteresis is not represented in UNSAT2. Means of accounting for seepage faces and plant transpiration are, however, included (Davis and Neuman, 1983).

UNSAT2 is based upon the Galerkin finite element method. One of the most notable features of UNSAT2 is the scheme whereby the mass matrix, which forms the coefficient of the time derivative, is mass-lumped. In essence, this means that off- diagonal terms in the element mass matrix are omitted. In some instances this approach leads to a more stable solution (Neuman, 1973) than would occur if a consistent mass matrix (mass matrix without lumping) were used. UNSAT2 is also distinctive in the sense that the code user is allowed to discretize the flow domain using both quadrilaterals and triangles. It should be noted, however, that the quadrilaterals are further subdivided within the code into triangles. Thus all computations are ultimately performed using linear triangular elements. The advantage of using simplex elements, as in this approach, is that it avoids the potentially burdensome task of numerical integration normally associated with first order isoparametric (quadrilateral) elements.

The equation solving scheme in UNSAT2 is classified as a bandsolver because it takes advantage of the banded nature of the global conductance matrix. Because the global matrix is symmetric, computations need only be carried out on the upper triangular portion of the matrix. To handle the nonlinear nature of the partially saturated flow problem, a Picard iteration scheme is employed.

Comments

Certainly one of the positive features of UNSAT2 is the utilization of linear triangular elements to the exclusion of all other types of elements. The use of these simplex elements avoids the need to orient element sides parallel to domain axes (Segerlind, 1984). Furthermore, sometimes costly numerical integration is completely avoided by using linear triangles. In addition, triangles also allow the boundaries of irregularly shaped domains to be handled quite readily. UNSAT2 also employs a dynamic dimensioning algorithm for allocating computer memory (or storage, in the case of a virtual memory system) to the various variables used in the FORTRAN program. This program enhancement eliminates the need to enlarge the size of all arrays used in the code; enlargement, when needed, is accomplished by increasing the size of one floating point array and one integer array.

Like TRUST, the original UNSAT2 code did not allow a direct steady state solution to be calculated. However, steady state conditions could be arrived at by allowing a simulation to run over very lengthy periods of time. A steady state version of the UNSAT2 code was developed by Yeh (1982) to circumvent potentially very long transient simulations. The usefulness of the modified UNSAT2 model is still limited because of the inherent problems with Picard iteration procedure used to solve the nonlinear system of equations.

Difficulties in achieving steady state solutions with UNSAT2 are probably reflective of the universally encountered problems with any simulator of this highly nonlinear form of moisture flow. Despite such drawbacks, the code's ability to handle a variety of transient problems (Davis and Neuman, 1983) has been documented. Yet there are a few additional features of UNSAT2 that we feel may limit its capacity to handle a variety of simulation conditions, which we mention here.

Moisture content values, as they vary with matric potential, are input to the model in tabulated form. Accordingly, specific moisture capacity, C, is determined in the model via linear slopes determined between tabulated moisture and suction data points. It is well known that specific moisture capacity exhibits a maximum value usually at a single value of pressure head. On either side of this maximum, values of C can drop off quickly to values of zero with changes in pressure head. The potential exists, therefore, for large changes in specific moisture capacity to occur over short ranges of pressure variation, and the linearly approximated values of C may not effectively catch important behavior of this parameter during the Picard iteration process. This may help to explain why the Picard procedure may fail to converge to a solution in partially saturated zones when large time steps are used. It also serves to illustrate why constitutive mathematical formulae relating moisture content to pressure head are sometimes employed in lieu of tabulated data; i.e. exact values of the slope of the characteristic curve can usually be obtained by differentiating the functional relationship between the two parameters. An additional technique for handling this potential problem is the chord-slope method (e.g. Huyakorn et al., 1984).

One final concern with UNSAT2 warrants mention. In particular, there is some indication that the mass-lumping procedure may lead to numerical error when applied to largely saturated domains (Huyakorn and Pinder, 1983). Although this technique apparently enhances the convergence of a solution in partially saturated zones, Frind and Verge (1978) report that the accuracy of some of their three-dimensional simulations of mostly saturated flow was adversely affected by the use of mass-lumping.

5.5 FEMWATER

The variable saturated flow simulator FEMWATER was developed at Oak Ridge National Laboratory by Yeh and Ward (1980). It is an extension of the work done by Reeves and Duguid (1976). Enhanced features of FEMWATER that specifically address the issue of mass balance computations are discussed by Yeh and Ward (1980) and Yeh (1981).

FEMWATER is a Galerkin finite element code designated to simulate two-dimensional variable saturated flow. It is programmed in FORTRAN IV. As with UNSAT2, the governing equation upon which FEMWATER was predicated is essentially the same as that used by SATURN, described in a following section. However, just as in TRUST, the FEMWATER code has also been designed to determine flow and storage parameters after physical properties have been entered into the model in their primitive forms. Therefore, rather than prompting the code user for a single value of specific storage, compressibilities of both water and media are read separately. Similarly, hydraulic conductivities are computed from input data consisting of intrinsic permeability, water density, gravitational constant and a fluid viscosity. Unlike TRUST, no attempts are made in FEMWATER to account for pressure effects on fluid density or skeletal deformation. Nor are hysteresis effects included.

In addition to accommodating first and second type boundaries, FEMWATER allows the use of a so-called rainfall- seepage boundary condition.

This last condition is apparently based on a head-dependent algorithm (Yeh and Ward, 1980) and bears some resemblance to the infiltration boundary (Davis and Neuman, 1983) scheme provided in UNSAT2. Seepage faces are also handled by FEMWATER.

Comments

Spatial discretization of flow domains simulated by FEMWATER is accomplished using quadrilateral elements. Utilization of these first order isoparametric elements is apparently advantageous in two ways:

- o Higher order accuracy is achieved (e.g. Tracy and Marino, 1987), than with linear triangular or linear rectangular elements; and
- o The elements easily conform to irregular boundaries of flow domains and subdomains.

Because quadrilaterals are included in the category of complex elements (e.g. Segerlind, 1984), there are no restrictions as to their orientation; i.e. it is not necessary to align element boundaries parallel to global coordinate axes. However, the computational burden usually increases when using quadrilaterals when compared with the computational needs associated with linear triangular or rectangular elements.

A direct solver is utilized in FEMWATER which takes advantage of the banded and symmetric nature (Yeh and Ward, 1980) of the model-generated global conductance matrix. Dirichlet (first type) boundary conditions are handled in the same fashion as UNSAT2; i.e. nondiagonal terms in the conductance matrix affected by prescribed head nodes are transferred to the load vector, while identity equations are generated for each Dirichlet node and are included in the global assembly process. The model user has the option of using either a consistent mass matrix or a lumped one. Picard iteration is applied to deal with the nonlinear nature of the variably saturated problem.

Perhaps the one feature of this code that most distinguishes it from other simulators is the means by which it computes Darcy velocities, and, consequently, carries out mass balance calculations. In contrast to other models (e.g. Reeves and Duguid, 1976; Huyakorn et al., 1984) that determines nodal flow velocities by numerically evaluating the spatial derivative of the final computed head field, FEMWATER solves for velocity components using an additional finite element formulation (Yeh and Ward, 1980; Yeh, 1981). The computed velocities are then in turn utilized to compute mass fluxes across boundaries. This last step contrasts with comparable schemes in UNSAT2 and SATURN, wherein mass fluxes at prescribed head nodes are determined via back-substitution.

The motivation for applying a separate Galerkin scheme to evaluate Darcy velocities is that such an approach assures veloctiy continuity at element boundaries and nodes. Discontinuity of velocity occurs when using the conventional method of evaluating spatial derivatives of the computed head field. This is a natural result of the finite element modeling procedure (Huyakorn and Pinder, 1983) when only one degree of freedom (i.e. head) is included in the numerical formulation. Discontinuity of velocities infers a violation of conservation of mass in a local sense.

Yeh (1981) argues that the generation of a continuous velocity field is essential to contaminant transport modeling, as large errors may result when solving the convective-dispersive equation using a discontinuous field. Because the additional Galerkin solution for velocities is an integral part of the FEMWATER code, the computed velocity field is also subsequently used to determine global mass balance during a simulation. Once again, the argument for carrying out this step is premised on the theory that if local mass balance is preserved, so too should global mass balance be achieved. Yeh and Ward (1981) reported significant reductions in mass balance error using FEMWATER when compared with more conventional schemes (e.g. Duguid and Reeves, 1976; Davis and Neuman, 1983) of computing boundary fluxes.

Advantages

As stated earlier, FEMWATER allows the opportunity of entering physical flow parameters in their primitive form into the code. This feature no doubt affords a greater interdisciplinary flexibility to some users. Another feature of FEMWATER that potentially contributes to its simulation versatility is its ability to handle the input of material property information via either tabular form or by constitutive relations. Thus, it is possible to avoid potential discontinuities in the determination of specific moisture capacity, C, by deriving analytical expression for the slope of the characteristic curve from the constitutive relationships. Unfortunately, the public version of FEMWATER does not utilize explicit formulae relating intrinsic permeability, moisture content and pressure head. Instead it is left up to the model user to choose his own functional relations, and to add FORTRAN statements to the code which will implement these relations during execution. Correspondingly, it is also necessary to add statements that serve to evaluate specific moisture capacity as pressure head changes. Consequently, although FEMWATER will automatically allow its users to input constitutive formulae parameters, there is some additional work involved in properly making use of these parameters.

FEMWATER incorporates an option to directly compute steady state solutions. However, as with both TRUST and UNSAT2, the program has difficulties when one attempting to apply the steady version of the FEMWATER code for large domains and for heterogeneous formations. This is due to the inherent problem in Picard iteration procedure.

Generally, FEMWATER requires long CPU time which may stem from the numerical algorithms associated with four-node quadrilateral elements. Although such elements provide an advantage over multiplex rectangular elements in the sense that their sides need not parallel coordinate axes, it is necessary with quadrilaterals to convert the global coordinates of their corner nodes to a local, or isoparametric, coordinate system. The use of the resulting so-called isoparametric elements is necessary if continuity (Segerlind, 1984) of the state variable (head) along interelement boundaries is to be maintained. A drawback of this procedure, however, is that necessary integration in the local isoparametric domain is much more complex (e.g. Huyakorn and Pinder, 1983) than when based on global coordinates. For all intents and purposes, numerical integration (e.g. Gaussian quadrature) then becomes a virtual

requirement if a numerical solution is to be attained. Consideration of computer operations suggest that the computational times associated with numerical quadrature will commonly exceed those based on direct analytical integration. Huyakorn et al. (1984) indicate that, in some cases, Gaussian quadrature can require more than 20 times the CPU time required by comparable analytical integration.

The difficulties posed by enlarged CPU times when performing numerical integration become even more significant in partially saturated flow simulation. The inherent nonlinearity of this type of problem requires hydraulic conductivities and specific moisture capacities to be updated at each iteration, and values for these parameters must in turn be interpolated onto the Gauss points employed in the numerical quadrature. Functional coefficient schemes do exist (e.g. Frind and Verge, 1978) that remove the need to numerically integrate at each iteration. A disadvantage of these latter approaches, however, is that finer and thus more spatial discretization may become necessary to preserve solution accuracy. Computational time in FEMWATER is also increased if the option to compute velocity components is used. According to Yeh (1981) the finite element method of computing velocities with two-dimensional problems enlarges CPU time by a factor of nearly three when compared with the conventional method of determining head gradients.

5.5 SATURN

The primary reference for this code is found in Huyakorn et al. (1984). As with UNSAT2 and FEMWATER, the model uses the Galerkin finite element method to approximate the Richard's equation for variably saturated flow under both steady and transient situations. It allows the use of either triangular or quadrilateral elements for discretizing the solution domain while a fully implicit finite difference scheme is used to discretize the time domain. Like UNSAT2, the solution is approximated by linear shape functions. Newton-Raphson iteration procedure is used to cop with the nonlinear algebraic equation set. Fluxes are evaluated at the center of each element.

Comments

The use of Newton-Raphson iteration procedure in SATURN may make it suitable for simulating flow through dry, coarse-textured materials or unsaturated fractured rocks. Furthermore, SATURN allows its users to input soil properties (i.e., hydraulic conductivity, moisture content, and pressure head) either in a tabular format or via constitutive functional relations. Regardless of which of these techniques is applied, specific moisture capacity information is generated by the chord-slope method of estimating derivatives, which has been shown to assist in arriving at stable solutions (Cooley, 1983) for some strongly nonlinear problems. It has been demonstrated that the chord-slope algorithm will in most cases result in better estimates of moisture capacity (Huyakorn, 1984) than do tabular input approaches where the value of moisture capacity is simply treated as a piecewise linearly continuous property of pressure head (e.g. UNSAT2). On the other hand, SATURN does not provide the option of inputting physical parameters in their so-called primitive forms, as is allowed in TRUST (e.g. Reisenauer, 1982) and FEMWATER (Yeh and Ward, 1980). Rather than asking for separate values of water and

media compressibility, SATURN looks for a single value of specific storage to be entered into the model. Unlike TRUST, it cannot represent skeletal deformation of porous media that may result from aquifer dewatering. To some extent, SATURN is restricted by its ability to solve only two-dimensional or axisymmetric problems. The SATURN code does contain an algorithm for modeling seepage faces. Additionally, SATURN evaluates the flux at the center of each element and as a result, the velocity field may not be continuous through out the simulation domain. This may present some problems in solute transport simulations.

5.7 TRACER3D

The TRACER3D model was developed by B. J. Travis at Los Alamos National Laboratory to model time-dependent two phase mass flow and chemical species transport in a three-dimensional, deformable, heterogeneous, reactive porous/fractured medium. The equations that comprise the TRACER3D model are the mass conservation equations for liquid and gas, and chemical species conservation equations, a reduced form of the momentum equations, and an equation of state plus several constitutive relations.

The governing partial differential equations are approximated by using a fully implicit, block centered, backward time finite difference scheme. Equations describing flow of liquid and gas are coupled and solved simultaneously for the pressures in each phase. Expressions derived by Brooks and Corey (1964) are used to represent the relative hydraulic conductivities of gas and liquid in the medium. An arithmetic mean is used to compute effective interface hydraulic conductivity. The solution technique used in the model is a Gauss-Seidel or SOR method for a nonlinear algebraic equation set. The model has been verified for water infiltration into a partially saturated column of soil, two-dimensional steady potential flow with a sink and a source, and steady flow with pressure-dependent permeability.

Comments

TRACER3D was written with flexibility in mind. It can handle problems ranging from steady, single phase, one-dimensional flow to transient, three-dimensional two-phase mass (air and liquid) flow and tracer transport in porous/fractured media. The trade off of its flexibility is its requirement of using a supercomputer to simulate flow and transport in any reasonable size of geologic systems. Test runs to validate the unsaturated flow simulation use soils (Yolo Light clay) of relatively mild nonlinearity in hydraulic characteristics. This does not warrant its suitability for coarse materials with high degree of nonlinear hydraulic characteristics curves. Based on our experiences, the Gauss-Seidel or SOR type iteration procedure often presents numerical convergence problems when it is applied to highly nonlinear equations. Although the model seems to be capable of simulating flow in fractures, no validation runs are shown.

5.8 HUYAKORN-3D

Huyakorn et al. (1986) developed a three-dimensional finite- element model for simulating water flow in variably saturated porous media. The

finite element formulation of the model is similar to that of SATURN. Three-dimensional Richard's equation is assumed to be the governing partial differential equation for the flow system. The Galerkin technique is used to approximate the solution. Rectangular and triangular prism elements are used to discretize the solution domain. The model is also capable of accommodating complex boundary conditions associated with seepage faces and infiltration or evaporation on the soil surface. An improved Picard iteration algorithm is implemented to deal with the nonlinearity of the equation. Matrix solution is achieved using a slice successive overrelaxation scheme that permits a fairly large number of nodal unknowns to be handled efficiently on small minicomputers.

Comments

The model has been validated for several different flow situations (Huyakorn et al., 1986) involving soils of relatively mild nonlinearity. The Picard iteration procedure used in the model may present convergence problems if the model is applied to coarse material or fractured rocks where large changes in hydraulic conductivity is expected.

5.9 BID2D

A boundary integral method has been used (Rasmussen et al., in press) to discretize and simultaneously solve steady liquid flow through a network of randomly-oriented, discrete fractures embedded within a porous medium. Experience with modeling two-dimensional flow within three dimensional networks of discrete fractures by Huang and Evans (1985) and by Rasmussen (1987) has resulted in the capability to discretize random networks of fractures embedded within an impermeable matrix. Fracture flow is characterized by defining physical and hydraulic parameters for each fracture.

The boundary integral method (BIM) has been widely applied within the field of fluid hydraulics and subsurface flow modeling (Lafe et al., 1981), although normally only for two dimensional applications. A few three dimensional applications have been reported (Liggett and Liu, 1983; Brebbia et al., 1984), as well as applications to flow through fractured rock (Shapiro and Andersson, 1983; Elsworth, 1986, 1987). Such studies have examined flow through homogenous media, or through layered media with homogeneous properties within each layer. Recent advances have also provided the ability to examine two dimensional flow through heterogeneous media (Lafe and Cheng, 1987). To illustrate the BIM method, an application is presented for solving the Laplace equation:

$$(5.7) \qquad \nabla^2 u = 0$$

where u is the potential. By discretizing the boundaries of the flow domain, a relationship between flow and head can be derived (Brebbia, 1978):

$$(5.8) \qquad [G] \langle q \rangle = [H] \langle u \rangle$$

where

q vector of fluxes normal to each boundary element, m/s;

u vector of pressure heads on each boundary element, m; and
G,H are matrices of weighting factors.

For two dimensional flow through fractures the elements of G and H are estimated using (Huyakorn and Pinder, 1983):

$$(5.9) \qquad g_{ij} = 1/2\pi \int \ln(1/r)\, d\Gamma$$

$$= D/2\pi \sum_k (w_k \ln(1/r_k))$$

and

$$(5.10) \qquad h_{ij} = 1/2\pi \int 1/r\, \delta r/\delta n\, d\Gamma$$

$$= -1/2\pi \sum_k (w_k\, s\, /\, r_k^2)$$

where

g_{ij}, h_{ij}	influence of flow, or head, at node j on node i,
r	distance from the point under consideration, i, to the point of application, j,
Γ	boundary segment for the point of application,
n	normal to the boundary segment,
k	index for the numerical integration points,
r_k	distance from the point under consideration to the numerical integration point,
w_k	numerical integration weighting factor,
s	normal distance from the point under consideration to the extension of the boundary segment for the point of application, and
D	length of the boundary segment for the point of application.

Special care must be taken to evaluate coefficients when nodes i and j share a common element. In this case, Equations (5.9) and (5.10) are estimated using:

$$(5.11) \qquad g_{ij} = r\,(1 - \ln(r))\,/\pi$$

and

$$(5.12) \qquad h_{ij} = \begin{cases} 0 & i = j \\ -\sum_j h_{ij} & i \neq j \end{cases}$$

The coefficients are estimated by numerical integration along a line. A linear variation in head and flow along the line is assumed. The linear weighting functions are:

$$(5.13) \qquad u(e) = (1-e)\, u_1/2 + (1+e)\, u_2/2$$

and

(5.14) $q(e) = (1-e)\ q_1/2 + (1+e)\ q_2/2$

where

e	dimensionless coordinate along the boundary segment,
u_1, u_2	heads at the endpoints of the boundary segment, and
q_1, q_2	flows at the endpoints of the boundary segment.

5.10 BID3D

The BIM2D formulation can be adapted for three dimensional flow. In this application, the elements of G and H in Equation (5.8) are estimated using (Huyakorn and Pinder, 1983):

(5.15) $$g_{ij} = 1/4\pi \int 1/r\ d\Omega$$

$$= 1/4\pi \sum_k (w_k/r_k)$$

and

(5.16) $$h_{ij} = 1/4\pi \int \delta(1/r)/\delta n\ d\Omega$$

$$= 1/4\pi \sum_k (w_k/r_k^3)$$

Where Ω is the boundary surface for the volume of interest. The g and h coefficients are estimated using gaussian integration over triangular areas (Cowper, 1973). In this study, linearly varying heads and fluxes were used. The triangular weighting functions are:

(5.17) $u(e,f) = e\ u_1 + f\ u_2 + (1-e-f)\ u_3$

and

(5.18) $q(e,f) = e\ q_1 + f\ q_2 + (1-e-f)\ q_3$

where

e,f	dimensionless coordinates over the triangular area,
$u_1, u_2, u3$	heads at the corners of the triangular boundary, and
q_1, q_2, u_3	flows at the corners of the triangular boundary.

The estimated fluxes can be integrated over each boundary element to give the total flow across each element. In two dimensions the boundary is a line requiring a line integration, while a surface integration must be performed in three dimensional flow problems. When flow between two intersecting fractures occurs, a boundary element is introduced to represent the line of intersection between the fracture planes. From mass balance considerations and equivalence of heads along the boundary, a larger matrix can be formed which is composed of sub-matrices of flow within each fracture plus the flow across the interface. The pure-fracture flow matrix equation is:

(5.19) $$[G_f] \langle q_f \rangle = [H_f] \langle u_f \rangle$$

or

(5.20) $$\begin{bmatrix} G_1 & G_{1i} & 0 \\ 0 & -G_{2i} & G_2 \end{bmatrix} \begin{Bmatrix} q_1 \\ q_i \\ q_1 \end{Bmatrix} = \begin{bmatrix} H_1 & H_{1i} & 0 \\ 0 & H_{2i} & H_2 \end{bmatrix} \begin{Bmatrix} h_1 \\ h_i \\ h_2 \end{Bmatrix}$$

where

G_1, H_1	matrices of weighting factors for fracture 1,
G_2, H_2	matrices of weighting factors for fracture 2,
G_{1i}, H_{1i}	matrices of weighting factors between nodes defining fracture 1 and interfacial nodes,
G_{2i}, H_{2i}	matrices of weighting factors between nodes defining fracture 2 and interfacial nodes,
q_1, u_1	flow and heads along the boundary of fracture 1,
q_2, u_2	flow and heads along the boundary of fracture 2, and
q_i, u_i	flow and heads along the interface.

For fracture flow which incorporates flow into and out of the fracture from the matrix, the matrix equation is:

(5.21) $$\nabla^2 u_f + q_m = 0$$

The flow through the matrix can be solved using:

(5.22) $$[G_m] \langle q_m \rangle = [H_m] \langle u_m \rangle$$

where the subscripted variables indicate matrix flow components, calculated using three dimensional weighting functions. The flow between the matrix and the fractures, across the boundary surface as well as the heads along the boundary surface, can be equated yielding the following equation for flow through the fracture:

(5.23) $$([G_f] + [G_m]) \langle q_f \rangle = [H_f] \langle u_f \rangle$$

where G_m is the flow across the fracture surface element from the matrix (Brebbia, 1978). This formulation allows simultaneous fracture and matrix flow through both a matrix of uniform hydraulic conductivity and embedded fractures. The model does not currently incorporate extreme changes in water content within the matrix or within fractures, but such a flow regime could be implemented by defining a discrete boundary at a wetting front. The resulting Green and Ampt formulation would yield fully saturated conditions behind the front and unsaturated conditions ahead of the front.

CHAPTER 6

EVALUATION METHODOLOGY

The simulation of fluid flow and solute transport in unsaturated fractured rocks at the Apache Leap Tuff Site is difficult, due, in part, to a lack of validated conceptual models for flow through unsaturated fractures as well as a lack of efficient numerical solution techniques for solving highly nonlinear partial differential equations. Also lacking are established laboratory and field measurement techniques for determining unsaturated hydraulic properties of fractured rocks which leads to a lack of reliable field and laboratory data. The degree of difficulty is further complicated by the spatial variability of the hydraulic properties of both matrix and fractures. In order to overcome these difficulties and to demonstrate the capability to simulate unsaturated flow and transport through fractured tuff, an incremental modeling approach will be adopted. Each incremental change in modeling capability will result in the ability to simulate additional levels of complexity. The simulation strategy is to progress from rather simple models to more rigorous ones as data and numerical skills become available.

6.1 Matrix Flow Characterization

Initially, the ability to simulate saturated flow through the matrix will be demonstrated for the purpose of determining the effect of spatial variability of the saturated matrix permeability on flow and transport. Once saturated flow has been examined, the ability to model unsaturated flow through the rock matrix will be added. Analytic stochastic models will be employed using techniques presented by Gelhar and Axeness (1983), Yeh (1985a,b,c), and Mantoglou and Gelhar (1987a,b,c). Three dimensional numerical models using the equivalent porous media formulation, such as TRUST, TRACER3D, and HUY3D will be also chosen for modeling flow through the matrix.

Hydraulic properties of the porous matrix at various depths at the existing nine boreholes will be determined from core samples and from in situ field experiments. The data will be analyzed to determine the degree of spatial variability of the hydraulic properties of the rock matrix. Geostatistics will be employed to determine variograms for properties of interest. The Apache Leap Tuff Site will then be discretized using three-dimensional elements without considering fractures. The hydraulic properties of the elements at unsampled locations will be estimated by using the variograms. Thus, a complete picture of hydraulic parameter distributions at the site will be available.

Various boundary conditions will be considered, including constant head and flux, step head and flux changes, and cyclic head and flux changes for annual cycles. Results from the analytic models will be compared to numerical procedures. Both models will be calibrated using available data including porosity and hydraulic conductivity functions obtained from oriented borehole cores, as well as measured borehole intake rates. Once flow and transport through saturated porous media have been

described, the effects of variable saturation will be investigated using estimates of the relative permeability functions obtained from laboratory analyses. Again, fracture flow will be ignored. Calibration data sets from neutron measurements of borehole water content will be used. Because the size of the field site is relatively large, and hydraulic parameters of the rock matrix may vary significantly in space, three dimensional models may fail to provide reliable solutions for flow situations due to numerical instabilities. This problem may force us to resort to the TOUGH or SATURN models which use the Newton-Raphson iteration procedure. However, use of this model will be limited to two dimensional cross-sections due to limitations of the model.

Solute transport will be simulated in order to develop travel time probability distributions. Simulations using stochastically generated parameters will be repeated in order to maximize the sample of potential flow paths. Enough realizations will be considered so that low probability events, corresponding to the tails of the expected distribution, are observed.

6.2 Fracture Flow Characterization

Concurrent with the developement of a porous media model of the rock matrix, flow through networks of discrete fractures will be examined. Initially, the inclusion of fractures will be made using these limiting scenarios:

- o Saturated fractures and an impermeable rock matrix;
- o Saturated fractures and a saturated rock matrix;
- o Desaturated fractures which impede matrix flow and a saturated rock matrix; and
- o Saturated horizontal fractures and desaturated vertical fractures which impede horizontal flow but do not affect vertical flow.

It may be possible that steady flow through a partially saturated, fractured porous rock can be understood without detailed knowledge of the discrete fracture network properties (Wang and Narasimhan, 1985). For large suctions, the rock matrix may be the main conduit for fluid flow. To test the validity of this supposition, simulations of flow in the rock matrix without fractures will be compared to the inclusion of discrete fractures. Boundary conditions similar to those employed in the matrix simulation models will again be applied.

Another supposition to be examined is the stochastic continuum concept which allows the use of equivalent porous media models (Neuman, 1987). The stochastic continuum representation of fracture hydraulic conductivity places less emphasis on fracture geometric data than on the results of hydraulic tests conducted on scales which are much greater than several fractures but smaller than a REV. Because of the large size of measurement, the erratic behavior of hydraulic properties may thus be removed and the use of the classic partial differential equations may thus be justified. This type of approach suggests that in situ hydraulic packer tests are necessary. The measured hydraulic properties then

represent the average properties over a scale which contains several fractures and the matrix but much smaller than the field site. Thus, the fractured geologic formation at the Apache Leap Tuff Site can be treated as a continuum with spatially varied hydraulic properties. The spatial variability of the properties is then characterized by a stochastic approach or geostatistics. Using classic flow models to predict flow and solute transport in such a medium may thus be appropriate.

The use of stochastic continuum approach could eliminate the difficulties of characterizing the complex fracture geometry. However, there are difficulties associated with the application of this concept to unsaturated fractured rocks. The major difficulty arises from a technological point of view. That is, how to conduct packer tests to measure unsaturated hydraulic properties (for instance, the hydraulic conductivity-suction relationship, and moisture release curves) in the field. Some innovative breakthroughs in monitoring technology seem to be necessary. The development of methodologies for solving inverse problems in unsaturated flow will also be needed. Finally, there is a need in developing an efficient and effective numerical scheme for solving the highly nonlinear unsaturated flow and transport equations.

Other models, including analytic stochastic models, dual porosity and discrete fracture models, will also be applied. These approaches require the knowledge of fracture hydraulic conductivity and suction relationships and the moisture retention characteristics of the fractures in addition to the fracture distribution. Although the distribution of the fractures at the Apache Leap site may be determined from the data collected at the boreholes, the unsaturated hydraulic properties of the fractures remain unknown. To circumvent the difficulty, we either have to rely on the fracture hydraulic conductivity model developed by Wang and Narasimhan (1985) to create hypothetical conductivity-suction relationship and moisture retention curve for the fracture, or use laboratory data from ongoing experiments.

Calibration of the fracture flow models will rely upon data sets generated from borehole intake rates of water and air. It is believed that ongoing laboratory experiments at the University of Arizona will provide additional calibration data sets for developing conceptual models for flow through unsaturated fractured rocks. Results of the experiments will provide parameters which relate fracture hydraulic conductivity to suction, as well as between moisture content and suction. This information will enhance the ability to quantify the relationship between discrete fracture geometry and its hydraulic properties. Appropriate parameters may then be measured in the field site to characterize the hydraulic properties of fractures.

Calibration of the solute transport portion of the flow models will require additional calibration data sets. The use of helium gas as a conservative gas phase tracer in fractures is a possible calibration tool. Relating gas phase velocities to fluid phase velocities may or may not be possible. Sampling volatile compounds in the fluid phase may be another means for obtaining transport calibration data sets.

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13. ABSTRACT (200 words or less)

The physical, hydraulic and pneumatic properties of variably saturated, fractured tuff are currently being evaluated at the Apache Leap Tuff Site, located near Superior, Arizona. Nine inclined boreholes, the deepest of which penetrate to a depth of thirty meters, have yielded over 270 m of oriented core. Field and laboratory data with regard to matrix and fracture properties are being collected which will be used to characterize the site. A description of the characterization parameters as well as field and laboratory techniques used to collect the parameters is presented. To extend the characterization to larger scales, as well as to interpret collected data, computer simulation modeling will be performed. A review and description of available computer models is presented. Recommendations for site characterization includes the use of analytic stochastic models, equivalent porous media models, and discrete fracture network models. Such models may accurately reproduce the expected dual porosity, three-dimensional characteristics of fluid flow at the Apache Leap Tuff Site. Also, the variable saturation which exists within fractures and the matrix at the site will also be reproduced. Simulation scenarios including constant head and flux surface boundary conditions, as well as slug and cyclic surface boundary conditions are recommended.

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